# References, Appendices \& All Parts Merged 

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## Lecture Notes and Problems

Beta version


## Essential Graduate Physics

Lecture Notes and Problems
Beta version, December 2013
(with later problem additions and typo corrections)
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## Preface

This is a series of lecture notes and problems on "Essential Graduate Physics", consisting of the following four parts:

> CM: Classical Mechanics (for a 1 -semester course), EM: Classical Electrodynamics ( 2 semesters), QM: Quantum Mechanics (2 semesters), and SM: Statistical Mechanics (1 semester).

The parts share a teaching style, structure, and (with few exceptions) notation, and are interlinked by extensive cross-referencing. I believe that due to this unity, the notes may be used for teaching these courses not only in the (preferred) sequence shown above, but in almost any order - or in parallel.

Each part is a two-component package consisting of:
(i) Lecture Notes chapter texts, ${ }^{2}$ with a list of exercise problems in the end of each chapter, and
(ii) Exercise and Test Problems with Model Solutions files.

The series also includes two brief reference appendices, MA: Selected Mathematical Formulas (16 pp.) and CA: Selected Physics Constants ( 2 pp ), and a list of references.

The series is a by-product of the so-called core physics courses I taught at Stony Brook University from 1991 to 2013. Reportedly, most physics departments require their graduate students to either take a set of similar courses or pass comprehensive exams based on an approximately similar body of knowledge. This is why I hope that my notes may be useful for both instructors and students of such courses, as well as for individual learners.

The motivation for composing the lecture notes (which had to be typeset because of my horrible handwriting) for Stony Brook students was my desperation to find textbooks I could actually use for teaching. First of all, the textbooks I could find, including the most influential Theoretical Physics series by L. Landau and E. Lifshitz, did not match my classes, which included experiment-oriented students, some PhD candidates from other departments, US college graduates with insufficient undergraduate background, and a few advanced undergraduates. Second, for the rigid time restrictions imposed on the core physics courses, most available textbooks are way too long, and using them would mean hopping from one topic to another, picking up a chapter here and a section there, at a high risk of losing the necessary background material and logical connections between course components - and students’ interest with them. On the other hand, many textbooks lack even brief discussions of several traditional and modern topics that I believe are necessary parts of every professional physicist's education. ${ }^{3,4}$

[^1]The main goal of my courses was to make students familiar with the basic notions and ideas of physics (hence the series' title), and my main effort was to organize the material in a logical sequence the students could readily follow and enjoy, at each new step understanding why exactly they need to swallow the next knowledge pill. As a back side of such a minimalistic goal, I believe that my texts may be used by advanced undergraduate physics students as well. Moreover, I hope that selected parts of the series may be useful for graduate students of other disciplines, including astronomy, chemistry, mechanical engineering, electrical, computer and electronic engineering, and material science.

At least since Confucius and Sophocles, i.e. for the last 2,500 years, teachers have known that students can master a new concept or method only if they have seen its application to at least a few particular problems. This is why in my notes, the range of theoretical physics methods is limited to the approaches that are indeed necessary for solution of the problems I had time to discuss, and the introduction of every new technique is always accompanied by an application example or two. Additional exercise problems are listed in the end of each chapter of the lecture notes, and may be used for homeworks. Individual readers are strongly encouraged to solve as many of these problems as possible. ${ }^{5}$

Detailed model solutions of the exercise problems (some with additional expansion of the lecture material), and several shorter problems suitable for tests (also with model solutions), are gathered in 6 separate files - one per semester. These files are available for both university instructors and individual readers - free of charge, but in return for a signed commitment to avoid unlimited distribution of the solutions - see p. vii below. For instructors, these files are available not only in the Adobe Systems' Portable Document Format (*.pdf), but also in the Microsoft Office 1997-2003 format (*.doc) free of macros, so that the problem assignments and solutions may be readily grouped, edited, etc., before their distribution to students, using either virtually any version of Microsoft Word or independent software tools - e.g., the public-domain OpenOffice.org.

I know that that my texts are far from perfection. In particular, some sacrifices made at the topic selection, always very subjective, were extremely painful. (Most regretfully, I could not find time for even a brief introduction to the general relativity. ${ }^{6}$ ) Moreover, it is very probable that despite all my effort and the great help from SBU students and teaching assistants, not all typos/errors have been weeded out. This is why all remarks (however candid) and suggestions by the readers would be highly appreciated. All significant contributions will be gratefully acknowledged - both online and in possible future editions of the series. ${ }^{7}$

[^2]
## Disclaimer

Since these materials are available free of charge, it is hard to imagine that somebody would blame their author for deceiving "customers" for his commercial gain. Still, I would like to go a little bit beyond the usual litigation-avoiding claims, ${ }^{8}$ and offer a word of caution to the potential reader, in order to preempt his or her possible later disappointment.

## This is NOT a course of theoretical physics - at least in the contemporary sense of the term

Though much of the included material is similar to that in textbooks on "theoretical physics" (most notably in the famous series by L. Landau and E. Lifshitz), this lecture note series is different from them by its emphasis on the basic concepts and ideas of physics, their relation to experimental data, and most important applications - rather than on sophisticated theoretical techniques. Indeed, the set of theoretical methods discussed in the notes is limited to the minimum necessary for quantitative understanding of the key notions of physics and for solving a few (or rather about a thousand :-) core problems. Moreover, because of the notes' shortness, I have not been able to cover some key fields of theoretical physics, most notably the general relativity and quantum field theory - beyond some introductory elements of quantum electrodynamics in QM Chapter 9. If you want to work in modern theoretical physics, you need to know much more than these lectures!

## Moreover, this is NOT a textbook - at least not the usual one

A usual textbook tries (though most commonly fails) to cover virtually all aspects of the addressed field. As a result, it is typically way too long for being fully read and understood by students during the time allocated for the corresponding course, so that the instructors are forced to pick up selected chapters and sections, frequently loosing narrative's logic lines. In contrast, these notes are much shorter (about 200 pages per semester), enabling their thorough reading - perhaps with just a few later sections dropped, depending on reader's interests. I have tried to mitigate the losses due to this minimalistic approach by providing extensive further reading recommendations on the topics I had no time to cover. The reader is highly encouraged to use these sources (and/or the corresponding chapters of more detailed textbooks) on any topic(s) of his or her special interest.

## Then, what these notes ARE and why you may like to use them (I think)

By tradition, graduate physics education consists of two main components: research experience and advanced physics courses. Unfortunately, the latter component is currently under pressure in many physics departments, apparently because of two reasons. On one hand, the average knowledge level of students entering graduate school is not improving, so that bringing them up to the level of contemporary research becomes increasingly difficult. On the other hand, the research itself is becoming more fragmented, so that the students frequently do not feel an immediate need for a broad physics

[^3]knowledge base for their PhD project success. Some thesis advisors, trying to maximize the time they could use students as a cheap laboratory workforce, do not help.

I believe that this trend toward the reduction of a broad physics education in graduate school is irresponsible. Experience shows that during his or her future research career, a typical current student will change research fields several times. Starting from scratch in a new field is hard - terribly hard in an advanced age (believe me :-). However, physics is fortunate to have a hard core of knowledge, that many other sciences lack. With this knowledge, the student will always feel in physics at home, while without it, he or she may not be able even to understand research literature in the new field, and would risk being reduced to auxiliary work roles - if any.

I have seen the main objective of my Stony Brook courses to give an introduction to this hard core of physics knowledge, at the same time trying to convey my own enchantment by the unparalleled beauty of the concepts and ideas of this science, and the remarkable logic of their fusion into a wonderful single construct. Let me hope that these notes relay not only the knowledge as such, but also at least a part of my enchantment.

## Versions and Acknowledgements

This is a preliminary ("Beta") version of the series. My plans are to publish, in a few years, its final version. Until that has happened, I commit to keeping the Beta stable. The only changes still to be made in it will be corrections of the typos noticed by the readers and myself, and minor stylistic edits.

I am extremely grateful to my faculty colleagues and other readers who commented on certain sections of the notes; here is their list (in the alphabetic order) ${ }^{9}$
A. Abanov, P. Allen, D. Averin, S. Berkovich, P.-T. de Boer, M. Fernandez-Serra, R. F. Hernandez, T. Konstantinova, A. Korotkov, V. Semenov, F. Sheldon, E. Tikhonov, X. Wang.
(Evidently, these kind people are not responsible for the remaining deficiencies.)
The Department of Physics and Astronomy of the Stony Brook University was very responsive to my requests of certain time ordering of my teaching assignments, that was beneficial for note writing and editing. The department, and the university as the whole, also provided a very friendly general environment for my work during the past 25 years.

A large part of my scientific background and experience, reflected in these materials, came from my education (and then research work) in the Department of Physics of Moscow State University.

And last but not least, I would like to thank my wife Lioudmila for several good advices on aesthetic aspects of note typesetting, and for all her love, care, and patience - without them, this project would be impossible.

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[^4]
## Problem Solution Request Templates

Requests should be sent to konstantin.likharev@stonybrook.edu in either of the following forms:

- an e-mail from a valid university address,
- a scanned copy of a signed letter - as an e-mail attachment.

Approximate contents:

## A. Request from a Prospective Instructor

Dear Dr. Likharev,
My plans are to use your lecture notes and/or problems of the Essential Graduate Physics series, part <select: CM, EM, QM, SM>, in my course <title> during <semester, year> in the <department, university>. I would appreciate sending me file Exercise and Test Problems with Model Solutions of that part of the series in the <select: .pdf, both .doc and .pdf> format(s).

I will avoid unlimited distribution of the solutions, in particular their posting on externally searchable Web sites. If I distribute the solutions among my students, I will ask them to adhere to the same restraint.

I will let you know of any significant typos / deficiencies I may find.
Sincerely, <signature, full name, university position, work phone number>

## B. Request from an Individual Learner

Dear Dr. Likharev,
My plans are to use your lecture notes and problems of the Essential Graduate Physics series, part(s) <select: CM, EM, QM, SM>, for my personal education. I would appreciate sending me file(s) Exercise and Test Problems with Model Solutions of that part(s) of the series.

I will not share the material with anyone, and will not use it for passing courses that are officially based on your series.

I will let you know of any significant typos / deficiencies I may find.
Sincerely, <signature, full name, present home address (in English), acting phone number>

## Notation

## Abbreviations

Eq. any formula (e.g., equation)
Fig. figure
Sec. section
c.c. complex conjugate
h. c. Hermitian conjugate
c.

## Fonts

$F, \not \subset$ scalar variables ${ }^{10}$
F, $\boldsymbol{7}$ vector variables
$\hat{F}, \hat{\not}$ scalar operators
$\hat{\mathbf{F}}, \hat{\boldsymbol{F}}$ vector operators
F matrix
$F_{j j}$, matrix element

## Parts of the series

CM: Classical Mechanics
EM: Classical Electrodynamics
QM: Quantum Mechanics
SM: Statistical Mechanics

## Symbols

- time differentiation operator $(d / d t)$
$\nabla$ spatial differentiation vector (del)
$\approx$ approximately equal to
$\sim$ of the same order as
$\propto$ proportional to
$\equiv$ equal to by definition (or evidently)
- scalar ("dot-") product
$\times$ vector ("cross-") product
- time averaging
$\rangle$ statistical averaging
[, ] commutator
\{, \} anticommutator


## Appendices

MA: Selected Mathematical Formulas
CA: Selected Physical Constants

## Prime signs

The prime signs ( ${ }^{\prime},{ }^{\prime \prime}$, etc) are used to distinguish similar variables or indices (such as $j$ and $j^{\prime}$ in the matrix element above), rather than to denote derivatives.

## Formulas

The most general and/or important formulas are highlighted with blue frames and short titles on the margins.

## Numbering

Chapter numbers are dropped in all references to formulas, figures, footnotes, and problems within the same chapter.

[^5]
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$$161814

$$
130+25=155
$$

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# Part CM: <br> Classical Mechanics 

Last corrections: 2019/07/31

A revised version of this material is now published by the IOP under the title
"Classical Mechanics: Lecture notes"
(Essential Advanced Physics - Volume 1, ISBN 978-0-7503-1398-8), with the model solutions of the exercise problems published under the title
"Classical Mechanics: Problems with solutions"
(Essential Advanced Physics - Volume 2, ISBN 978-0-7503-1401-5)

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Additional file (available upon request):
Exercise and Test Problems with Model Solutions (136 + 40 = 176 problems; 227 pp.)

## This <br>  <br> $\square$



## Chapter 1. Review of Fundamentals

After elaborating a bit on the title and contents of the course, this short introductory chapter lists the basic notions and facts of the classical mechanics, that are supposed to be known to the reader from undergraduate studies. ${ }^{1}$ Due to this reason, the explanations are very brief.

### 1.1. Mechanics and dynamics

A more fair title of this course would be Classical Mechanics and Dynamics, because the notions of mechanics and dynamics, though much intertwined, are still somewhat different. Term mechanics, in its narrow sense, means deriving the equations of motion of point-like particles and their systems (including solids and fluids), solution of these equations, and interpretation of the results. Dynamics is a more ambiguous term; it may mean, in particular:
(i) the part of mechanics that deals with motion (in contrast to statics);
(ii) the part of mechanics that deals with reasons for motion (in contrast to kinematics);
(iii) the part of mechanics that focuses on its two last tasks, i.e. the solution of the equations of motion and discussion of the results.

The last definition invites a question. It may look that mechanics and dynamics are just two sequential steps of a single process; why should they be considered separate disciplines? The main reason is that the many differential equations of motion, obtained in classical mechanics, also describe processes in different systems, so that their analysis may reveal important features of these systems as well. For example, the famous ordinary differential equation

$$
\begin{equation*}
\ddot{x}+\omega_{0}^{2} x=0 \tag{1.1}
\end{equation*}
$$

describes sinusoidal 1D oscillations not only of a mass on a spring, but also of an electric or magnetic field in a resonator, and many other systems. Similarly, the well-known partial differential equation

$$
\begin{equation*}
\left(\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}-\nabla^{2}\right) f(\mathbf{r}, t)=0 \tag{1.2}
\end{equation*}
$$

where $v$ is a constant and $\nabla^{2}$ is the Laplace operator, ${ }^{2}$ describes not only acoustic waves in an elastic mechanical continuum (solid or fluid), but also electromagnetic waves in a non-dispersive media, certain chemical reactions, etc. Thus the results of analysis of the dynamics described by these equations may be reused for applications well beyond mechanics.

[^6]To summarize, term "dynamics" is so ambiguous ${ }^{3}$ that, after some hesitation, I have opted to using for this course the traditional name Classical Mechanics, implying its broader meaning, which includes (similarly to Quantum Mechanics and Statistical Mechanics) studies of dynamics of some nonmechanical systems.

### 1.2. Kinematics: Basic notions

The basic notions of kinematics may be defined in various ways, and some mathematicians pay a lot of attention to analyzing such systems of axioms and relations between them. In physics, we typically stick to less rigorous ways (in order to proceed faster to particular problems), and end debating a definition as soon as everybody in the room agrees that we are all speaking about the same thing. Let me hope that the following notions used in classical mechanics do satisfy this criterion:
(i) All the Euclidean geometry notions, including the geometric point (the mathematical abstraction for the position of a very small object), straight line, etc.
(ii) The orthogonal, linear ("Cartesian") coordinates ${ }^{4} r_{j}$ of a geometric point in a particular reference frame - see Fig. $1 .{ }^{5}$


Fig. 1.1. Cartesian coordinates and radius-vector of a point/particle.

The coordinates may be used to define the point's radius-vector ${ }^{6}$
${ }^{3}$ Another important issue is: Definition (iii) of dynamics is suspiciously close to the part of mathematics devoted to the differential equation analysis; what is the difference? To answer, we have to dip, for just a second, into the philosophy of physics. Physics may be described as an art (and a bit of science :-) of description of Mother Nature by mathematical means; hence in many cases the approaches of a mathematician and a physicist to a problem are very similar. The main difference is that physicists try to express the results of their analysis in terms of system's motion rather than function properties, and as a result develop some sort of intuition ("gut feeling") about how other, apparently similar, systems may behave, even if their exact equations of motion are somewhat different - or not known at all. The intuition so developed has an enormous heuristic power, and most discoveries in physics have been made through gut-feeling-based insights rather than by plugging one formula into another one.
${ }^{4}$ In these notes the Cartesian coordinates are denoted either as either $\left\{r_{1}, r_{2}, r_{3}\right\}$ or $\{x, y, z\}$, depending on convenience in the particular case. Note that axis numbering is important for operations like the vector ("cross") product; the "correct" (meaning generally accepted) numbering order is such that rotation $\mathbf{n}_{1} \rightarrow \mathbf{n}_{2} \rightarrow \mathbf{n}_{3} \rightarrow \mathbf{n}_{1} \ldots$ looks counterclockwise if watched from a point with all $r_{i}>0-$ see Fig. 1.
${ }^{5}$ In references to figures, formulas, problems and sections within the same chapter of these notes, the chapter number is dropped for brevity.
${ }^{6}$ From the point of view of the tensor theory (in which the physical vectors like $\mathbf{r}$ are considered the rank-1 tensors), it would be more natural to use superscripts in the components $r_{j}$ and other "contravariant" vectors. However, the superscripts may be readily confused with the power signs, and I will postpone this notation (as well as the implied summation over the repeated indices) until the discussion of relativity in EM Chapter 9.

Radius -vector

Euclidean metric

Velocity

Acceleration
and its acceleration:

$$
\begin{equation*}
\mathbf{a}(t) \equiv \frac{d \mathbf{v}}{d t} \equiv \dot{\mathbf{v}}=\ddot{\mathbf{r}} . \tag{1.6}
\end{equation*}
$$

Since the above definitions of vectors $\mathbf{r}, \mathbf{v}$, and a depend on the chosen reference frame (are "reference-frame-specific"), there is a need to relate those vectors as observed in different frames. Within the Euclidean geometry, for two reference frames with the corresponding axes parallel in the moment of interest (Fig. 2), the relation between the radius-vectors is very simple:
Radiusvector's transformation

$$
\begin{equation*}
\mathbf{r}=\sum_{j=1}^{3} \mathbf{n}_{j} r_{j} \tag{1.3}
\end{equation*}
$$

where $\mathbf{n}_{1}, \mathbf{n}_{2}, \mathbf{n}_{3}$ are the unit vectors along coordinate axis directions, with the Euclidean metric:
which is independent, in particular, of the distribution of matter in space.
(iii) The time - as described by a continuous scalar variable (say, $t$ ), typically considered an independent argument of various physical observables, in particular the point's radius-vector $\mathbf{r}(t)$. By accepting Eq. (4), and an implicit assumption that time $t$ runs similarly in all reference frames, we subscribe to the notion of the absolute ("Newtonian") space/time, and hence abstain from a discussion of relativistic effects. ${ }^{7}$
(iv) The (instant) velocity of the point,

$$
\begin{equation*}
\mathbf{v}(t) \equiv \frac{d \mathbf{r}}{d t} \equiv \dot{\mathbf{r}}, \tag{1.5}
\end{equation*}
$$

$$
\begin{equation*}
\left.\mathbf{r}\right|_{\text {in } O^{\prime}}=\left.\mathbf{r}\right|_{\text {in } O}+\left.\mathbf{r}_{O}\right|_{\text {in } O^{\prime}} \tag{1.7}
\end{equation*}
$$



Fig. 1.2. Coordinate transfer between two reference frames.

[^7]If the frames move versus each other by translation only (no mutual rotation!), similar relations are valid for velocity and acceleration as well:

$$
\begin{align*}
& \left.\mathbf{v}\right|_{\text {in } O^{\prime}}=\left.\mathbf{v}\right|_{\text {in } O}+\left.\mathbf{v}_{O}\right|_{\text {in } O^{\prime}},  \tag{1.8}\\
& \left.\mathbf{a}\right|_{\text {in } O^{\prime}}=\left.\mathbf{a}\right|_{\text {in } O}+\left.\mathbf{a}_{O}\right|_{\text {in } O^{\prime}} . \tag{1.9}
\end{align*}
$$

In the case of mutual rotation of the reference frames, notions like $\left.\mathbf{v}_{O}\right|_{\text {in } O}$, are not well defined. (Indeed, different points of a rigid body connected to frame $O$ may have different velocities in frame $O^{\prime}$.) As a result, the transfer laws for velocities and accelerations are more complex than those given by Eqs. (8) and (9). It will be more natural for me to discuss them in the end of Chapter 5 that is devoted to rigid body motion.
(v) The particle: a localized physical object whose size is negligible, and shape unimportant for the given problem. Note that the last qualification is extremely important. For example, the size and shape of a Space Shuttle are not too important for the discussion of its orbital motion, but are paramount when its landing procedures are being developed. Since classical mechanics neglects the quantum mechanical uncertainties, ${ }^{8}$ particle's position, at any particular instant $t$, may be identified with a single geometric point, i.e. one radius-vector $\mathbf{r}(t)$. Finding the laws of motion $\mathbf{r}(t)$ of all particles participating in the given problem is frequently considered the final goal of classical mechanics.

### 1.3. Dynamics: Newton laws

Generally, the classical dynamics is fully described (in addition to the kinematic relations given above) by three Newton laws. ${ }^{9}$ In contrast to the impression some textbooks on theoretical physics try to create, these laws are experimental in nature, and cannot be derived from purely theoretical arguments. ${ }^{10}$

I am confident that the reader of these notes is already familiar with the Newton laws, in one or another formulation. Let me note only that in some formulations the $l^{\text {st }}$ Newton law looks just as a particular case of the $2^{\text {nd }}$ law - for the case of zero net force acting on a particle. In order to avoid this duplication, the $1^{\text {st }}$ law may be formulated as the following postulate:

- There exists at least one reference frame, called inertial, in which any free particle (i.e. a $1^{\text {st }}$ Newton particle isolated from the rest of the Universe) moves with $\mathbf{v}=$ const, i.e. with $\mathbf{a}=0$.

According to Eq. (9), this postulate immediately means that there is also an infinite number of inertial frames, because all frames $O^{\prime}$ moving without rotation or acceleration relative to the postulated inertial frame $O$ (i.e. having $\left.\mathbf{a}_{O}\right|_{\text {in }} O^{\prime}=0$ ) are also inertial.

[^8]On the other hand, the $2^{\text {nd }}$ and $3^{\text {rd }}$ Newton laws may be postulated together in the following elegant way. Each particle, say number $k$, may be characterized by a scalar constant (called mass $m_{k}$ ), such that at any interaction of $N$ particles (isolated from the rest of the Universe), in any inertial system,

$$
\begin{equation*}
\mathbf{P} \equiv \sum_{k=1}^{N} m_{k} \mathbf{v}_{k}=\text { const. } \tag{1.10}
\end{equation*}
$$

(Each component of this sum,

$$
\begin{equation*}
\mathbf{p}_{k} \equiv m_{k} \mathbf{v}_{k}, \tag{1.11}
\end{equation*}
$$

is called the mechanical momentum of the corresponding particle, and the whole sum $\mathbf{P}$, the total momentum of the system.)

Let us apply this postulate to just two interacting particles. Differentiating Eq. (10), written for this case, over time, we get

$$
\begin{equation*}
\dot{\mathbf{p}}_{1}=-\dot{\mathbf{p}}_{2} \tag{1.12}
\end{equation*}
$$

Let us give the derivative $\dot{\mathbf{p}}_{1}$ (i.e., a vector) the name of force $\mathbf{F}_{1}$ excerted on particle 1. In our current case, when the only possible source of force is particle 2, the force may be denoted as $\mathbf{F}_{12}$. Similarly, $\mathbf{F}_{21} \equiv \dot{\mathbf{p}}_{2}$, so that we get the $3^{\text {rd }}$ Newton law

3rd Newton law

$$
\begin{equation*}
\mathbf{F}_{12}=-\mathbf{F}_{21} . \tag{1.13}
\end{equation*}
$$

Now, returning to the general case of several interacting particles, we see that an additional (but very natural) assumption that all partial forces $\mathbf{F}_{k k^{\prime}}$ acting on particle $k$ add up as vectors, leads to the general form of the $2^{\text {nd }}$ Newton law ${ }^{11}$

$$
\begin{equation*}
m_{k} \mathbf{a}_{k} \equiv \dot{\mathbf{p}}_{k}=\sum_{k^{\prime} \neq k} \mathbf{F}_{k k^{\prime}} \equiv \mathbf{F}_{k}, \tag{1.14}
\end{equation*}
$$

that allows a clear interpretation of the mass as a measure of particle's inertia.
As a matter of principle, if the dependence of all pair forces $\mathbf{F}_{k k^{\prime}}$ of particle positions (and generally maybe of time as well) is known, Eq. (14) augmented with kinematic relations (4) and (5), allows the calculation of the laws of motion $\mathbf{r}_{k}(t)$ of all particles of the system. For example, for one particle the $2^{\text {nd }}$ law (14) gives the ordinary differential equation of the second order,

$$
\begin{equation*}
m \ddot{\mathbf{r}}=\mathbf{F}(\mathbf{r}, t) \tag{1.15}
\end{equation*}
$$

that may be integrated - either analytically or numerically.
For certain cases, this is very simple. As an elementary example, the Newton's gravity field
Newton's gravity law
(where $\mathbf{R} \equiv \mathbf{r}-\mathbf{r}$ ' is the distance between particles of masses $m$ and $m^{\prime}$ ) ${ }^{12}$, is virtually uniform and may be approximated as

[^9]\[

$$
\begin{equation*}
\mathbf{F}=m \mathbf{g}, \tag{1.16b}
\end{equation*}
$$

\]

Uniform gravity field
with the vector $\mathbf{g} \equiv\left(G m^{\prime} / r^{\prime 3}\right) \mathbf{r}^{\prime}$ being constant, for local, relatively small-scale motions, with $r \ll r^{\prime} .{ }^{13}$ As a result, $m$ in Eq. (15) cancels, it is reduced to just $\ddot{\mathbf{r}}=\mathbf{g}$, and may be easily integrated twice:

$$
\begin{gather*}
\dot{\mathbf{r}}(t) \equiv \mathbf{v}(t)=\int_{0}^{t} \mathbf{g} d t^{\prime}+\mathbf{v}(0)=\mathbf{g} t+\mathbf{v}(0)  \tag{1.17}\\
\mathbf{r}(t)=\int_{0}^{t} \mathbf{v}\left(t^{\prime}\right) d t^{\prime}+\mathbf{r}(0)=\mathbf{g} \frac{t^{2}}{2}+\mathbf{v}(0) t+\mathbf{r}(0) \tag{1.18}
\end{gather*}
$$

thus giving the full solution of all those undergraduate problems on the projectile motion, which should be so familiar to the reader.

All this looks (and indeed is) very simple, but in most other cases leads to more complex calculations. As an example, let us consider another simple problem: a bead of mass $m$ sliding, without friction, along a round ring of radius $R$ in a gravity field obeying Eq. (16b) - see Fig. 3.


Fig. 1.3. Bead moving on a vertical ring.

Suppose we are only interested in bead's velocity $v$ in the lowest point, after it has been dropped from the rest at the rightmost position. If we want to solve this problem using only the Newton laws, we have to do the following steps:
(i) consider the bead in an arbitrary intermediate position on a ring, described, for example by the angle $\theta$ shown in Fig. 3;
(ii) draw all the forces acting on the particle - in our current case, the gravity force $m \mathbf{g}$ and the reaction force $\mathbf{N}$ exerted by the ring;

[^10](iii) write the $2^{\text {nd }}$ Newton law for two nonvanishing components of the bead acceleration, say for its vertical and horizontal components $a_{x}$ and $a_{y}$;
(iv) recognize that in the absence of friction, the force $\mathbf{N}$ should be normal to the ring, so that we can use two additional equations, $N_{x}=-N \sin \theta$ and $N_{y}=N \cos \theta$;
(v) eliminate unknown variables $N, N_{x}$, and $N_{y}$ from the resulting system of four equations, thus getting a single second-order differential equation for one variable, for example $\theta$;
(vi) integrate this equation once to get the expression relating the velocity $\dot{\theta}$ and the angle $\theta$; and, finally,
(vii) using our specific initial condition ( $\dot{\theta}=0$ at $\theta=\pi / 2$ ), find the final velocity as $v=R \dot{\theta}$ at $\theta=0$.

All this is very much doable, but please agree that the procedure it too cumbersome for such a simple problem. Moreover, in many other cases even writing equations of motion along relevant coordinates is very complex, and any help the general theory may provide is highly valuable. In many cases, such help is given by conservation laws; let us review the most general of them.

### 1.4. Conservation laws

(i) Energy conservation is arguably the most general law of physics, but in mechanics it takes a more humble form of mechanical energy conservation that has limited applicability. To derive it, we first have to define the kinetic energy of a particle as

Kinetic energy

$$
\begin{equation*}
T \equiv \frac{m}{2} v^{2} \tag{1.19}
\end{equation*}
$$

and then recast its differential as ${ }^{14}$

$$
\begin{equation*}
d T=d\left(\frac{m}{2} v^{2}\right)=d\left(\frac{m}{2} \mathbf{v} \cdot \mathbf{v}\right)=m \mathbf{v} \cdot d \mathbf{v}=m \frac{d \mathbf{v} \cdot d \mathbf{r}}{d t}=\frac{d \mathbf{p}}{d t} \cdot d \mathbf{r} . \tag{1.20}
\end{equation*}
$$

Now plugging in the momentum's derivative from the $2^{\text {nd }}$ Newton law, $d \mathbf{p} / d t=\mathbf{F}$, where $\mathbf{F}$ is the full force acting on the particle, we get relation $d T=\mathbf{F} \cdot d \mathbf{r}$. Its integration along particle's trajectory between some points $A$ and $B$ gives the relation that is sometimes called the work-energy principle:

Energy-
work
principle

$$
\begin{equation*}
\Delta T \equiv T\left(\mathbf{r}_{B}\right)-T\left(\mathbf{r}_{A}\right)=\int_{A}^{B} \mathbf{F} \cdot d \mathbf{r} \tag{1.21}
\end{equation*}
$$

where the integral in the right-hand part is called the work of the force $\mathbf{F}$ on the path from $A$ to $B$.
The further step may be made only for potential (also called "conservative") forces that may be presented as (minus) gradients of some scalar function $U(\mathbf{r})$, called the potential energy. ${ }^{15}$ The vector operator $\nabla$ (called either del or nabla) of spatial differentiation ${ }^{16}$ allows a very compact expression of this fact:

[^11]\[

$$
\begin{equation*}
\mathbf{F}=-\nabla U \tag{1.22}
\end{equation*}
$$

\]

For example, for the uniform gravity field (16b),

$$
\begin{equation*}
U=m g h+\text { const }, \tag{1.23}
\end{equation*}
$$

where $h$ is the vertical coordinate directed "up" - opposite to the direction of the vector $\mathbf{g}$.
Integrating the tangential component $F_{\tau}$ of the vector $\mathbf{F}$, given by Eq. (22), along an arbitrary path connecting points $A$ and $B$, we get

$$
\begin{equation*}
\int_{A}^{B} F_{\tau} d r \equiv \int_{A}^{B} \mathbf{F} \cdot d \mathbf{r}=U\left(\mathbf{r}_{A}\right)-U\left(\mathbf{r}_{B}\right), \tag{1.24}
\end{equation*}
$$

i.e. work of potential forces may be presented as the difference of values of function $U(\mathbf{r})$ in the initial and final point of the path. (Note that according to Eq. (24), work of a potential force on any closed trajectory, with $\mathbf{r}_{A}=\mathbf{r}_{B}$, is zero.)

Now returning to Eq. (21) and comparing it with Eq. (24), we see that

$$
\begin{equation*}
T\left(\mathbf{r}_{B}\right)-T\left(\mathbf{r}_{A}\right)=U\left(\mathbf{r}_{A}\right)-U\left(\mathbf{r}_{B}\right), \tag{1.25}
\end{equation*}
$$

so that the total mechanical energy $E$, defined as

$$
\begin{equation*}
E \equiv T+U \tag{1.26}
\end{equation*}
$$

is indeed conserved:

$$
\begin{equation*}
E\left(\mathbf{r}_{A}\right) \equiv E\left(\mathbf{r}_{B}\right), \tag{1.27}
\end{equation*}
$$

[^12]If we sum up the resulting Eqs. (14) for all particles of the system then, due to the $3^{\text {rd }}$ Newton law (13), the contributions of all internal forces to this double sum in the right-hand part cancel, and we get the equation

System's momentum evolution

$$
\begin{equation*}
\dot{\mathbf{P}}=\mathbf{F}^{(\mathrm{ext})}, \quad \text { where } \mathbf{F}^{(e x t)} \equiv \sum_{k=1}^{N} \mathbf{F}_{k}^{(\mathrm{ext})} \tag{1.30}
\end{equation*}
$$

which tells us that the translational motion of the system as the whole is similar to that of a single particle, under the effect of the net external force $\mathbf{F}^{(\text {ext })}$. As a simple sanity check, if the external forces have a zero sum, we return to postulate (10). Just one reminder: Eq. (30), just as its precursor Eq. (14), is only valid in an inertial reference frame.
(iii) Angular momentum of a particle ${ }^{18}$ is defined as the following vector:

Angular momentum: definition

$$
\begin{equation*}
\mathbf{L} \equiv \mathbf{r} \times \mathbf{p} \tag{1.31}
\end{equation*}
$$

where $\mathbf{a} \times \mathbf{b}$ means the vector (or "cross-") product of the vector operands. ${ }^{19}$ Now, differentiating Eq. (31) over time, we get

$$
\begin{equation*}
\dot{\mathbf{L}}=\dot{\mathbf{r}} \times \mathbf{p}+\mathbf{r} \times \dot{\mathbf{p}} \tag{1.32}
\end{equation*}
$$

In the first product, $\dot{\mathbf{r}}$ is just the velocity vector $\mathbf{v}$ which is parallel to the particle momentum $\mathbf{p}=\mathrm{mv}$, so that this product vanishes, since the vector product of any two parallel vectors is zero. In the second product, $\dot{\mathbf{p}}$ equals the full force $\mathbf{F}$ acting on the particle, so that Eq. (32) is reduced to

Angular
momentum: evolution

Torque
where vector

$$
\begin{equation*}
\dot{\mathbf{L}}=\boldsymbol{\tau} \tag{1.33}
\end{equation*}
$$

is called the torque of force $\mathbf{F}$. (Note that the torque is evidently reference-frame specific - and again, the frame has to be inertial for Eq. (33) to be valid.) For an important particular case of a central force $\mathbf{F}$ that is parallel to the radius vector $\mathbf{r}$ of a particle (as measured from the force source point), the torque vanishes, so that (in that particular reference frame only!) the angular momentum is conserved:

$$
\begin{equation*}
\mathbf{L}=\text { const. } \tag{1.35}
\end{equation*}
$$

For a system of $N$ particles, the total angular momentum is naturally defined as

$$
\begin{equation*}
\mathbf{L} \equiv \sum_{k=1}^{N} \mathbf{L}_{k} . \tag{1.36}
\end{equation*}
$$

Differentiating this equation over time, using Eq. (33) for each $\dot{\mathbf{L}}_{k}$, and again partitioning each force in a accordance with Eq. (29), we get

[^13]\[

$$
\begin{equation*}
\dot{\mathbf{L}}=\sum_{\substack{k, k^{\prime}=1 \\ k \neq k}}^{N} \mathbf{r}_{k} \times \mathbf{F}_{k k^{\prime}}+\boldsymbol{\tau}^{(e x t)}, \quad \text { where } \boldsymbol{\tau}^{(e x t)} \equiv \sum_{k=1}^{N} \mathbf{r}_{k} \times \mathbf{F}_{k}^{(e x t)} \tag{1.37}
\end{equation*}
$$

\]

The first (double) sum may be always divided into pairs of the type $\left(\mathbf{r}_{k} \times \mathbf{F}_{k k^{\prime}}+\mathbf{r}_{k^{\prime}} \times \mathbf{F}_{k^{\prime} k}\right)$. With a natural assumption of the central forces $\left(\mathbf{F}_{k k^{\prime}} \| \mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right.$ ), each of these pairs equals zero. Indeed, in this case both components of the pair are vectors perpendicular to the plane passed through positions of both particles and the reference frame origin, i.e. to the plane of drawing of Fig. 4. Also, due to the $3^{\text {rd }}$ Newton law (13) the two forces are equal and opposite, and the magnitude of each term in the sum may be presented as $\left|F_{k k^{\prime}}\right| h_{k k^{\prime}}$, with equal "lever arms" $h_{k k^{\prime}}=h_{k^{\prime} k}$. As a result, each sum $\left(\mathbf{r}_{k} \times \mathbf{F}_{k k^{\prime}}+\mathbf{r}_{k^{\prime}} \times \mathbf{F}_{k^{\prime} k}\right)$, and hence the whole double sum in Eq. (37) vanish, and it is reduced to a very simple result,

$$
\begin{equation*}
\dot{\mathbf{L}}=\boldsymbol{\tau}^{(\mathrm{ext})} \tag{1.38}
\end{equation*}
$$

that is similar to Eq. (33) for a single particle, and is the angular analog of Eq. (30). In particular, Eq. (38) shows that if the full external torque $\tau^{(\text {ext })}$ vanishes by some reason (e.g., if the system of particles is isolated from the rest of the Universe), the conservation law (35) is valid for the full angular momentum $\mathbf{L}$, even if its individual components $\mathbf{L}_{k}$ are not conserved due to inter-particle interactions.


Fig. 1.4. Internal and external forces, and the internal torque cancellation in a system of two particles.

From the mathematical point of view, most conservation laws present the first integrals of motion which sometimes liberate us from the necessity to integrate the second-order differential equations of motion, following from the Newton laws, twice.

### 1.5. Potential energy and equilibrium

Another important role of the potential energy $U$, especially for dissipative systems whose total mechanical energy $E$ is not conserved because it may be drained to the environment, is finding the positions of equilibrium (sometimes called the fixed points of the system under analysis) and analyzing their stability with respect to small perturbations. For a single particle, this is very simple: force (22) vanishes at each extremum (minimum or maximum) of the potential energy. ${ }^{20}$ Of those fixed points, only the minimums of $U(\mathbf{r})$ are stable - see Sec. 3.2 below for a discussion of this point.

[^14]A slightly more subtle case is a particle with potential energy $U(\mathbf{r})$, subjected to an additional external force $\mathbf{F}^{(\text {ext })}(\mathbf{r})$. In this case, the stable equilibrium is reached at the minimum of not function $U(\mathbf{r})$, but of what is sometimes called the Gibbs potential energy

$$
\begin{equation*}
U_{\mathrm{G}}(\mathbf{r}) \equiv U(\mathbf{r})-\int^{\mathbf{r}} \mathbf{F}^{(\mathrm{ext})}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime} \tag{1.39}
\end{equation*}
$$

which is defined, just as $U(\mathbf{r})$ is, to an arbitrary constant. The proof of Eq. (39) is very simple: in an extremum of this function, the total force acting on the particle,

$$
\begin{equation*}
\mathbf{F}^{(\mathrm{tot})}=\mathbf{F}+\mathbf{F}^{(\mathrm{ext})} \equiv-\nabla U+\nabla \int^{\mathbf{r}} \mathbf{F}^{(\mathrm{ext})}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime}=-\nabla U_{\mathrm{G}} \tag{1.40}
\end{equation*}
$$

vanishes, as it should. ${ }^{21}$ For the simplest (and very frequent) case of the applied force independent on particle's position, the Gibbs potential energy is just

$$
\begin{equation*}
U_{\mathrm{G}}(\mathbf{r}) \equiv U(\mathbf{r})-\mathbf{F}^{(\mathrm{ext})} \cdot \mathbf{r}+\text { const } . \tag{1.41}
\end{equation*}
$$

This is all very straightforward, but since the notion of $U_{\mathrm{G}}$ is not well known to some students, ${ }^{22}$ let me offer a very simple example. Consider a 1D deformation of the usual elastic spring providing the returning force $(-\kappa x)$, where $x$ is the deviation from spring's equilibrium. In order for the force to comply with Eq. (22), its potential energy should equal to $U=\kappa x^{2} / 2+$ const, so that its minimum corresponds to $x=0$. This works fine until the spring comes under effect of a nonvanishing external force $F$, say independent of $x$. Then the equilibrium deformation of the spring, $x_{0}=F / \kappa$, evidently corresponds not to the minimum of $U$ but rather to that of the Gibbs potential energy (41): $U_{\mathrm{G}}=U-F x=\kappa x^{2} / 2-F x+$ const.

### 1.6. OK, we've got it - can we go home now?

Not yet. In many cases the conservation laws discussed above provide little help, even in systems without dissipation. Consider for example a generalization of the bead-on-the-ring problem shown in Fig. 3, in which the ring is rotated by external forces, with a constant angular velocity $\omega$, about its vertical diameter (Fig. 5). ${ }^{23}$ In this problem (to which I will repeatedly return below, using it as

[^15]an analytical mechanics "testbed"), none of the three conservation laws listed in the last section, holds. In particular, bead's energy,
\[

$$
\begin{equation*}
E=\frac{m}{2} v^{2}+m g h, \tag{1.42}
\end{equation*}
$$

\]

is not constant, because the external forces rotating the ring may change it. Of course, we still can solve the problem using the Newton laws, but this is even more complex than for the above case of the ring at rest, in particular because the force $\mathbf{N}$ exerted on the bead by the ring now may have three rather than two Cartesian components, which are not simply related. One can readily see that if we could exclude the so-called reaction forces such as $\mathbf{N}$, that ensure external constraints of the particle motion, in advance, that would help a lot. Such an exclusion may be provided by analytical mechanics, in particular its Lagrangian formulation, which will be discussed in the next chapter.


Fig. 1.5. Bead sliding along a rotating ring.

An even more important motivation for analytical mechanics is given by dynamics of "nonmechanical" systems, for example, of the electromagnetic field - possibly interacting with charged particles, conducting bodies, etc. In many such systems, the easiest (and sometimes the only practicable) way to find the equations of motion is to derive then from the Lagrangian or Hamiltonian function of the system. In particular, the Hamiltonian formulation of the analytical mechanics (to be discussed in Chapter 10) offers a direct pathway to deriving Hamiltonian operators of systems, which is the standard entry point for analysis of their quantum-mechanical properties.

### 1.7. Self-test problems

1.1. A bicycle, ridden with velocity $v$ on a wet pavement, has no mudguards on its wheels. How far behind should the following biker ride to avoid being splashed over? Neglect the air resistance effects.
1.2. Two round disks of radius $R$ are firmly connected with a coaxial cylinder of a smaller radius $r$, and a thread is wound on the resulting spool. The spool is placed on a horizontal surface, and thread's end is being pooled out at angle $\varphi$-see Fig. on the right. Assuming that the spool does not slip on the surface, what direction would it roll?

(Sometimes the device is called the "Watt's governor", after the famous engineer J. Watts who used it in 1788 in one of his first steam engines, though it had been used in European windmills at least since the 1600s.)
1.3. Calculate the equilibrium shape of a flexible, heavy rope of length $l$, with a constant mass $\mu$ per unit length, if it is hung in a uniform gravity field between two points separated by a horizontal distance $d$ - see Fig. on the right.

1.4. A uniform, long, thin bar is placed horizontally on two similar round cylinders rotating toward each other with the same angular velocity $\omega$ and displaced by distance $d$ - see Fig. on the right. Calculate the laws of relatively slow horizontal motions of the bar within the plane of drawing for both possible directions of cylinder rotation, assuming that the friction force between the slipping surfaces of the bar and each cylinder obeys the usual simple law $|F|=\mu N$, where $N$ is the normal
 pressure force between them, and $\mu$ is a constant (velocityindependent) coefficient. Formulate the condition of validity of your result.
1.5. A small block slides, without friction, down a smooth slide that ends with a round loop of radius $R$ - see Fig. on the right. What smallest initial height $h$ allows the block to make its way around the loop without dropping from the slide, if it is launched with negligible initial velocity?

1.6. A satellite of mass $m$ is being launched from height $H$ over the surface of a spherical planet with radius $R$ and mass $M \gg m$ - see Fig. on the right. Find the range of initial velocities $\mathbf{v}_{0}$ (normal to the radius) providing closed orbits above the planet's surface.

1.7. Prove that the thin-uniform-disk model of a galaxy describes small harmonic oscillations of stars inside it along the direction normal to the disk, and calculate the frequency of these oscillations in terms of the Newton's gravitational constant $G$ and the average density $\rho$ of the star/dust matter of the galaxy.
1.8. Derive the differential equations of motion for small oscillations of two similar pendula coupled with a spring (see Fig. on the right), within the vertical plane. Assume that at the vertical position of both pendula, the spring is not stretched $(\Delta L=0)$.

1.9. One of popular futuristic concepts of travel is digging a straight railway tunnel through the Earth and letting a train go through it, without initial velocity - driven only by gravity. Calculate train's travel time through such a tunnel, assuming that the Earth's density $\rho$ is constant, and neglecting the friction and planet rotation effects.
1.10. A small bead of mass $m$ may slide, without friction, along a light string, stretched with a force $\mathscr{T} \gg m g$ between two points separated by a horizontal distance $2 d-$ see Fig. on the right. Calculate the frequency of horizontal oscillations of the bead about its equilibrium position.

1.11. Find the acceleration of a rocket due to the working jet motor, and explore the resulting equation of rocket's motion.

Hint: For the sake of simplicity, you may consider a 1D motion.
1.12. Prove the following virial theorem: ${ }^{24}$ for a set of $N$ particles performing a periodic motion,

$$
\bar{T}=-\frac{1}{2} \sum_{k=1}^{N} \overline{\mathbf{F}_{k} \cdot \mathbf{r}_{k}},
$$

where (as everywhere in these notes), the top bar means time averaging - in this case over the motion period. What does the virial theorem say about:
(i) the 1 D motion of a particle in a confining potential $U(x)=a x^{2 s}$, with $a>0$ and $s>0$, and
(ii) the orbital motion of a particle moving in a central potential $U(r)=-C / r$ ?

Hint: Explore the time derivative of the following scalar function of time: $G(t) \equiv \sum_{k=1}^{N} \mathbf{p}_{k} \cdot \mathbf{r}_{k}$.

[^16]
## Chapter 2. Lagrangian Formalism

The goal of this chapter is to describe the Lagrangian formulation of analytical mechanics, which is extremely useful for obtaining the differential equations of motion (and sometimes their first integrals) not only for mechanical systems with holonomic constraints, but also other dynamic systems.

### 2.1. Lagrange equations

In many cases, the constraints imposed on 3D motion of a system of $N$ particles may be described by $N$ vector (i.e. $3 N$ scalar) algebraic equations

$$
\begin{equation*}
\mathbf{r}_{k}=\mathbf{r}_{k}\left(q_{1}, q_{2}, \ldots, q_{j}, \ldots, q_{J}, t\right), \quad 1 \leq k \leq N \tag{2.1}
\end{equation*}
$$

where $q_{j}$ are certain generalized coordinates which (together with constraints) completely define the system position, and $J \leq 3 N$ is the number of the actual degrees of freedom. The constraints that allow such description are called holonomic. ${ }^{1}$

For example, for our testbed, bead-on-rotating-ring problem (see Fig. 1.5 and Fig. 1 below) $J=$ 1, because taking into account the constraints imposed by the ring, bead's position may be uniquely determined by just one generalized coordinate - for example, its polar angle $\theta$. Indeed, selecting the reference frame as shown in Fig. 1 and using the well-known formulas for the spherical coordinates, ${ }^{2}$ we see that in this case Eq. (1) in Cartesian coordinates has the form

$$
\begin{equation*}
\mathbf{r} \equiv\{x, y, z\}=\{R \sin \theta \cos \varphi, R \sin \theta \sin \varphi, R \cos \theta\}, \quad \text { where } \varphi=\omega t+\text { const } \tag{2.2}
\end{equation*}
$$

where the constant depends on the exact selection of axes $x$ and $y$ and the time origin. Since $\varphi(t)$ is a fixed function of time, and $R$ is a fixed constant, the position of particle in space at any instant $t$ is indeed completely determined by the value of its only generalized coordinate $\theta$. Note that the dimensionality of the generalized coordinate may be different from that of Cartesian coordinates (meters)!


Fig. 2.1. Bead on a rotating ring as a example of the system with just one degree of freedom: $J=1$.

[^17]Now returning to the general case of $J$ degrees of freedom, let us consider a set of small variations (alternatively called "virtual displacements") $\delta q_{j}$ allowed by the constraints. Virtual displacements differ from the actual small displacements (described by differentials $d q_{j}$ proportional to time variation $d t$ ) in that $\delta q_{j}$ describes not the system's motion as such, but rather its possible variation see Fig. 1.


Fig. 2.2. Actual displacement $d q_{j}$ vs. the virtual one (i.e. variation) $\delta q_{j}$.

Generally, operations with variations are the subject of a special field of mathematics, the calculus of variations. ${ }^{3}$ However, the only math background necessary for our current purposes is the understanding that operations with variations are similar to those with the usual differentials, though we need to watch carefully what each variable is a function of. For example, if we consider the variation of the radius-vectors (1), at a fixed time $t$, as a function of independent variations $\delta q_{j}$, we may use the usual formula for the differentiation of a function of several arguments: ${ }^{4}$

$$
\begin{equation*}
\delta \mathbf{r}_{k}=\sum_{j} \frac{\partial \mathbf{r}_{k}}{\partial q_{j}} \delta q_{j} \tag{2.3}
\end{equation*}
$$

Now let us break the force acting upon the $k$-th particle into two parts: the frictionless, constraining part $\mathbf{N}_{k}$ of the reaction force and the remaining part $\mathbf{F}_{k}$ - including the force components from other sources and possibly the friction part of the reaction force. Then the $2^{\text {nd }}$ Newton law for $k$-th particle of the system may be presented as

$$
\begin{equation*}
m_{k} \dot{\mathbf{v}}_{k}-\mathbf{F}_{k}=\mathbf{N}_{k} \tag{2.4}
\end{equation*}
$$

Since any variation of the motion has to be allowed by the constraints, its 3 N -dimensional vector with $N$ 3D-vector components $\delta \mathbf{r}_{k}$ has to be perpendicular to the 3 N -dimensional vector of the constraining forces, also with $N$ 3D-vector components $\mathbf{N}_{k}$. (For example, for the problem shown in Fig. 2.1, the virtual displacement vector $\delta \mathbf{r}_{k}$ may be directed only along the ring, while the constraining force $\mathbf{N}$, exerted by the ring, has to be perpendicular to that direction.) This condition may be expressed as

$$
\begin{equation*}
\sum_{k} \mathbf{N}_{k} \cdot \delta \mathbf{r}_{k}=0, \tag{2.5}
\end{equation*}
$$

[^18]where the scalar product of 3 N -dimensional vectors is defined exactly as that of 3 D vectors, i.e. as the sum of the products of the corresponding components of the operands. The substitution of Eq. (4) into Eq. (5) results in the so-called D'Alembert principle: ${ }^{5}$

D'Alembert principle

$$
\begin{equation*}
\sum_{k}\left(m_{k} \dot{\mathbf{v}}_{k}-\mathbf{F}_{k}\right) \cdot \delta \mathbf{r}_{k}=0 \tag{2.6}
\end{equation*}
$$

Now we may plug Eq. (3) into Eq. (6) to get

$$
\begin{equation*}
\sum_{j}\left\{\sum_{k} m_{k} \dot{\mathbf{v}}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}}-\boldsymbol{7}_{j}\right\} \delta q_{j}=0 \tag{2.7}
\end{equation*}
$$

where scalars $\mathcal{7}_{j}$, called generalized forces, are defined as follows: ${ }^{6}$

$$
\begin{equation*}
\boldsymbol{7}_{j} \equiv \sum_{k} \mathbf{F}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}} . \tag{2.8}
\end{equation*}
$$

Now we may use the standard argument of the calculus of variations: in order for the left-hand part of Eq. (7) to be zero for an arbitrary selection of independent variations $\delta q_{j}$, the expressions in the curly brackets, for every $j$, should equal zero. This gives us a set of $J$ equations

$$
\begin{equation*}
\sum_{k} m_{k} \dot{\mathbf{v}}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}}-\boldsymbol{\gamma}_{j}=0 \tag{2.9}
\end{equation*}
$$

let us present them in a more convenient form. First, using the differentiation by parts to calculate the following time derivative:

$$
\begin{equation*}
\frac{d}{d t}\left(\mathbf{v}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}}\right)=\dot{\mathbf{v}}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}}+\mathbf{v}_{k} \frac{d}{d t}\left(\frac{\partial \mathbf{r}_{k}}{\partial q_{j}}\right) \tag{2.10}
\end{equation*}
$$

we may notice that the first term in the right-hand part is exactly the scalar product in the first term of Eq. (9).

Second, let us use another key fact of the calculus of variations (which is, essentially, evident from Fig. 3): the differentiation of a variable over time and over the generalized coordinate variation (at fixed time) are interchangeable operations.


Fig. 2.3. Variation of the differential (of any function $f$ ) equals the differential of its variation.

[^19]As a result, in the second term on the right-hand part of Eq. (10) we may write

$$
\begin{equation*}
\frac{d}{d t}\left(\frac{\partial \mathbf{r}_{k}}{\partial q_{j}}\right)=\frac{\partial}{\partial q_{j}}\left(\frac{d \mathbf{r}_{k}}{d t}\right) \equiv \frac{\partial \mathbf{v}_{k}}{\partial q_{j}} \tag{2.11}
\end{equation*}
$$

Finally, let us differentiate of Eq. (1) over time:

$$
\begin{equation*}
\mathbf{v}_{k} \equiv \frac{d \mathbf{r}_{k}}{d t}=\sum_{j} \frac{\partial \mathbf{r}_{k}}{\partial q_{j}} \dot{q}_{j}+\frac{\partial \mathbf{r}_{k}}{\partial t} \tag{2.12}
\end{equation*}
$$

This equation shows that particle velocities $\mathbf{v}_{k}$ may be considered as linear functions of the generalized velocities $\dot{q}_{j}$ considered as independent variables, with proportionality coefficients

$$
\begin{equation*}
\frac{\partial \mathbf{v}_{k}}{\partial \dot{q}_{j}}=\frac{\partial \mathbf{r}_{k}}{\partial q_{j}} \tag{2.13}
\end{equation*}
$$

With the account of Eqs. (10), (11), and (13), Eq. (9) turns into

$$
\begin{equation*}
\frac{d}{d t} \sum_{k} m_{k} \mathbf{v}_{k} \cdot \frac{\partial \mathbf{v}_{k}}{\partial \dot{q}_{j}}-\sum_{k} m_{k} \mathbf{v}_{k} \frac{\partial \mathbf{v}_{k}}{\partial q_{j}}-\mathcal{Z}_{j}=0 \tag{2.14}
\end{equation*}
$$

This result may be further simplified by making, for the total kinetic energy of the system,

$$
\begin{equation*}
T \equiv \sum_{k} \frac{m_{k}}{2} v_{k}^{2}=\frac{1}{2} \sum_{k} m_{k} \mathbf{v}_{k} \cdot \mathbf{v}_{k} \tag{2.15}
\end{equation*}
$$

the same commitment as for $\mathbf{v}_{k}$, i.e. considering $T$ a function of not only the generalized coordinates $q_{j}$ and time $t$, but also of the generalized velocities $\dot{q}_{i}$ - as variables independent of $q_{j}$ and $t$. Then we may calculate the partial derivatives of $T$ as

$$
\begin{equation*}
\frac{\partial T}{\partial q_{j}}=\sum_{k} m_{k} \mathbf{v}_{k} \cdot \frac{\partial \mathbf{v}_{k}}{\partial q_{j}}, \quad \frac{\partial T}{\partial \dot{q}_{j}}=\sum_{k} m_{k} \mathbf{v}_{k} \cdot \frac{\partial \mathbf{v}_{k}}{\partial \dot{q}_{j}} \tag{2.16}
\end{equation*}
$$

and notice that they are exactly the two sums participating in Eq. (14). As a result, we get a system of $J$ Lagrange equations, ${ }^{7}$

$$
\begin{equation*}
\frac{d}{d t} \frac{\partial T}{\partial \dot{q}_{j}}-\frac{\partial T}{\partial q_{j}}-7_{j}=0, \quad \text { for } j=1,2, \ldots, J \tag{2.17}
\end{equation*}
$$

Their big advantage over the initial Newton law equations (4) is that the Lagrange equations do not include the constraining forces $\mathbf{N}_{\mathrm{k}}$.

This is as far as we can go for arbitrary forces. However, if all the forces may be expressed in the form similar but somewhat more general than Eq. (1.31), $\mathbf{F}_{k}=-\nabla_{k} U\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \ldots, \mathbf{r}_{N}, t\right.$, where $U$ is the

[^20]effective potential energy of the system, ${ }^{8}$ and $\operatorname{sign} \nabla_{k}$ denotes differentiation over coordinates of $k$-th particle, we may recast Eq. (8) into a simpler form:
\[

$$
\begin{equation*}
\boldsymbol{Z}_{j} \equiv \sum_{k} \mathbf{F}_{k} \cdot \frac{\partial \mathbf{r}_{k}}{\partial q_{j}}=-\sum_{k}\left(\frac{\partial U}{\partial x_{k}} \cdot \frac{\partial x_{k}}{\partial q_{j}}+\frac{\partial U}{\partial y_{k}} \cdot \frac{\partial y_{k}}{\partial q_{j}}+\frac{\partial U}{\partial z_{i}} \cdot \frac{\partial z_{i}}{\partial q_{j}}\right) \equiv-\frac{\partial U}{\partial q_{j}} . \tag{2.18}
\end{equation*}
$$

\]

Since we assume that $U$ depends only on particle coordinates (and possibly time), but not velocities, $\partial U / \partial \dot{q}_{j}=0$, with the substitution of Eq. (18), the Lagrange equation (17) may be presented in its canonical form

Canonical Lagrange equations

$$
\begin{equation*}
\frac{d}{d t} \frac{\partial L}{\partial \dot{q}_{j}}-\frac{\partial L}{\partial q_{j}}=0, \quad \text { where } L \equiv T-U \tag{2.19a}
\end{equation*}
$$

where $L$ is called the Lagrangian function (or just the "Lagrangian"), defined as

$$
\begin{equation*}
L \equiv T-U . \tag{2.19b}
\end{equation*}
$$

It is crucial to distinguish this function from the mechanical energy (1.26), $E=T+U$.
Using the Lagrangian formalism in practice, the reader should always remember that:
(i) Each system has only one Lagrange function $L$, but is described by $J \geq 1$ Lagrange equations of motion (for $j=1,2, \ldots, J$ ).
(ii) Differentiating $T$, we have to consider the generalized velocities $\dot{q}_{j}$ as independent variables, ignoring the fact they are actually the time derivatives of $q_{j}$.

### 2.2. Examples

As the first, simplest example, consider a particle constrained to move along one axis (say, $x$ ):

$$
\begin{equation*}
T=\frac{m}{2} \dot{x}^{2}, \quad U=U(x, t) \tag{2.20}
\end{equation*}
$$

In this case, it is natural to consider $x$ as the (only) generalized coordinate, and $\dot{x}$ as the generalized velocity, so that

$$
\begin{equation*}
L \equiv T-U=\frac{m}{2} \dot{x}^{2}-U(x, t) . \tag{2.21}
\end{equation*}
$$

Considering $\dot{x}$ an independent variable, we get $\partial L / \partial \dot{x}=m \dot{x}$, and $\partial L / \partial x=-\partial U / \partial x$, so that the Lagrange equation of motion (only one equation in this case of the single degree of freedom!) yields

$$
\begin{equation*}
\frac{d}{d t}(m \dot{x})-\left(-\frac{\partial U}{\partial x}\right)=0, \tag{2.22}
\end{equation*}
$$

[^21]evidently the same result as the $x$-component of the $2^{\text {nd }}$ Newton law with $F_{x}=-\partial U / \partial x$. This is a good sanity check, but we see that the Lagrange formalism does not provide too much advantage in this particular case.

This advantage is, however, evident for our testbed problem - see Fig. 1. Indeed, taking the polar angle $\theta$ for the (only) generalized coordinate, we see that in this case the kinetic energy depends not only on the generalized velocity, but also on the generalized coordinate: ${ }^{9}$

$$
\begin{align*}
& T=\frac{m}{2} R^{2}\left(\dot{\theta}^{2}+\omega^{2} \sin ^{2} \theta\right), \quad U=-m g z+\text { const }=-m g R \cos \theta+\text { const },  \tag{2.23}\\
& L \equiv T-U=\frac{m}{2} R^{2}\left(\dot{\theta}^{2}+\omega^{2} \sin ^{2} \theta\right)+m g R \cos \theta+\text { const. }
\end{align*}
$$

Here it is especially important to remember that at substantiating the Lagrange equation, $\theta$ and $\dot{\theta}$ have to be treated as independent arguments of $L$, so that

$$
\begin{equation*}
\frac{\partial L}{\partial \dot{\theta}}=m R^{2} \dot{\theta}, \quad \frac{\partial L}{\partial \theta}=m R^{2} \omega^{2} \sin \theta \cos \theta-m g R \sin \theta \tag{2.24}
\end{equation*}
$$

giving us the following equation of motion:

$$
\begin{equation*}
\frac{d}{d t}\left(m R^{2} \dot{\theta}\right)-\left(m R^{2} \omega^{2} \sin \theta \cos \theta-m g R \sin \theta\right)=0 \tag{2.25}
\end{equation*}
$$

As a sanity check, at $\omega=0$, Eq. (25) is reduced to the correct equation of the usual pendulum:

$$
\begin{equation*}
\ddot{\theta}+\Omega^{2} \sin \theta=0, \quad \text { where } \Omega \equiv\left(\frac{g}{R}\right)^{1 / 2} . \tag{2.26}
\end{equation*}
$$

We will explore the full dynamic equation (25) in more detail later, but please note how simple its derivation was - in comparison with writing the Newton laws and then excluding the reaction force.

Next, though the Lagrangian formalism was derived from the Newton law for mechanical systems, the resulting equations (19) are applicable to other dynamic systems, especially those for which the kinetic and potential energies may be readily expressed via some generalized coordinates. As the simplest example, consider the well-known connection (Fig. 4) of a capacitor with capacitance $C$ to an inductive coil with self-inductance $L .{ }^{10}$ (Electrical engineers frequently call it the $L C$ tank circuit.)


Fig. 2.4. $L C$ tank circuit.

[^22]As the reader certainly knows, at relatively low frequencies we may use the so-called lumpedcircuit approximation, in which the total energy of the system as the sum of two components, the electric energy $E_{C}$ localized inside the capacitor, and the magnetic energy $E_{L}$ localized inside the inductance coil

$$
\begin{equation*}
E_{C}=\frac{Q^{2}}{2 C}, \quad E_{L}=\frac{L I^{2}}{2} \tag{2.27}
\end{equation*}
$$

Since the electric current $I$ through the coil and the electric charge $Q$ on the capacitor are connected by the charge continuity equation $d Q / d t=I$ (evident from Fig. 4), it is natural to declare the charge a generalized coordinate, and the current, the generalized velocity. With this choice, the electrostatic energy $E_{C}(Q)$ may be treated as the potential energy $U$ of the system, and the magnetic energy $E_{L}(I)$, as its kinetic energy $T$. With this attribution, we get

$$
\begin{equation*}
\frac{\partial T}{\partial \dot{q}} \equiv \frac{\partial E_{L}}{\partial I}=L I \equiv L \dot{Q}, \quad \frac{\partial T}{\partial q} \equiv \frac{\partial E_{L}}{\partial Q}=0, \quad \frac{\partial U}{\partial q} \equiv \frac{\partial E_{C}}{\partial Q}=\frac{Q}{C} \tag{2.28}
\end{equation*}
$$

so that the Lagrange equation of motion is

$$
\begin{equation*}
\frac{d}{d t}(L \dot{Q})-\left(-\frac{Q}{C}\right)=0 \tag{2.29}
\end{equation*}
$$

Note, however, that the above choice of the generalized coordinate and velocity is not unique. Instead, one can use as the generalized coordinate the magnetic flux $\Phi$ through the inductive coil, related to the common voltage $V$ across the circuit (Fig. 4) by Faraday's induction law $V=-d \Phi / d t$. With this choice, $(-V)$ becomes the generalized velocity, $E_{L}=\Phi^{2} / 2 L$ should be understood as the potential energy, and $E_{C}=C V^{2} / 2$ treated as the kinetic energy. It is straightforward to verify that for this choice, the resulting Lagrange equation of motion is equivalent to Eq. (29). If both parameters of the circuit, $L$ and $C$, are constant in time, Eq. (29) is just the harmonic oscillator equation similar to Eq. (1.1), and describes sinusoidal oscillations with frequency

$$
\begin{equation*}
\omega_{0}=\frac{1}{(L C)^{1 / 2}} . \tag{2.30}
\end{equation*}
$$

This is of course a very well known result that may be derived in the more standard way by equating the voltage drops across the capacitor $(V=Q / C)$ and the inductor $\left(V=-L d I / d t=-L d^{2} Q / d t^{2}\right)$. However, the Lagrangian approach is much more convenient for more complex systems, for example, for the description of electromagnetic field and its interaction with charged relativistic particles. ${ }^{11}$

### 2.3. Hamiltonian function and energy

The canonical form (19) of the Lagrange equation has been derived using Eq. (18), which is formally similar to Eq. (1.22) for a potential force. Does this mean that the system described by Eq. (19) always conserves energy? Not necessarily, because the "potential energy" $U$, that participates in Eq. (18), may depend not only on the generalized coordinates, but on time as well. Let us start the analysis of this issue with the introduction of two new (and very important!) notions: the generalized momenta corresponding to each generalized coordinate $q_{j}$,

[^23]\[

$$
\begin{equation*}
p_{j} \equiv \frac{\partial L}{\partial \dot{q}_{j}} \tag{2.31}
\end{equation*}
$$

\]

and the Hamiltonian function ${ }^{12}$

$$
\begin{equation*}
H \equiv \sum_{j} \frac{\partial L}{\partial \dot{q}_{j}} \dot{q}_{j}-L \equiv \sum_{j} p_{j} \dot{q}_{j}-L \tag{2.32}
\end{equation*}
$$

In order to see whether the Hamiltonian function is conserved, let us differentiate its definition (32) over time:

$$
\begin{equation*}
\frac{d H}{d t}=\sum_{j}\left[\frac{d}{d t}\left(\frac{\partial L}{\partial \dot{q}_{j}}\right) \dot{q}_{j}+\frac{\partial L}{\partial \dot{q}_{j}} \ddot{q}_{j}\right]-\frac{d L}{d t} . \tag{2.33}
\end{equation*}
$$

If we want to make use of the Lagrange equation (19), the last derivative has to be calculated considering $L$ as a function of independent arguments $q_{j}, \dot{q}_{j}$, and $t$ :

$$
\begin{equation*}
\frac{d L}{d t}=\sum_{j}\left(\frac{\partial L}{\partial q_{j}} \dot{q}_{j}+\frac{\partial L}{\partial \dot{q}_{j}} \ddot{q}_{j}\right)+\frac{\partial L}{\partial t}, \tag{2.34}
\end{equation*}
$$

where the last term is the derivative of $L$ as an explicit function of time. We see that the last term in the square brackets of Eq. (33) immediately cancels with the last term in the parentheses of Eq. (34). Moreover, using the Lagrange equation (19) for the first term in the square brackets of Eq. (33), we see that it cancels with the first term in the parentheses of Eq. (34). Thus we arrive at a very simple and important result:

$$
\begin{equation*}
\frac{d H}{d t}=-\frac{\partial L}{\partial t} \tag{2.35}
\end{equation*}
$$

Hamiltonian function
and coincides with particle's mechanical energy $E=T+U$. Since the Lagrangian does not depend on time explicitly, both $H$ and $E$ are conserved.

However, it is not always that simple! Indeed, let us return again to our testbed problem (Fig. 1). In this case, the generalized momentum corresponding to the generalized coordinate $\theta$ is

$$
\begin{equation*}
p_{\theta} \equiv \frac{\partial L}{\partial \dot{\theta}}=m R^{2} \dot{\theta} \tag{2.39}
\end{equation*}
$$

and Eq. (32) yields:

$$
\begin{align*}
H & \equiv p_{\theta} \dot{\theta}-L=m R^{2} \dot{\theta}^{2}-\left[\frac{m}{2} R^{2}\left(\dot{\theta}^{2}+\omega^{2} \sin ^{2} \theta\right)+m g R \cos \theta\right]+\mathrm{const}  \tag{2.40}\\
& =\frac{m}{2} R^{2}\left(\dot{\theta}^{2}-\omega^{2} \sin ^{2} \theta\right)-m g R \cos \theta+\text { const. }
\end{align*}
$$

This means that (as soon as $\omega \neq 0$ ), the Hamiltonian function differs from the mechanical energy

$$
\begin{equation*}
E \equiv T+U=\frac{m}{2} R^{2}\left(\dot{\theta}^{2}+\omega^{2} \sin ^{2} \theta\right)-m g R \cos \theta+\text { const } . \tag{2.41}
\end{equation*}
$$

The difference, $E-H=m R^{2} \omega^{2} \sin ^{2} \theta$ (besides an inconsequential constant), may change at bead's motion along the ring, so that although $H$ is an integral of motion (since $\partial L / \partial t=0$ ), energy $E$ is not conserved.

Let us find out when do these two functions, $E$ and $H$, coincide. In mathematics, there is a notion of a homogeneous function $f\left(x_{1}, x_{2}, \ldots\right)$ of degree $\lambda$, defined in the following way: for an arbitrary constant $a$,

$$
\begin{equation*}
f\left(a x_{1}, a x_{2}, \ldots\right)=a^{\lambda} f\left(x_{1}, x_{2}, \ldots\right) \tag{2.42}
\end{equation*}
$$

Such functions obey the following Euler theorem: ${ }^{13}$

$$
\begin{equation*}
\sum_{j} \frac{\partial f}{\partial x_{j}} x_{j}=\lambda f \tag{2.43}
\end{equation*}
$$

that may be readily proven by differentiating both parts of Eq. (42) over $a$ and then setting this parameter to the particular value $a=1$. Now, consider the case when the kinetic energy is a quadratic form of all generalized velocities $\dot{q}_{j}$ :

$$
\begin{equation*}
T=\sum_{j, j^{\prime}} t_{j j^{\prime}}\left(q_{1}, q_{2}, \ldots, t\right) \dot{q}_{j} \dot{q}_{j^{\prime}}, \tag{2.44}
\end{equation*}
$$

with no other terms. It is evident that such $T$ satisfies the definition of a homogeneous function of the velocities with $\lambda=2,{ }^{14}$ so that the Euler theorem (43) gives

$$
\begin{equation*}
\sum_{j} \frac{\partial T}{\partial \dot{q}_{j}} \dot{q}_{j}=2 T . \tag{2.45}
\end{equation*}
$$

[^24]But since $U$ is independent of the generalized velocities, $\partial L / \partial \dot{q}_{j}=\partial T / \partial \dot{q}_{j}$, and the left-hand part of Eq. (45) is exactly the first term in the definition (32) of the Hamiltonian function, so that in this case

$$
\begin{equation*}
H=2 T-L=2 T-(T-U)=T+U=E . \tag{2.46}
\end{equation*}
$$

So, for the kinetic energy of the type (44), for example a free particle with the kinetic energy considered as a function of its Cartesian velocities,

$$
\begin{equation*}
T=\frac{m}{2}\left(v_{x}^{2}+v_{y}^{2}+v_{z}^{2}\right), \tag{2.47}
\end{equation*}
$$

the notions of the Hamiltonian function and mechanical energy are identical. (Indeed, some textbooks, very regretfully, do not distinguish these notions at all!) However, as we have seen from our bead-on-the-rotating-ring example, this is not always true. For that problem, the kinetic energy, in addition to the term proportional to $\dot{\theta}^{2}$, has another, velocity-independent term - see the first of Eqs. (23) - and hence is not a quadratic-homogeneous function of the angular velocity.

Thus, Eq. (36) expresses a new conservation law, generally different from that of the mechanical energy conservation.

### 2.4. Other conservation laws

Looking at the Lagrange equation (19), we immediately see that if $L \equiv T-U$ as a whole is independent of some generalized coordinate $q_{j}, \partial L / \partial q_{j}=0,{ }^{15}$ then the corresponding generalized momentum is an integral of motion: ${ }^{16}$

$$
\begin{equation*}
p_{j} \equiv \frac{\partial L}{\partial \dot{q}_{j}}=\text { const. } \tag{2.48}
\end{equation*}
$$

For example, for a 1D particle with Lagrangian (21), momentum $p_{x}$ is conserved if the potential energy is constant (the $x$-component of force is zero) - of course. As a less obvious example, let us consider a 2D motion of a particle in the field of central forces. If we use polar coordinates $r$ and $\varphi$ in the role of the generalized coordinates, the Lagrangian function, ${ }^{17}$

$$
\begin{equation*}
L \equiv T-U=\frac{m}{2}\left(\dot{r}^{2}+r^{2} \dot{\varphi}^{2}\right)-U(r) \tag{2.49}
\end{equation*}
$$

is independent of $\varphi$ and hence the corresponding generalized momentum,

$$
\begin{equation*}
p_{\varphi} \equiv \frac{\partial L}{\partial \dot{\varphi}}=m r^{2} \dot{\varphi} \tag{2.50}
\end{equation*}
$$

[^25]is conserved. This is just a particular (2D) case of the angular momentum conservation - see Eq. (1.24). Indeed, for the 2D motion within the $[x, y]$ plane, the angular momentum vector,
\[

\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}=\left|$$
\begin{array}{ccc}
\mathbf{n}_{x} & \mathbf{n}_{y} & \mathbf{n}_{z}  \tag{2.51}\\
x & y & z \\
m \dot{x} & m \dot{y} & m \dot{z}
\end{array}
$$\right|,
\]

has only one nonvanishing component, perpendicular to the motion plane:

$$
\begin{equation*}
L_{z}=x(m \dot{y})-y(m \dot{x}) . \tag{2.52}
\end{equation*}
$$

Differentiating the well-known relations between the polar and Cartesian coordinates,

$$
\begin{equation*}
x=r \cos \varphi, \quad y=r \sin \varphi, \tag{2.53}
\end{equation*}
$$

over time, and plugging the result into Eq. (52), we see that $L_{z}=m r^{2} \dot{\varphi}=p_{\varphi}$.
Thus the Lagrangian formalism provides a powerful way of searching for non-evident integrals of motion. On the other hand, if such conserved quantity is evident or known a priori, it is helpful for the selection of the most appropriate generalized coordinates, giving the simplest Lagrange equations. For example, in the last problem, if we have known in advance that $p_{\varphi}$ had to be conserved, this could provide a motivation for using angle $\varphi$ as one of generalized coordinates.

### 2.5. Exercise problems

In each of Problems 2.1-2.10:
(i) introduce a set of convenient generalized coordinate(s) $q_{j}$ of the system,
(ii) write down Lagrangian $L$ as a function of $q_{j}, \dot{q}_{j}$, and (if appropriate) time,
(iii) write down the Lagrangian equation(s) of motion,
(iv) calculate the Hamiltonian function $H$; find out whether it is conserved,
(v) calculate energy $E$; is $E=H$ ?; is energy conserved?
(vi) any other evident integrals of motion?
2.1. Double pendulum - see Fig. on the right. Consider only the motion confined to a vertical plane containing the suspension point.

2.2. Stretchable pendulum (i.e. a mass hung on an elastic cord that exerts force $F$ $=-\kappa\left(l-l_{0}\right)$, where $\kappa$ and $l_{0}$ are positive constants), confined to a vertical plane:

2.3. Fixed-length pendulum hanging from a horizontal support whose motion law $x_{0}(t)$ is fixed. (No vertical plane constraint here.)

2.4. A pendulum of mass $m$ hung on another point mass $m$ ' that may slide, without friction, along a straight horizontal rail (see Fig. on the right). Its motion is confined to the vertical plane that contains the rail.
2.5. A bead of mass $m$, sliding without friction along a light string stretched by fixed force $T$, between two horizontally displaced points - see Fig. on the right. Here, in contrast to the similar Problem 1.10, string tension $T$ may be comparable with bead's weight mg , and
 the motion is not restricted to the vertical plane.
2.6. A bead of mass $m$, sliding without friction along a light string of fixed length $2 l$, which is hung between two points, horizontally displaced by distance $2 d<2 l-$ see Fig. on the right. As in the previous problem, the motion is not restricted to the vertical plane.

2.7. A block of mass $m$ that can slide, without friction, along the inclined plane surface of a heavy wedge with mass $m^{\prime}$. The wedge is free to move, also without friction, along a horizontal surface - see Fig. on the right. (Both motions are within the vertical plane containing the steepest slope line.)
2.8. The two-pendula system that was the subject of Problem $1.8-$ see Fig. on the right.

2.9. A system of two similar, inductively-coupled LC circuits - see Fig. on the right.

2.10.* A small Josephson junction, i.e. a system of two superconductors coupled by Cooper-pair tunneling through a thin insulating layer that separates them (see Fig. on the right).


Hints:
(i) At not very high frequencies (whose quantum $\hbar \omega$ is lower than the binding energy $2 \Delta$ of the Cooper pairs), the Josephson effect may be described by coupling energy

$$
U(\varphi)=-E_{\mathrm{J}} \cos \varphi+\text { const },
$$

where constant $E_{\mathrm{J}}$ describes the coupling strength, and variable $\varphi$ (called the Josephson phase difference) is related to voltage $V$ across the junction via the famous frequency-to-voltage relation

$$
\frac{d \varphi}{d t}=\frac{2 e}{\hbar} V,
$$

where $e \approx 1.6 \times 10^{-19} \mathrm{C}$ is the fundamental electric charge and $\hbar \approx 1.054 \times 10^{-34} \mathrm{~J} \cdot \mathrm{~s}$ is the Planck constant. ${ }^{18}$ (ii) The junction (as any system of two close conductors) has a substantial electric capacitance $C$.

[^26]

## Chapter 3. A Few Simple Problems

In this chapter, I will review the solutions of a few simple but very important problems of particle motion, that may be reduced to one dimension, including the famous "planetary" problem of two particles interacting via a spherically-symmetric potential. In the process, we will discuss several methods that will be useful for the analysis of more complex systems.

### 3.1. One-dimensional and 1D-reducuble systems

If a particle is confined to motion along a straight line (say, axis $x$ ), its position, of course, is completely defined by this coordinate. In this case, as we already know, particle's Lagrangian is given by Eq. (2.21):

$$
\begin{equation*}
L=T(\dot{x})-U(x, t), \quad T(\dot{x})=\frac{m}{2} \dot{x}^{2} \tag{3.1}
\end{equation*}
$$

so that the Lagrange equation of motion (2.22)

$$
\begin{equation*}
m \ddot{x}=-\frac{\partial U(x, t)}{\partial x} \tag{3.2}
\end{equation*}
$$

is just the $x$-component of the $2^{\text {nd }}$ Newton law.
It is convenient to discuss the dynamics of such really $1 D$ systems in the same breath with that of effectively $1 D$ systems whose position, due to holonomic constraints and/or conservation laws, is also fully determined by one generalized coordinate $q$, and whose Lagrangians may be presented in a form similar to Eq. (1):

$$
\begin{equation*}
L=T_{\mathrm{ef}}(\dot{q})-U_{\mathrm{ef}}(q, t), \quad T_{\mathrm{ef}}=\frac{m_{\mathrm{ef}}}{2} \dot{q}^{2} \tag{3.3}
\end{equation*}
$$

where $m_{\mathrm{ef}}$ is some constant which may be considered as the effective mass of the system, and the function $U_{\text {ef }}$ its effective potential energy. In this case the Lagrange equation (2.19) describing the system dynamics has a form similar to Eq. (2):

$$
\begin{equation*}
m_{\mathrm{ef}} \ddot{q}=-\frac{\partial U_{\mathrm{ef}}(q, t)}{\partial q} . \tag{3.4}
\end{equation*}
$$

As an example, let us return again to our testbed system shown in Fig. 1.5. We have already seen that for that system, having one degree of freedom, the genuine kinetic energy $T$, expressed by the first of Eqs. (2.23), is not a quadratically-homogeneous function of the generalized velocity. However, the system's Lagrangian (2.23) still may be presented in form (3),

$$
\begin{equation*}
L=\frac{m}{2} R^{2} \dot{\theta}^{2}+\frac{m}{2} R^{2} \omega^{2} \sin ^{2} \theta+m g R \cos \theta+\mathrm{const}=T_{\mathrm{ef}}-U_{\mathrm{ef}}, \tag{3.5}
\end{equation*}
$$

if we take

$$
\begin{equation*}
T_{\mathrm{ef}} \equiv \frac{m}{2} R^{2} \dot{\theta}^{2}, \quad U_{\mathrm{ef}} \equiv-\frac{m}{2} R^{2} \omega^{2} \sin ^{2} \theta-m g R \cos \theta+\text { const. } \tag{3.6}
\end{equation*}
$$

In this new partitioning of function $L$, which is legitimate because $U_{\text {ef }}$ depends only on the generalized coordinate $\theta$, but not on the corresponding generalized velocity, $T_{\text {ef }}$ includes only a part of the full kinetic energy $T$ of the bead, while $U_{\text {ef }}$ includes not only the real potential energy $U$ of the bead in the gravity field, but also an additional term related to ring rotation. (As we will see in Sec. 6.6, this term may be interpreted as the effective potential energy due to the inertial centrifugal "force".)

Returning to the general case of effectively 1D systems with Lagrangian (3), let us calculate their Hamiltonian function, using its definition (2.32):

$$
\begin{equation*}
H=\frac{\partial L}{\partial \dot{q}} \dot{q}-L=m_{\mathrm{ef}} \dot{q}^{2}-\left(T_{\mathrm{ef}}-U_{\mathrm{ef}}\right)=T_{\mathrm{ef}}+U_{\mathrm{ef}} \tag{3.7}
\end{equation*}
$$

So, $H$ is expressed via $T_{\text {ef }}$ and $U_{\text {ef }}$ exactly as the mechanical energy $E$ is expressed via genuine $T$ and $U$.

### 3.2. Equilibrium and stability

Autonomous systems are defined as the dynamic systems whose equations of motion do not depend on time. For 1D (and effectively 1D) systems obeying Eq. (4), this means that their function $U_{\text {ef }}$, and hence the Lagrangian function (5) should not depend on time explicitly. According to Eqs. (2.35), in such systems the Hamiltonian function (7), i.e. the sum $T_{\text {ef }}+U_{\text {ef }}$, is an integral of motion. However, be careful! This may not be true for system's mechanical energy $E$; for example, as we already know from Sec. 2.2, for our testbed problem, with the generalized coordinate $q=\theta$ (Fig. 2.1), $H \neq E$.

According to Eq. (4), an autonomous system, at appropriate initial conditions, may stay in equilibrium at one or several stationary (alternatively called fixed) points $q_{n}$, corresponding to either the minimum or a maximum of the effective potential energy (see Fig. 1):

$$
\begin{equation*}
\frac{d U_{\mathrm{ef}}}{d q}\left(q_{n}\right)=0 \tag{3.8}
\end{equation*}
$$



In order to explore the stability of such fixed points, let us analyze the dynamics of small deviations

$$
\begin{equation*}
\widetilde{q}(t) \equiv q(t)-q_{n} \tag{3.9}
\end{equation*}
$$

from the equilibrium. For that, let us expand function $U_{\text {ef }}(\mathrm{q})$ in the Taylor series at a fixed point,

$$
\begin{equation*}
U_{\mathrm{ef}}(q)=U_{\mathrm{ef}}\left(q_{n}\right)+\frac{d U_{\mathrm{ef}}}{d q}\left(q_{n}\right) \widetilde{q}+\frac{1}{2} \frac{d^{2} U_{\mathrm{ef}}}{d q^{2}}\left(q_{n}\right) \widetilde{q}^{2}+\ldots \tag{3.10}
\end{equation*}
$$

The first term in the right-hand part, $U_{\text {ef }}\left(q_{n}\right)$, is arbitrary and does not affect motion. The next term, linear in deviation $\widetilde{q}$, is equal zero - see the fixed point definition (8). Hence the fixed point stability is determined by the next term, quadratic in $\widetilde{q}$, more exactly by its coefficient,

$$
\begin{equation*}
\kappa_{\mathrm{ef}} \equiv \frac{d^{2} U_{\mathrm{ef}}}{d q^{2}}\left(q_{n}\right) \tag{3.11}
\end{equation*}
$$

which plays the role of the effective spring constant. Indeed, neglecting the higher terms of the Taylor expansion (10), ${ }^{1}$ we see that Eq. (4) takes the familiar form - cf. Eq. (1.1):

$$
\begin{equation*}
m_{\mathrm{ef}} \ddot{\tilde{q}}+\kappa_{\mathrm{ef}} \widetilde{q}=0 . \tag{3.12}
\end{equation*}
$$

I am confident that the reader of these notes knows everything about this equation, but since we will soon run into similar but more complex equations, let us review the formal procedure of its solution. From the mathematical standpoint, Eq. (12) is an ordinary, linear differential equation of the second order, with constant coefficients. The theory of such equations tells us that its general solution (for any initial conditions) may be presented as

$$
\begin{equation*}
\widetilde{q}(t)=c_{+} e^{\lambda_{+} t}+c_{-} e^{\lambda_{-} t} \tag{3.13}
\end{equation*}
$$

where constants $c_{ \pm}$are determined by initial conditions, while the so-called characteristic exponents $\lambda_{ \pm}$ are completely defined by the equation itself. In order to find the exponents, it is sufficient to plug just one partial solution, $\exp \{\lambda t\}$, into the equation. In our simple case (12), this yields the following characteristic equation:

$$
\begin{equation*}
m_{\mathrm{ef}} \lambda^{2}+\kappa_{\mathrm{ef}}=0 \tag{3.14}
\end{equation*}
$$

If the ratio $k_{\mathrm{ef}} / m_{\mathrm{ef}}$ is positive, ${ }^{2}$ i.e. the fixed point corresponds to the minimum of potential energy (e.g., points $q_{0}$ and $q_{2}$ in Fig. 1), the characteristic equation yields

$$
\begin{equation*}
\lambda_{ \pm}= \pm i \omega_{0}, \quad \omega_{0} \equiv\left(\frac{\kappa_{\mathrm{ef}}}{m_{\mathrm{ef}}}\right)^{1 / 2} \tag{3.15}
\end{equation*}
$$

(where $i$ is the imaginary unit, $i^{2}=-1$ ), so that Eq. (13) describes sinusoidal oscillations of the system,

$$
\begin{equation*}
\widetilde{q}(t)=c_{+} e^{+i \omega_{0} t}+c_{-} e^{-i \omega_{0} t}=c_{c} \cos \omega_{0} t+c_{s} \sin \omega_{0} t \tag{3.16}
\end{equation*}
$$

with eigenfrequency (or "own frequency") $\omega_{0}$, about the fixed point which is thereby stable. On the other hand, at the potential energy maximum ( $k_{\mathrm{ef}}<0$, e.g., at point $q_{1}$ in Fig. 1), we get

$$
\begin{equation*}
\lambda_{ \pm}= \pm \lambda, \quad \lambda \equiv\left(\frac{\left|\kappa_{\mathrm{ef}}\right|}{m_{\mathrm{ef}}}\right)^{1 / 2}, \quad \widetilde{q}(t)=c_{+} e^{+\lambda t}+c_{-} e^{-\lambda t} . \tag{3.17}
\end{equation*}
$$

Since the solution has an exponentially growing part, ${ }^{3}$ the fixed point is unstable.

[^27]Note that the quadratic expansion of function $U_{\text {ef }}(q)$, given by Eq. (10), is equivalent to a linear expansion of the effective force:

$$
\begin{equation*}
F_{\mathrm{ef}} \equiv-\left.\frac{d U_{\mathrm{ef}}}{d q}\right|_{q=q_{n}} \approx-\kappa_{\mathrm{ef}} \widetilde{q}, \tag{3.18}
\end{equation*}
$$

immediately resulting in the linear equation (12). Hence, in order to analyze the stability of a fixed point $q_{n}$, it is sufficient to linearize the equation of motion in small deviations from that point, and study possible solutions of the resulting linear equation.

As an example, let us return to our testbed problem (Fig. 2.1) whose function $U_{\text {ef }}$ we already know - see the second of Eqs. (6). With it, the equation of motion (4) becomes

$$
\begin{equation*}
m R^{2} \ddot{\theta}=-\frac{d U_{\mathrm{ef}}}{d \theta}=m R^{2}\left[\omega^{2} \cos \theta-\Omega^{2}\right] \sin \theta, \text { i.e. } \ddot{\theta}=\left[\omega^{2} \cos \theta-\Omega^{2}\right] \sin \theta \tag{3.19}
\end{equation*}
$$

where $\Omega \equiv(g / R)^{1 / 2}$ is the frequency of small oscillations of the system at $\omega=0$ - see Eq. (2.26). ${ }^{4}$ From requirement (8), we see that on any $2 \pi$-long segment of angle $\theta,{ }^{5}$ the system may have four fixed points:

$$
\begin{equation*}
\theta_{0}=0, \quad \theta_{1}=\pi, \quad \theta_{2,3}= \pm \cos ^{-1} \frac{\Omega^{2}}{\omega^{2}} \tag{3.20}
\end{equation*}
$$

The last two fixed points, corresponding to the bead rotating on either side of the ring, exist only if the angular velocity $\omega$ of ring rotation exceeds $\Omega$. (In the limit of very fast rotation, $\omega \gg \Omega$, Eq. (20) yields $\theta_{2,3} \rightarrow \pm \pi / 2$, i.e. the stationary positions approach the horizontal diameter of the ring - in accordance with physical intuition.)

In order to analyze the fixed point stability, similarly to Eq. (9), we plug $\theta=\theta_{n}+\widetilde{\theta}$ into Eq. (19) and Taylor-expand the trigonometric functions of $\theta$ up to the first term in $\widetilde{\theta}$ :

$$
\begin{equation*}
\ddot{\tilde{\theta}}=\left[\omega^{2}\left(\cos \theta_{n}-\sin \theta_{n} \widetilde{\theta}\right)-\Omega^{2}\right]\left(\sin \theta_{n}+\cos \theta_{n} \widetilde{\theta}\right) \tag{3.21}
\end{equation*}
$$

Generally, this equation may be linearized further by purging its right-hand part of the term proportional to $\widetilde{\theta}^{2}$; however in this simple case, Eq. (21) is already convenient for analysis. In particular, for the fixed point $\theta_{0}=0$ (corresponding to the bead position at the bottom of the ring), we have $\cos \theta_{0}=1$ and $\sin \theta_{0}=0$, so that Eq. (21) is reduced to a linear differential equation

$$
\begin{equation*}
\ddot{\tilde{\theta}}=\left(\omega^{2}-\Omega^{2}\right) \tilde{\theta} \tag{3.22}
\end{equation*}
$$

whose characteristic equation is similar to Eq. (14) and yields

$$
\begin{equation*}
\lambda^{2}=\omega^{2}-\Omega^{2}, \quad \text { for } \theta \approx \theta_{0} \tag{3.23a}
\end{equation*}
$$

[^28]This result shows that if $\omega<\Omega$, when both roots $\lambda$ are imaginary, this fixed point is stable. However, as the rotation speed $\omega$ is increased beyond $\Omega$, the roots become real, $\lambda_{ \pm}=\left(\omega^{2}-\Omega^{2}\right)^{1 / 2}$, with one of them positive, so that the fixed point becomes unstable beyond this threshold, i.e. as soon as fixed points $\theta_{2,3}$ exist. An absolutely similar calculations for other fixed points yield

$$
\begin{align*}
& \lambda^{2}=\Omega^{2}+\omega^{2}>0, \quad \text { for } \theta \approx \theta_{1}  \tag{3.23b}\\
& \lambda^{2}=\Omega^{2}-\omega^{2}, \quad \text { for } \theta \approx \theta_{2,3} \tag{3.23c}
\end{align*}
$$

These results show that fixed point $\theta_{1}$ (bead on the top of the ring) is always unstable - just as we could foresee, while the side fixed points $\theta_{2,3}$ are stable as soon as they exist (at $\omega>\Omega$ ).

Thus, our fixed-point analysis may be summarized in a simple way: an increase of the ring rotation speed $\omega$ beyond a certain threshold value, equal to $\Omega$ (2.26), causes the bead to move on one of the ring sides, oscillating about one of the fixed points $\theta_{2,3}$. Together with the rotation about the vertical axis, this motion yields quite a complex spatial trajectory as observed from a lab frame, so it is fascinating that we could analyze it qualitatively in such a simple way.

Later in this course we will repeatedly use the linearization of the equations of motion for the analysis of stability of more complex systems, including those with energy dissipation.

### 3.3. Hamiltonian 1D systems

The autonomous systems that are described by time-independent Lagrangians, are frequently called Hamiltonian, because their Hamiltonian function $H$ (again, not necessarily equal to the genuine mechanical energy $E!$ ) is conserved. In our current 1D case, described by Eq. (3),

$$
\begin{equation*}
H=\frac{m_{\mathrm{ef}}}{2} \dot{q}^{2}+U_{\mathrm{ef}}(q)=\text { const } \tag{3.24}
\end{equation*}
$$

This is the first integral of motion. Solving Eq. (24) for $\dot{q}$, we get the first-order differential equation,

$$
\begin{equation*}
\frac{d q}{d t}= \pm\left\{\frac{2}{m_{\mathrm{ef}}}\left[H-U_{\mathrm{ef}}(q)\right]\right\}^{1 / 2}, \tag{3.25}
\end{equation*}
$$

which may be readily integrated:

$$
\begin{equation*}
\pm\left(\frac{m_{\mathrm{ef}}}{2}\right)^{1 / 2} \int_{q\left(t_{0}\right)}^{q(t)} \frac{d q^{\prime}}{\left[H-U_{\mathrm{ef}}\left(q^{\prime}\right)\right]^{1 / 2}}=t-t_{0} \tag{3.26}
\end{equation*}
$$

Since constant $H$ (as well as the proper sign before the integral - see below) is fixed by initial conditions, Eq. (26) gives the reciprocal form, $t=t(q)$, of the desired law of system motion, $q(t)$. Of course, for any particular problem the integral in Eq. (26) still has to be worked out, either analytically or numerically, but even the latter procedure is typically much easier than the numerical integration of the initial, second-order differential equation of motion, because at addition of many values (to which the numerical integration is reduced ${ }^{6}$ ) the rounding errors are effectively averaged out.

[^29]Moreover, Eqs. (24)-(25) also allow a general classification of 1D system motion. Indeed:
(i) If $H>U_{\text {ef }}(q)$ in the whole range of interest, the effective kinetic energy $T_{\text {ef }}$ (3) is always positive. Hence derivative $d q / d t$ cannot change sign, so that the effective velocity retains the sign it had initially. This is the unbound motion in one direction (Fig. 2a).
(ii) Now let the particle approach a classical turning point $A$ where $H=U_{\text {ef }}(x)$ - see Fig. 2b. ${ }^{7}$ According to Eqs. (25), (26), at that point the particle velocity vanishes, while its acceleration, according to Eq. (4), is still finite. Evidently, this corresponds to the particle reflection from the "potential wall", with the change of velocity sign.
(iii) If, after the reflection from point $A$, the particle runs into another classical turning point $B$ (Fig. 2c), the reflection process is repeated again and again, so that the particle is bound to a periodic motion between two turning points.

(c)

Fig. 3.2. Graphical representation of Eq. (25) for three different cases: (a) unbound motion, with the velocity sign conserved, (b) reflection from the "classical turning point", accompanied with the velocity sign change, and (c) bound, periodic motion between two turning points - schematically. (d) Effective potential energy (6) of the bead on the rotating ring (Fig. 1.5) for $\omega>\Omega$, in units of $2 m g R$.

The last case of periodic oscillations presents large practical interest, and the whole next chapter will be devoted to a detailed analysis of this phenomenon and numerous associated effects. Here I will only note that Eq. (26) immediately enables us to calculate the oscillation period:

$$
\begin{equation*}
\tau=2\left(\frac{m_{\mathrm{ef}}}{2}\right)^{1 / 2} \int_{B}^{A} \frac{d q}{\left[H-U_{\mathrm{ef}}(q)\right]^{1 / 2}} \tag{3.27}
\end{equation*}
$$

[^30]where the additional upfront factor 2 accounts for two time intervals: for the motion from $B$ to A and back (Fig. 2c). Indeed, according to Eq. (25), in each classically allowed point $q$ the velocity magnitude is the same, so that these time intervals are equal to each other. ${ }^{8}$

Now let us link Eq. (27) to the fixed point analysis carried out in the previous section. As Fig. 2c shows, if $H$ is reduced to approach $U_{\min }$, the oscillations described by Eq. (27) take place at the very bottom of "potential well", about a stable fixed point $q_{0}$. Hence, if the potential energy profile is smooth enough, we may limit the Taylor expansion (10) by the quadratic term. Plugging it into Eq. (27), and using the mirror symmetry of this particular problem about the fixed point $q_{0}$, we get

$$
\begin{equation*}
\tau=4\left(\frac{m_{\mathrm{ef}}}{2}\right)^{1 / 2} \int_{0}^{A} \frac{d \widetilde{q}}{\left[H-\left(U_{\min }+\kappa_{\mathrm{ef}} \widetilde{q}^{2} / 2\right)\right]^{1 / 2}}=\frac{4}{\omega_{0}} I, \quad \text { with } I \equiv \int_{0}^{1} \frac{d \xi}{\left(1-\xi^{2}\right)^{1 / 2}}, \tag{3.28}
\end{equation*}
$$

where $\xi \equiv \widetilde{q} / A$, with $A \equiv\left(2 / \kappa_{\mathrm{ef}}\right)^{1 / 2}\left[H-U_{\mathrm{min}}\right]^{1 / 2}$ being the classical turning point, i.e. the oscillation amplitude, and $\omega_{0}$ is the eigenfrequency given by Eq. (15). Taking into account that the elementary integral $I$ in that equation equals $\pi / 2,{ }^{9}$ we finally get

$$
\begin{equation*}
\tau=\frac{2 \pi}{\omega_{0}} \tag{3.29}
\end{equation*}
$$

as it should be for harmonic oscillations (16). Note that the oscillation period does not depend on the oscillation amplitude $A$, i.e. on the difference $\left(H-U_{\min }\right)$ - while it is small.

### 3.4. Planetary problems

Leaving a more detailed study of oscillations for the next chapter, let us now discuss the socalled planetary systems ${ }^{10}$ whose description, somewhat surprisingly, may be also reduced to an effectively 1D problem. Consider two particles that interact via a conservative, central force $\mathbf{F}_{21}=-\mathbf{F}_{12}$ $=\mathbf{n}_{r} F(r)$, where $r$ and $\mathbf{n}_{r}$ are, respectively, the magnitude and direction of the distance vector $\mathbf{r} \equiv \mathbf{r}_{1}-\mathbf{r}_{2}$ connecting the two particles (Fig. 3).


Fig. 3.3. Vectors in the "planetary" problem.
${ }^{8}$ Note that the dependence of points $A$ and $B$ on the "energy" $H$ is not necessarily continuous. For example, for our testbed problem, whose effective potential energy is plotted in Fig. 2d (for a particular value of $\omega>\Omega$ ), a gradual increase of $H$ leads to a sudden jump, at $H=H_{1}$, of point $B$ to position $B^{\prime}$, corresponding to a sudden switch from oscillations about one fixed point $\theta_{2,3}$ to oscillations about two adjacent fixed points (before the beginning of a persistent rotation along the ring at $H>H_{2}$ ).
${ }^{9}$ Introducing a new variable $\zeta$ by relation $\xi \equiv \sin \zeta$, we get $d \xi=\cos \zeta d \zeta=\left(1-\xi^{2}\right)^{1 / 2} d \zeta$, so that the function under the integral is just $d \zeta$.
${ }^{10}$ This name is very conditional, because this group of problems includes, for example, charged particle scattering (see Sec. 3.7 below).

Generally, two particles moving without constrains in 3D space, have $3+3=6$ degrees of freedom that may be described, e.g., by their Cartesian coordinates $\left\{x_{1}, y_{1}, z_{1}, x_{2}, y_{2}, z_{2}\right\}$ However, for this particular form of interaction, the following series of tricks allows the number of essential degrees of freedom to be reduced to just one.

First, the central, conservative force of particle interaction may be described by timeindependent potential energy $U(r)$. Hence the Lagrangian of the system is

$$
\begin{equation*}
L \equiv T-U(r)=\frac{m_{1}}{2} \dot{\mathbf{r}}_{1}^{2}+\frac{m_{2}}{2} \dot{\mathbf{r}}_{2}^{2}-U(r) . \tag{3.30}
\end{equation*}
$$

Let us perform the transfer from the initial six scalar coordinates of the particles to six generalized coordinates: three Cartesian components of the distance vector

$$
\begin{equation*}
\mathbf{r} \equiv \mathbf{r}_{1}-\mathbf{r}_{2} \tag{3.31}
\end{equation*}
$$

and three components of vector

$$
\begin{equation*}
\mathbf{R} \equiv \frac{m_{1} \mathbf{r}_{1}+m_{2} \mathbf{r}_{2}}{M}, \quad M \equiv m_{1}+m_{2} \tag{3.32}
\end{equation*}
$$

which defines the position of the center of mass of the system. Solving the system of two linear equations (31) and (32) for the $\mathbf{r}_{1}$ and $\mathbf{r}_{2}$, we get

$$
\begin{equation*}
\mathbf{r}_{1}=\mathbf{R}+\frac{m_{2}}{M} \mathbf{r}, \quad \mathbf{r}_{2}=\mathbf{R}-\frac{m_{1}}{M} \mathbf{r} \tag{3.33}
\end{equation*}
$$

Plugging these relations into Eq. (30), we may reduce it to

$$
\begin{equation*}
L=\frac{M}{2} \dot{\mathbf{R}}^{2}+\frac{m}{2} \dot{\mathbf{r}}^{2}-U(r) \tag{3.34}
\end{equation*}
$$

where $m$ is the so-called reduced mass:

$$
\begin{equation*}
m \equiv \frac{m_{1} m_{2}}{M}, \quad \text { so that } \frac{1}{m} \equiv \frac{1}{m_{1}}+\frac{1}{m_{2}} \tag{3.35}
\end{equation*}
$$

Reduced mass

Note that according to Eq. (35), the reduced mass is lower than that of the lightest component of the two-body system. If one of $m_{1,2}$ is much less that is counterpart (like it is in most star-planet or planetsatellite systems), then with a good precision $m \cong \min \left[m_{1}, m_{2}\right]$.

Since the Lagrangian function (34) depends only on $\dot{\mathbf{R}}$ rather than $\mathbf{R}$ itself, according to our discussion in Sec. 2.4, the Cartesian components of $R$ are cyclic coordinates, and the corresponding generalized momenta are conserved:

$$
\begin{equation*}
P_{j} \equiv \frac{\partial L}{\partial \dot{R}_{j}}=M \dot{R}_{j}=\text { const }, \quad j=1,2,3 . \tag{3.36}
\end{equation*}
$$

Physically, this is just the conservation law for the full momentum $\mathbf{P} \equiv M \mathbf{R}$ of our system, due to absence of external forces. Actually, in the axiomatics used in Sec. 1.3 this law is postulated - see Eq. (1.10) - but now we may attribute momentum $\mathbf{P}$ to a certain geometric point, the center of mass $\mathbf{R}$. In particular, since according to Eq. (36) the center moves with constant velocity in the inertial reference
frame used to write Eq. (30), we may create a new inertial frame with the origin at point $\mathbf{R}$. In this new frame, $\mathbf{R} \equiv 0$, so that vector $\mathbf{r}$ (and hence scalar $r$ ) remain the same as in the old frame (because the frame transfer vector adds equally to $\mathbf{r}_{1}$ and $\mathbf{r}_{2}$, and cancels in $\mathbf{r}=\mathbf{r}_{1}-\mathbf{r}_{2}$ ), and the Lagrangian (34) is now reduced to

$$
\begin{equation*}
L=\frac{m}{2} \dot{\mathbf{r}}^{2}-U(r) . \tag{3.37}
\end{equation*}
$$

Thus our initial problem has been reduced to just three degrees of freedom - three scalar components of vector $\mathbf{r}$. Moreover, Eq. (37) shows that dynamics of vector $\mathbf{r}$ of our initial, two-particle system is identical to that of the radius-vector of a single particle with the effective mass $m$, moving in the central potential field $U(r)$.

## 3.5. $2^{\text {nd }}$ Kepler law

Two more degrees of freedom may be excluded from the planetary problem by noticing that according to Eq. (1.35), the angular momentum $\mathbf{L}=\mathbf{r} \times \mathbf{p}$ of our effective particle is also conserved, both in magnitude and direction. Since the direction of $\mathbf{L}$ is, by its definition, perpendicular to both of $\mathbf{r}$ and $\mathbf{v}$ $=\mathbf{p} / m$, this means that particle's motion is confined to a plane (whose orientation in space is determined by the initial directions of vectors $\mathbf{r}$ and $\mathbf{v}$ ). Hence we can completely describe particle's position by just two coordinates in that plane, for example by distance $r$ to the center, and the polar angle $\varphi$. In these coordinates, Eq. (37) takes the form identical to Eq. (2.49):

$$
\begin{equation*}
L=\frac{m}{2}\left(\dot{r}^{2}+r^{2} \dot{\varphi}^{2}\right)-U(r) . \tag{3.38}
\end{equation*}
$$

Moreover, the latter coordinate, polar angle $\varphi$, may be also eliminated by using the conservation of angular momentum's magnitude, in the form of Eq. (2.50): ${ }^{11}$

$$
\begin{equation*}
L_{z}=m r^{2} \dot{\varphi}=\text { const. } \tag{3.39}
\end{equation*}
$$

A direct corollary of this conservation is the so-called $2^{\text {nd }}$ Kepler law: ${ }^{12}$ the radius-vector $\mathbf{r}$ sweeps equal areas $A$ in equal times. Indeed, in the linear approximation in $d A \ll A$, the area differential $d A$ equals to the area of a narrow right triangle with the base being the arc differential $r d \varphi$, and the height equal to $r$-see Fig. 4. As a result, according to Eq. (39), the time derivative of the area,

$$
\begin{equation*}
\frac{d A}{d t}=\frac{r(r d \varphi) / 2}{d t}=\frac{1}{2} r^{2} \dot{\varphi}=\frac{L_{z}}{2 m}, \tag{3.40}
\end{equation*}
$$

remains constant. Integration of this equation over an arbitrary (not necessarily small!) time interval proves the $2^{\text {nd }}$ Kepler law.

[^31]

Fig. 3.4. Area differential in the polar coordinates.

Now note that since $\partial L / \partial t=0$, the Hamiltonian function $H$ is also conserved, and since, according to Eq. (38), the kinetic energy of the system is a quadratic-homogeneous function of the generalized velocities $\dot{r}$ and $\dot{\varphi}, H=E$, so that the system energy $E$,

$$
\begin{equation*}
E=\frac{m}{2} \dot{r}^{2}+\frac{m}{2} r^{2} \dot{\varphi}^{2}+U(r), \tag{3.41}
\end{equation*}
$$

is also a first integral of motion. ${ }^{13}$ But according to Eq. (39), the second term of Eq. (41) may be presented as

$$
\begin{equation*}
\frac{m}{2} r^{2} \dot{\varphi}^{2}=\frac{L_{z}^{2}}{2 m r^{2}} \tag{3.42}
\end{equation*}
$$

so that energy (41) may be expressed as that of a 1D particle moving along axis $r$,

$$
\begin{equation*}
E=\frac{m}{2} \dot{r}^{2}+U_{\mathrm{ef}}(r) \tag{3.43}
\end{equation*}
$$

in the following effective potential:

$$
\begin{equation*}
U_{\mathrm{ef}}(r) \equiv U(r)+\frac{L_{z}^{2}}{2 m r^{2}} \tag{3.44}
\end{equation*}
$$

Effective
potential energy

So the planetary motion problem has been reduced to the dynamics of an effectively 1 D system. ${ }^{14}$
Now we may proceed just like we did in Sec. 3, with due respect for the very specific effective potential (44) which, in particular, diverges at $r \rightarrow 0$ - possibly besides the very special case of an exactly radial motion, $L_{z}=0$. In particular, we may solve Eq. (43) for $d r / d t$ to get

$$
\begin{equation*}
d t=\left(\frac{m}{2}\right)^{1 / 2} \frac{d r}{\left[E-U_{\mathrm{ef}}(r)\right]^{1 / 2}} \tag{3.45}
\end{equation*}
$$

The integration of this relation allows us not only to get a direct relation between time $t$ and distance $r$, similar to Eq. (26),

[^32]\[

$$
\begin{equation*}
t= \pm\left(\frac{m}{2}\right)^{1 / 2} \int \frac{d r}{\left[E-U_{\mathrm{ef}}(r)\right]^{1 / 2}}= \pm\left(\frac{m}{2}\right)^{1 / 2} \int \frac{d r}{\left[E-U(r)-L_{z}^{2} / 2 m r^{2}\right]^{1 / 2}}, \tag{3.46}
\end{equation*}
$$

\]

but also do a similar calculation of angle $\varphi$. Indeed, integrating Eq. (39),

$$
\begin{equation*}
\varphi \equiv \int \dot{\varphi} d t=\frac{L_{z}}{m} \int \frac{d t}{r^{2}} . \tag{3.47}
\end{equation*}
$$

and plugging $d t$ from Eq. (45), we get an explicit expression for particle's trajectory $\varphi(r)$ :

$$
\begin{equation*}
\varphi= \pm \frac{L_{z}}{(2 m)^{1 / 2}} \int \frac{d r}{r^{2}\left[E-U_{\text {ef }}(r)\right]^{1 / 2}}= \pm \frac{L_{z}}{(2 m)^{1 / 2}} \int \frac{d r}{r^{2}\left[E-U(r)-L_{z}^{2} / 2 m r^{2}\right]^{1 / 2}} \tag{3.48}
\end{equation*}
$$

Note that according to Eq. (39), derivative $d \varphi / d t$ does not change sign at the reflection from any classical turning point $r \neq 0$, so that, in contrast to Eq. (46), the sign in the right-hand part of Eq. (48) is uniquely determined by the initial conditions and cannot change during the motion.

Let us use these results, valid for any interaction law $U(r)$, for the planetary motion's classification. The following cases should be distinguished. (Following a good tradition, in what follows I will select the arbitrary constant in the potential energy in the way to provide $U_{\text {ef }} \rightarrow 0$ at $r \rightarrow \infty$.)

If the particle interaction is attractive, and the divergence of the attractive potential at $r \rightarrow 0$ is faster than $1 / r^{2}$, then $U_{\text {ef }}(r) \rightarrow-\infty$ at $r \rightarrow 0$, so that at appropriate initial conditions $(E<0)$ the particle may drop on the center even if $L_{z} \neq 0$ - the event called the capture. On the other hand, with $U(r)$ either converging or diverging slower than $1 / r^{2}$ at $r \rightarrow 0$, the effective energy profile $U_{\text {eff }}(r)$ has the shape shown schematically in Fig. 5. This is true, in particular, for the very important case

Attractive Coulomb potential

$$
\begin{equation*}
U(r)=-\frac{\alpha}{r}, \quad \alpha>0 \tag{3.49}
\end{equation*}
$$

which describes, in particular, the Coulomb (electrostatic) interaction of two particles with electric charges of the opposite sign, and Newton's gravity law (1.16a). This particular case will be analyzed in the following section, but now let us return to the analysis of an arbitrary attractive potential $U(r)<0$ leading to the effective potential shown in Fig. 5, when the angular-momentum term dominates at small distances $r$.


Fig. 3.5. Effective potential profile of, and two types of motion in an attractive central field.

According to the analysis of Sec. 3, such potential profile, with a minimum at some distance $r_{0}$, may sustain two types of motion, depending on the energy $E$ (which is of course determined by the initial conditions):
(i) If $E>0$, there is only one classical turning point where $E=U_{\mathrm{ef}}$, so that distance $r$ either grows with time from the very beginning, or (if the initial value of $\dot{r}$ was negative) first decreases and then, after the reflection from the increasing potential $U_{\text {ef }}$, starts to grow indefinitely. The latter case, of course, describes scattering.
(ii) On the opposite, if the energy is within the range

$$
\begin{equation*}
U_{\text {ef }}\left(r_{0}\right) \leq E<0, \tag{3.50}
\end{equation*}
$$

the system moves periodically between two classical turning points $r_{\text {min }}$ and $r_{\text {max }}$. These oscillations of distance $r$ correspond to the bound orbital motion of our effective particle about the attracting center. ${ }^{15}$

Let us start with the discussion of the bound motion, with energy within the range (50). If energy has its minimal possible value,

$$
\begin{equation*}
E=U_{\mathrm{ef}}\left(r_{0}\right)=\min \left[U_{\mathrm{ef}}(r)\right], \tag{3.51}
\end{equation*}
$$

the distance cannot change, $r=r_{0}=$ const, so that the orbit is circular, with the radius $r_{0}$ satisfying the condition $d U_{\mathrm{ef}} / d r=0$. Let us see whether this result allows for an elementary explanation. Using Eq. (44) we see that the condition for $r_{0}$ may be written as

$$
\begin{equation*}
\frac{L_{z}^{2}}{m r_{0}^{3}}=\left.\frac{d U}{d r}\right|_{r=r_{0}} . \tag{3.52}
\end{equation*}
$$

Since in a circular motion, velocity $\mathbf{v}$ is perpendicular to the radius vector $\mathbf{r}, L_{z}$ is just $m r_{0} v$, the left-hand part of Eq. (52) equals $m v^{2} / r_{0}$, while its right-hand part is just the magnitude of the attractive force, so that this equation expresses the well-known $2^{\text {nd }}$ Newton law for the circular motion. Plugging this result into Eq. (47), we get a linear law of angle change, $\varphi=\omega t+$ const, with angular velocity

$$
\begin{equation*}
\omega=\frac{L_{z}}{m r_{0}^{2}}=\frac{v}{r_{0}}, \tag{3.53}
\end{equation*}
$$

and hence the rotation period $\tau_{\varphi} \equiv 2 \pi / \omega$ obeys the elementary relation

$$
\begin{equation*}
\tau_{\varphi}=\frac{2 \pi r_{0}}{v} \tag{3.54}
\end{equation*}
$$

Now, let the energy be above its minimum value. Using Eq. (46) just as in Sec. 3, we see that distance $r$ now oscillates with period

$$
\begin{equation*}
\tau_{r}=(2 m)^{1 / 2} \int_{r_{\min }}^{r_{\max }} \frac{d r}{\left[E-U(r)-L_{z}^{2} / 2 m r^{2}\right]^{1 / 2}} \tag{3.55}
\end{equation*}
$$

[^33]This period is, in general, different from $\tau_{\varphi}$. Indeed, the change of angle $\varphi$ between two sequential points of the nearest approach, that follows from Eq. (48),

$$
\begin{equation*}
|\Delta \varphi|=2 \frac{L_{z}}{(2 m)^{1 / 2}} \int_{\mathrm{r}_{\min }}^{r_{\max }} \frac{d r}{r^{2}\left[E-U(r)-L_{z}^{2} / 2 m r^{2}\right]^{1 / 2}}, \tag{3.56}
\end{equation*}
$$

is generally different from $2 \pi$. Hence, the general trajectory of the bound motion has a spiral shape see, e.g., an illustration in Fig. 6.


Fig. 3.6. Typical open orbit of a particle moving in a non-Coulomb central field.

## 3.6. $1^{\text {st }}$ and $3^{\text {rd }}$ Kepler laws

The situation is special, however, for a very important particular case, namely that of the Coulomb potential described by Eq. (49). Indeed, plugging this potential into Eq. (48), we get

$$
\begin{equation*}
\varphi= \pm \frac{L_{z}}{(2 m)^{1 / 2}} \int \frac{d r}{r^{2}\left(E+\alpha / r-L_{z}^{2} / 2 m r^{2}\right)^{1 / 2}} . \tag{3.57}
\end{equation*}
$$

This is a table integral, ${ }^{16}$ equal to

$$
\begin{equation*}
\varphi= \pm \cos ^{-1} \frac{L_{z}^{2} / m \alpha r-1}{\left(1+2 E L_{z}^{2} / m \alpha^{2}\right)^{1 / 2}}+\text { const } \tag{3.58}
\end{equation*}
$$

The reciprocal function, $r(\varphi)$, is $2 \pi$-periodic:

$$
\begin{equation*}
r=\frac{p}{1+e \cos (\varphi+\text { const })}, \tag{3.59}
\end{equation*}
$$

Elliptic orbit
nd its parameters
so that at $E<0$, the orbit a closed line, ${ }^{17}$ characterized with the following parameters:

$$
\begin{equation*}
p \equiv \frac{L_{z}^{2}}{m \alpha}, \quad e \equiv\left[1+\frac{2 E L_{z}^{2}}{m \alpha^{2}}\right]^{1 / 2} \tag{3.60}
\end{equation*}
$$

[^34]The physical meaning of these parameters is very simple. Indeed, according to the general Eq. (52), in the Coulomb potential, for which $d U / d r=\alpha / r^{2}$, we see that $p$ is just the circular orbit radius ${ }^{18}$ for given $L_{z}: r_{0}=L_{z}{ }^{2} / m \alpha \equiv p$, and

$$
\begin{equation*}
\min \left[U_{\mathrm{ef}}(r)\right] \equiv U_{\mathrm{ef}}\left(r_{0}\right)=-\frac{\alpha^{2} m}{2 L_{z}^{2}}, \tag{3.61}
\end{equation*}
$$

Using this equality, parameter $e$ (called eccentricity) may be presented just as

$$
\begin{equation*}
e=\left\{1-\frac{E}{\min \left[U_{\mathrm{ef}}(r)\right]}\right\}^{1 / 2} . \tag{3.62}
\end{equation*}
$$

Analytical geometry tells us that Eq. (59), with $e<1$, is one of canonical forms for presentation of an ellipse, with one of its two focuses located at the origin. This fact is known as the $1^{\text {st }}$ Kepler law. Figure 7 shows the relation between the main dimensions of the ellipse and parameters $p$ and $e .{ }^{19}$


Fig. 3.7. Ellipse, and its special points and dimensions.

In particular, the major axis $a$ and minor axis $b$ are simply related to $p$ and $e$ and hence, via Eqs. (60), to the motion integrals $E$ and $L_{z}$ :

$$
\begin{equation*}
a=\frac{p}{1-e^{2}}=\frac{\alpha}{2|E|}, \quad b=\frac{p}{\left(1-e^{2}\right)^{1 / 2}}=\frac{L_{z}}{(2 m|E|)^{1 / 2}} . \tag{3.63}
\end{equation*}
$$

As was mentioned above, at $E \rightarrow \min \left[U_{\text {ef }}(r)\right]$ the orbit is almost circular, with $r(\varphi) \cong r_{0}=p$. On the contrary, as $E$ is increased to approach zero (its maximum value for the closed orbit), then $e \rightarrow 1$, so that the aphelion point $r_{\max }=p /(1-e)$ tends to infinity, i.e. the orbit becomes extremely extended. If the energy is exactly zero, Eq. (59) (with $e=1$ ) is still valid for all values of $\varphi$ (except for one special point $\varphi=\pi$ where $r$ becomes infinite) and describes a parabolic (i.e. open) trajectory. At $E>0$, Eq. (59) is still valid within a certain sector of angles $\varphi$ (in that it yields positive results for $r$ ), and describes an open, hyperbolic trajectory - see the next section.

For $E<0$, the above relations also allow a ready calculation of the rotation period $\tau_{\equiv} \tau_{r}=\tau_{\varphi}$. (In the case of a closed trajectory, $\tau_{r}$ and $\bar{T}_{\varphi}$ have to coincide.) Indeed, it is well known that the ellipse area $A=\pi a b$. But according to the $2^{\text {nd }}$ Kepler law (40), $d A / d t=L_{z} / 2 m=$ const. Hence

[^35]\[

$$
\begin{equation*}
\tau=\frac{A}{d A / d t}=\frac{\pi a b}{L_{z} / 2 m} . \tag{3.64a}
\end{equation*}
$$

\]

Using Eqs. (60) and (63), this result may be presented in several other forms:

$$
\begin{equation*}
\tau=\frac{\pi p^{2}}{\left(1-e^{2}\right)^{3 / 2}\left(L_{z} / 2 m\right)}=\pi \alpha\left(\frac{m}{2|E|^{3}}\right)^{1 / 2}=2 \pi a^{3 / 2}\left(\frac{m}{\alpha}\right)^{1 / 2} \tag{3.64b}
\end{equation*}
$$

Since for the Newtonian gravity (1.16a), $\alpha=G m_{1} m_{2}=G m M$, at $m_{1} \ll m_{2}$ (i.e. $m \ll M$ ) this constant is proportional to $m$, and the last form of Eq. (64b) yields the $3^{\text {rd }}$ Kepler law: periods of motion of different planets in the same central field, say that of our Sun, scale as $T \propto a^{3 / 2}$. Note that in contrast to the $2^{\text {nd }}$ Kepler law (that is valid for any central field), the $1^{\text {st }}$ and $3^{\text {rd }}$ Kepler laws are potentialspecific.

### 3.7. Classical theory of elastic scattering

If $E>0$, the motion is unbound for any interaction potential. In this case, the two most important parameters of the particle trajectory are the scattering angle $\theta$ and impact parameter $b$ (Fig. 8), and the main task for theory is to find the relation between them in the given potential $U(r)$. For that, it is convenient to note that $b$ is related to two conserved quantities, particle's energy ${ }^{20} E$ and its angular momentum $L_{z}$, in a simple way: ${ }^{21}$

$$
\begin{equation*}
L_{z}=b(2 m E)^{1 / 2} \tag{3.65}
\end{equation*}
$$

Hence the angular contribution to the effective potential (44) may be presented as

$$
\begin{equation*}
\frac{L_{z}^{2}}{2 m r^{2}}=E \frac{b^{2}}{r^{2}} \tag{3.66}
\end{equation*}
$$

Second, according to Eq. (48), the trajectory sections from infinity to the nearest approach point ( $r=$ $r_{\text {min }}$ ), and from that point to infinity, have to be similar, and hence correspond to equal angle changes $\varphi_{0}$ - see Fig. 8.


Fig. 3.8. Main geometric parameters of the scattering problem.

[^36]Hence we may apply the general Eq. (48) to just one of the sections, say $\left[r_{\min }, \infty\right.$ ], to find the scattering angle:

$$
\begin{equation*}
\theta=\pi-2 \varphi_{0}=\pi-2 \frac{L_{z}}{(2 m)^{1 / 2}} \int_{r_{\min }}^{\infty} \frac{d r}{r^{2}\left[E-U(r)-L_{z}^{2} / 2 m r^{2}\right]^{1 / 2}}=\pi-2 \int_{r_{\min }}^{\infty} \frac{b d r}{r^{2}\left[1-U(r) / E-b^{2} / r^{2}\right]^{1 / 2}} \cdot( \tag{3.67}
\end{equation*}
$$

In particular, for the Coulomb potential (49), now with an arbitrary sign of $\alpha$, we can apply the same table integral as in the previous section to get ${ }^{22}$

$$
\begin{equation*}
\theta=\left|\pi-2 \cos ^{-1} \frac{\alpha / 2 E b}{\left[1+(\alpha / 2 E b)^{2}\right]^{1 / 2}}\right| \tag{3.68a}
\end{equation*}
$$

This result may be more conveniently rewritten as

$$
\begin{equation*}
\tan \frac{|\theta|}{2}=\frac{|\alpha|}{2 E b} \tag{3.68b}
\end{equation*}
$$

Very clearly, the scattering angle's magnitude increases with the potential strength $\alpha$, and decreases as either the particle energy or the impact parameter (or both) are increased.

The general equation (67) and the Coulomb-specific relations (68) present a formally complete solution of the scattering problem. However, in a typical experiment on elementary particle scattering the impact parameter $b$ of a single particle is random and unknown. In this case, our results may be used to obtain statistics of the scattering angle $\theta$, in particular the so-called differential cross-section ${ }^{23}$

$$
\begin{equation*}
\frac{d \sigma}{d \Omega} \equiv \frac{1}{n} \frac{d N}{d \Omega}, \tag{3.69}
\end{equation*}
$$

where $n$ is the average number of the incident particles per unit area, and $d N$ is the average number of particles scattered into a small solid angle range $d \Omega$. For a spherically-symmetric scattering center, which provides an axially-symmetric scattering pattern, $d \sigma / d \Omega$ may be calculated by counting the number of incident particles within a small range $d b$ of the impact parameter:

$$
\begin{equation*}
d N=n 2 \pi b d b \tag{3.70}
\end{equation*}
$$

and hence scattered into the corresponding small solid angle range $d \Omega=2 \pi \sin \theta d \theta$. Plugging these relations into Eq. (69), we get the following general geometric relation:

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\frac{b}{\sin \theta}\left|\frac{d b}{d \theta}\right| \tag{3.71}
\end{equation*}
$$

In particular, for the Coulomb potential (49), a straightforward differentiation of Eq. (68) yields the so-called Rutherford scattering formula

[^37]Rutherford scattering formula

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\left(\frac{\alpha}{4 E}\right)^{2} \frac{1}{\sin ^{4}(\theta / 2)} \tag{3.72}
\end{equation*}
$$

This result, which shows very strong scattering to small angles (so strong that the integral that expresses the full cross-section $\sigma$ is formally diverging at $\theta \rightarrow 0$ ), ${ }^{24}$ and weak backscattering (scattering to angles $\theta \approx \pi$ ) was historically extremely significant: in the early 1910s its good agreement with $\alpha$ particle scattering experiments carried out by E. Rutherford's group gave a strong justification for "planetary" models of atoms, with electrons moving about very small nuclei.

Note that elementary particle scattering is frequently accompanied with electromagnetic radiation and/or other processes leading to the loss of the initial mechanical energy of the system, leading to inelastic scattering, that may give significantly different results. (In particular, a capture of an incoming particle becomes possible even for a Coulomb attracting center.) Also, quantum-mechanical effects may be important at scattering, so that the above results should be used with caution.

### 3.8. Exercise problems

3.1. For the system considered in Problem 2.5 (a bead sliding along a string with fixed tension $T$, see Fig. on the right), analyze small oscillations of the bead near the equilibrium.

3.2. Calculate the functional dependence of period $\tau$ of oscillations of a 1D particle of mass $m$ in potential $U(q)=\alpha q^{2 n}$ (where $\alpha>0$, and $n$ is a positive integer) on energy $E$. Explore the limit $n \rightarrow \infty$.
3.3. Explain why the term $m r^{2} \dot{\varphi}^{2} / 2$, recast in accordance with Eq. (42), cannot be merged with $U(r)$ in Eq. (38), to form an effective 1D potential energy $U(r)-L_{z}{ }^{2} / 2 m r^{2}$, with the second term's sign opposite to that given by Eq. (44). We have done an apparently similar thing for our testbed, bead-on-rotating-ring problem in the very end of Sec. 1 - see Eq. (3.6); why cannot the same trick work for the planetary problem? Besides a formal explanation, discuss the physics behind this difference.
3.4. A dumbbell, consisting of two equal masses $m$ on a light rod of length $l$, can slide without friction along a vertical ring of radius $R$, rotated about its vertical diameter with constant angular velocity $\omega$ - see Fig. on the right. Derive the condition of stability of the lower horizontal position of the dumbbell.


[^38]3.5. ${ }^{25}$ Analyze the dynamics of the so-called spherical pendulum - a point mass hung, in a uniform gravity field $\mathbf{g}$, on a light cord of length $l$, with no motion's confinement to a vertical plane. In particular:
(i) find the integrals of motion and reduce the problem to a 1 D one,
(ii) calculate the time period of the possible circular motion around the vertical axis,
(iii) explore small deviations from the circular motion. (Are the pendulum orbits closed?)
3.6. The orbits of Mars and Earth around the Sun may be well approximated as circles, with a radii ratio of $3 / 2$. Use this fact, and the Earth year duration (which you should know :-), to calculate the time of travel to Mars spending least energy, neglecting the planets' size and the effects of their gravitational fields on the spacecraft.
3.7. Derive first-order and second-order differential equations for $u \equiv 1 / r$ as a function of $\varphi$, describing the trajectory of particle's motion in a central potential $U(r)$. Spell out the latter equation for the particular case of the Coulomb potential (3.49) and discuss the result.
3.8. For motion in the central potential
$$
U(r)=-\frac{\alpha}{r}+\frac{\beta}{r^{2}},
$$
(i) find the orbit $r(\varphi)$, for positive $\alpha$ and $\beta$, and all possible ranges of energy $E$;
(ii) prove that in the limit $\beta \rightarrow 0$, and for energy $E<0$, the orbit may be represented as a slowly rotating ellipse;
(iii) express the angular velocity of this slow orbit rotation via parameters $\alpha$ and $\beta$ of the potential, particle's mass $m$, its energy $E$, and the angular momentum $L_{z}$.
3.9. A particle is moving in the field of an attractive central force, with potential
$$
U(r)=-\frac{\alpha}{r^{n}}, \quad \text { where } \alpha n>0
$$

For what values of $n$ is a circular orbit stable?
3.10. Determine the condition for a particle of mass $m$, moving under the effect of a central attractive force

$$
\mathbf{F}=-\alpha \frac{\mathbf{r}}{r^{3}} \exp \left\{-\frac{r}{R}\right\}
$$

where $\alpha$ and $R$ are positive constants, to have a stable circular orbit.
3.11. A particle of mass $m$, with angular momentum $L_{z}$, moves in the field of an attractive central force with a distance-independent magnitude $F$. If particle's energy $E$ is slightly higher than the value $E_{\min }$ corresponding to the circular orbit of the particle, what is the time period of its radial oscillations? Compare the period with that of the circular orbit at $E=E_{\min }$.

[^39]3.12. For particle scattering in a repulsive Coulomb field, calculate the minimum approach distance $r_{\text {min }}$ and velocity $v_{\text {min }}$ at that point, and analyze their dependence on the impact parameter $b$ (see Fig. 3.8 of the lecture notes) and the initial velocity $v_{\infty}$ of the particle.
3.13. A particle is launched from afar, with impact parameter $b$, toward an attracting center with central potential
$$
U(r)=-\frac{\alpha}{r^{n}}, \quad \text { with } n>2, \alpha>0
$$
(i) Express the minimum distance between the particle and the center via $b$, if the initial kinetic energy $E$ of the particle is barely sufficient for escaping the capture by the attracting center.
(ii) Calculate capture's full cross-section; explore the limit $n \rightarrow 2$.
3.14. A meteorite with initial velocity $v_{\infty}$ approaches an atmosphere-free planet of mass $M$ and radius $R$.
(i) Find the condition on the impact parameter $b$ for the meteorite to hit planet's surface.
(ii) If the meteorite barely avoids the collision, what is its scattering angle?
3.15. Calculate the differential and full cross-sections of the classical, elastic scattering of small particles by a hard sphere of radius $R$.
3.16. The most famous ${ }^{26}$ confirmation of Einstein's general relativity theory has come from the observation, by A. Eddington and his associates, of light's deflection by the Sun, during the May 1919 solar eclipse. Considering light photons as classical particles propagating with the light speed $v_{0} \rightarrow c \approx$ $2.998 \times 10^{8} \mathrm{~m} / \mathrm{s}$, and the astronomic data for Sun's mass, $M_{S} \approx 1.99 \times 10^{30} \mathrm{~kg}$, and radius, $R_{S} \approx$ $0.6957 \times 10^{9} \mathrm{~m}$, calculate the nonrelativistic mechanics' prediction for the angular deflection of the light rays grazing the Sun's surface.

[^40]

## Chapter 4. Oscillations

In this course, oscillations in $1 D$ (and effectively 1D) systems are discussed in detail, because of their key importance for physics and engineering. We will start with the so-called "linear" oscillator whose differential equation of motion is linear and hence allows the full analytical solutions, and then proceed to "nonlinear" and parametric systems whose dynamics may be only explored by either approximate analytical or numerical methods.

### 4.1. Free and forced oscillations

In Sec. 3.2 we briefly discussed oscillations in a very important Hamiltonian system - a 1D harmonic oscillator described by a simple 1D Lagrangian ${ }^{1}$

$$
\begin{equation*}
L \equiv T(\dot{q})-U(q)=\frac{m}{2} \dot{q}^{2}-\frac{\kappa}{2} q^{2}, \tag{4.1}
\end{equation*}
$$

whose Lagrangian equation of motion,

$$
\begin{equation*}
m \ddot{q}+\kappa q=0, \quad \text { i.e. } \ddot{q}+\omega_{0}^{2} q=0, \quad \text { with } \omega_{0}^{2} \equiv \frac{\kappa}{m} \geq 0, \tag{4.2}
\end{equation*}
$$

is a linear homogeneous differential equation. Its general solution is presented by Eq. (3.16), but it is frequently useful to recast it into another, amplitude-phase form:

$$
\begin{equation*}
q(t)=u \cos \omega_{0} t+v \sin \omega_{0} t=A \cos \left(\omega_{0} t-\varphi\right) \tag{4.3a}
\end{equation*}
$$

where $A$ is the amplitude and $\varphi$ the phase of the oscillations, which are determined by the initial conditions. Mathematically, it is frequently easier to work with sinusoidal functions as complex exponents, by rewriting Eq. (3a) in one more form: ${ }^{2}$

$$
\begin{equation*}
q(t)=\operatorname{Re}\left[A e^{-i\left(\omega_{0} t-\varphi\right)}\right]=\operatorname{Re}\left[a e^{-i \omega_{0} t}\right] \tag{4.3b}
\end{equation*}
$$

where $a$ is the complex amplitude of the oscillations:

$$
\begin{equation*}
a \equiv A e^{i \varphi}, \quad|a|=A, \quad \operatorname{Re} a=A \cos \varphi=u, \quad \operatorname{Im} a=A \sin \varphi=v . \tag{4.4}
\end{equation*}
$$

Equations (3) represent the so-called free oscillations of the system, that are physically due to the initial energy of the system. At an account for dissipation, i.e. energy leakage out of the system, such oscillations decay with time. The simplest model of this effect is represented by an additional linear friction ("drag") force that is proportional to the generalized velocity and directed opposite to it:
${ }^{1}$ For the notation simplicity, in this chapter I will drop indices "ef" in the energy components $T$ and $U$, and parameters like $m, \kappa$, etc. However, the reader should still remember that $T$ and $U$ do not necessarily coincide with the real kinetic and potential energies (even if those energies may be uniquely identified) - see Sec. 3.1.
${ }^{2}$ Note that this is the so-called physics convention. Most engineering texts use the opposite sign in the imaginary exponent, $\exp \{-i \omega t\} \rightarrow \exp \{i \omega t\}$, with the corresponding sign implications for intermediate formulas, but (of course) similar final results for real variables.

$$
\begin{equation*}
F_{v}=-\eta \dot{q}, \tag{4.5}
\end{equation*}
$$

where constant $\eta$ is called the drag coefficient. ${ }^{3}$ The inclusion of this force modifies the equation of motion (2) to become

$$
\begin{equation*}
m \ddot{q}+\eta \dot{q}+\kappa q=0 \tag{4.6a}
\end{equation*}
$$

This equation is frequently presented in the form

$$
\begin{equation*}
\ddot{q}+2 \delta \ddot{q}+\omega_{0}^{2} q=0, \quad \text { with } \delta \equiv \frac{\eta}{2 m} \tag{4.6b}
\end{equation*}
$$

Free
oscillator
with
damping
where parameter $\delta$ is called the damping coefficient. Note that Eq. (6) is still a linear homogeneous second-order differential equation, and its general solution still has the form of the sum (3.13) of two exponents of the type $\exp \{\lambda t\}$, with arbitrary pre-exponential coefficients. Plugging such an exponent into Eq. (4), we get the following algebraic characteristic equation for $\lambda$ :

$$
\begin{equation*}
\lambda^{2}+2 \delta \lambda+\omega_{0}^{2}=0 \tag{4.7}
\end{equation*}
$$

Solving this quadratic equation, we get

$$
\begin{equation*}
\lambda_{ \pm}=-\delta \pm i \omega_{0}^{\prime}, \quad \text { where } \omega_{0}^{\prime} \equiv\left(\omega_{0}^{2}-\delta^{2}\right)^{1 / 2} \tag{4.8}
\end{equation*}
$$

so that for not very high damping $\left(\delta<\omega_{0}\right)^{4}$ we get the following generalization of Eq. (3):

$$
\begin{equation*}
q_{\text {free }}(t)=c_{+} e^{\lambda_{+} t}+c_{-} e^{\lambda_{-} t}=\left(u_{0} \cos \omega_{0}^{\prime} t+v_{0} \sin \omega_{0}{ }^{\prime} t\right) e^{-\delta t}=A_{0} e^{-\delta t} \cos \left(\omega_{0}{ }^{\prime} t-\varphi_{0}\right) . \tag{4.9}
\end{equation*}
$$

The result shows that, besides a certain correction to the free oscillation frequency (which is very small in the most interesting case of low damping, $\delta \ll \omega_{0}$ ), the energy dissipation leads to an exponential decay of oscillation amplitude with time constant $\tau=1 / \delta$ :

$$
\begin{equation*}
A=A_{0} e^{-t / \tau}, \quad \text { where } \tau \equiv \frac{1}{\delta}=\frac{2 m}{\eta} . \tag{4.10}
\end{equation*}
$$

A convenient, dimensionless measure of damping is the so-called quality factor $Q$ (or just $Q$ factor ) which is defined as $\omega_{0} / 2 \delta$, and may be rewritten in several other useful forms:

[^41]\[

$$
\begin{equation*}
Q \equiv \frac{\omega_{0}}{2 \delta}=\frac{m \omega_{0}}{\eta}=\frac{(m \kappa)^{1 / 2}}{\eta}=\pi \frac{\tau}{\tau}=\frac{\omega_{0} \tau}{2}, \tag{4.11}
\end{equation*}
$$

\]

where $T=2 \pi / \omega_{0}$ is the oscillation period in the absence of damping - see Eq. (3.29). Since the oscillation energy $E$ is proportional to their amplitude squared, i.e. decays as $\exp \{-2 t / \tau\}$, with time constant $\tau / 2$, the last form of Eq. (11) may be used to rewrite the $Q$-factor in one more form:

$$
\begin{equation*}
Q=\omega_{0} \frac{E}{(-\dot{E})} \equiv \omega_{0} \frac{E}{\mathcal{P}}, \tag{4.12}
\end{equation*}
$$

where $\mathcal{P}$ is the dissipation power. (Two other useful ways to measure $Q$ will be discussed in a minute.) The range of $Q$-factors of important oscillators is very broad, all the way from $Q \sim 10$ for a human leg (with relaxed muscles), to $Q \sim 10^{4}$ of the quartz crystals used in "electronic" clocks and watches, all the way up to $Q \sim 10^{12}$ for microwave cavities with superconducting walls.

In contrast to the decaying free oscillations, the forced oscillations, induced by an external force $F(t)$, may maintain their amplitude infinitely, even at nonvanishing damping. This process may be described by a still linear but now inhomogeneous differential equation

$$
\begin{equation*}
m \ddot{q}+\eta \dot{q}+\kappa q=F(t) \tag{4.13a}
\end{equation*}
$$

or, more conveniently, by the following generalization of Eq. (6b):

$$
\begin{equation*}
\ddot{q}+2 \delta \dot{q}+\omega_{0}^{2} q=f(t), \quad \text { where } f(t) \equiv F(t) / m \tag{4.13b}
\end{equation*}
$$

For a particle of mass $m$, confined to a straight line, Eq. (12a) is just an expression of the $2^{\text {nd }}$ Newton law (or rather one of its Cartesian component). More generally, according to Eq. (1.41), Eq. (13) is valid for any dissipative 1D system whose Gibbs potential energy (1.39) has the form $U_{\mathrm{G}}(q, t)=\kappa q^{2} / 2-F(t) q$.

The forced-oscillation solutions may be analyzed by two mathematically equivalent methods whose relative convenience depends on the character of function $f(t)$.
(i) Frequency domain. Let us present function $f(t)$ as a Fourier sum of sinusoidal harmonics: ${ }^{5}$

$$
\begin{equation*}
f(t)=\sum_{\omega} f_{\omega} e^{-i \omega t} \tag{4.14}
\end{equation*}
$$

Then, due to linearity of Eq. (13), its general solution may be presented as a sum of the decaying free oscillations (9) with frequency $\omega_{0}$ ', independent of function $F(t)$, and forced oscillations due to each of the Fourier components of the force: ${ }^{6}$

General solution of Eq. (13)

$$
\begin{equation*}
q(t)=q_{\text {free }}(t)+q_{\text {forced }}(t), \quad q_{\text {forced }}(t)=\sum_{\omega} a_{\omega} e^{-i \omega t} \tag{4.15}
\end{equation*}
$$

Plugging Eq. (15) into Eq. (13), and requiring the factors before each $e^{-i \omega t}$ in both parts to be equal, we get

[^42]\[

$$
\begin{equation*}
a_{\omega}=f_{\omega} \chi(\omega), \tag{4.16}
\end{equation*}
$$

\]

where complex function $\chi(\omega)$, in our particular case equal to

$$
\begin{equation*}
\chi(\omega)=\frac{1}{\left(\omega_{0}^{2}-\omega^{2}\right)-2 i \omega \delta} \tag{4.17}
\end{equation*}
$$

is called either the response function or (especially for non-mechanical oscillators) the generalized susceptibility. From here, the real amplitude of oscillations under the effect of a sinusoidal force that may be represented by just one Fourier harmonic of the sum (15), is

$$
\begin{equation*}
A_{\omega} \equiv\left|a_{\omega}\right|=\left|f_{\omega} \| \chi(\omega)\right|, \quad \text { with }|\chi(\omega)|=\frac{1}{\left[\left(\omega_{0}^{2}-\omega^{2}\right)^{2}+(2 \omega \delta)^{2}\right]^{1 / 2}} \tag{4.18}
\end{equation*}
$$

Forced oscillation's amplitude

This formula describes, in particular, an increase of the oscillation amplitude $A_{\omega}$ at $\omega \rightarrow \omega_{0}$ - see Fig. 1. At the exact resonance,

$$
\begin{equation*}
|\chi(\omega)|_{\omega=\omega_{0}}=\frac{1}{2 \omega_{0} \delta}, \tag{4.19}
\end{equation*}
$$

so that, according to Eq. (11), the ratio of the oscillator response magnitudes at $\omega=\omega_{0}$ and at $\omega=0$ $\left(|\chi(\omega)|_{\omega=0}=1 / \omega_{0}^{2}\right)$ is exactly equal to the $Q$-factor. Thus, the response increase is especially strong in the low damping limit ( $\delta \ll \omega_{0}$, i.e. $Q \gg 1$ ); moreover at $Q \rightarrow \infty$ and $\omega \rightarrow \omega_{0}$ the response diverges. (This fact is very useful for the approximate methods to be discussed later in this chapter.) This is of course the classical description of the famous phenomenon of resonance, so ubiquitous in physics.


Fig. 4.1. Resonance in a harmonic oscillator (13), for several values of the $Q$-factor.

Due to the increase of the resonance peak height, its width is inversely proportional to $Q$. Quantitatively, in the most interesting low-damping limit, $Q \gg 1$, the reciprocal $Q$-factor gives the normalized value of the so-called FWHM ("full-width at half-maximum") of the resonance curve:

$$
\begin{equation*}
\frac{\Delta \omega}{\omega_{0}}=\frac{1}{Q} \tag{4.20}
\end{equation*}
$$

Indeed, $\Delta \omega$ is defined as the difference ( $\omega_{+}-\omega_{\text {. }}$ ) between the two values of $\omega$ at that the square of oscillator response function, $|\chi(\omega)|^{2}$ (proportional to the oscillation energy), equals a half of its
resonance value (19). In the low damping limit, both these points are very close to $\omega_{0}$, so that in the first (linear) approximation in $\left(\omega-\omega_{0}\right) \ll \omega_{0}, \omega$ we can take $\left(\omega_{0}{ }^{2}-\omega^{2}\right) \equiv-\left(\omega+\omega_{0}\right)\left(\omega-\omega_{0}\right) \approx(-2 \omega \xi) \approx\left(-2 \omega_{0} \xi\right)$, where

$$
\begin{equation*}
\xi \equiv \omega-\omega_{0} \tag{4.21}
\end{equation*}
$$

is a convenient parameter called detuning. (We will repeatedly use it later in this chapter.) In this approximation, the second of Eqs. (18) is reduced to

$$
\begin{equation*}
|\chi(\omega)|^{2}=\frac{1}{4 \omega^{2}\left(\delta^{2}+\xi^{2}\right)} \tag{4.22}
\end{equation*}
$$

As a result, points $\omega_{ \pm}$correspond to $\xi^{2}=\delta^{2}$, i.e. $\omega_{ \pm}=\omega_{0} \pm \delta=\omega_{0}(1 \pm 1 / 2 Q)$, so that $\Delta \omega \equiv \omega_{+}-\omega_{-}=$ $\omega_{0} / Q$, thus proving Eq. (20).
(ii) Time domain. Returning to the general problem of linear oscillations, one may argue that Eqs. (9), (15)-(17) provide a full solution of the forced oscillation problem. This is formally correct, but this solution may be very inconvenient if the external force is far from sinusoidal function of time. In this case, we should first calculate the complex amplitudes $f_{\omega}$ participating in the Fourier sum (14). In the general case of non-periodic $f(t)$, this is actually the Fourier integral,

$$
\begin{equation*}
f(t)=\int_{-\infty}^{+\infty} f_{\omega} e^{-i \omega t} d t \tag{4.23}
\end{equation*}
$$

so that $f_{\omega}$ should be calculated using the reciprocal Fourier transform,

$$
\begin{equation*}
f_{\omega}=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} f\left(t^{\prime}\right) e^{i \omega t^{\prime}} d t^{\prime} \tag{4.24}
\end{equation*}
$$

Now we can use Eq. (16) for each Fourier component of the resulting forced oscillations, and rewrite the last of Eqs. (15) as

$$
\begin{align*}
q_{\text {forced }}(t) & =\int_{-\infty}^{+\infty} a_{\omega} e^{-i \omega t} d \omega=\int_{-\infty}^{+\infty} \chi(\omega) f_{\omega} e^{-i \omega t} d \omega=\int_{-\infty}^{+\infty} d \omega \chi(\omega) \frac{1}{2 \pi} \int_{-\infty}^{+\infty} d t^{\prime} f\left(t^{\prime}\right) e^{i \omega\left(t^{\prime}-t\right)} \\
& =\int_{-\infty}^{+\infty} d t^{\prime} f\left(t^{\prime}\right)\left[\frac{1}{2 \pi} \int_{-\infty}^{+\infty} d \omega \chi(\omega) e^{i \omega\left(t^{\prime}-t\right)}\right], \tag{4.25}
\end{align*}
$$

with the response function $\chi(\omega)$ given, in our case, by Eq. (17). Besides requiring two integrations, Eq. (25) is conceptually uncomforting: it seems to indicate that the oscillator's coordinate at time $t$ depends not only on the external force exerted at earlier times $t^{\prime}<t$, but also in future times. This would contradict one of the most fundamental principles of physics (and indeed, science as a whole), the causality: no effect may precede its cause.

Fortunately, a straightforward calculation (left for reader's exercise) shows that the response function (17) satisfies the following rule: ${ }^{7}$

[^43]\[

$$
\begin{equation*}
\int_{-\infty}^{+\infty} \chi(\omega) e^{-i \omega \tau} d \omega=0, \quad \text { for } \tau<0 \tag{4.26}
\end{equation*}
$$

\]

This fact allows the last form of Eq. (25) to be rewritten in either of the following equivalent forms:

$$
\begin{equation*}
q_{\text {forced }}(t)=\int_{-\infty}^{t} f\left(t^{\prime}\right) G\left(t-t^{\prime}\right) d t^{\prime}=\int_{0}^{\infty} f(t-\tau) G(\tau) d \tau \tag{4.27}
\end{equation*}
$$

Linear system's response

Temporal
Green's function
is called the (temporal) Green's function of the system. According to Eq. (26), $G(\tau)=0$ for all $\tau<0$.
While the second form of Eq. (27) is more convenient for calculations, its first form is more clear conceptually. Namely, it expresses the linear superposition principle in time domain, and may be interpreted as follows: the full effect of force $f(t)$ on an oscillator (actually, any linear system ${ }^{8}$ ) may be described as a sum of effects of short pulses of duration $d t^{\prime}$ and magnitude $f\left(t^{\prime}\right)$ :

$$
\begin{equation*}
q_{\text {forced }}(t)=\lim _{\Delta t^{\prime} \rightarrow 0} \sum_{t^{\prime}=-\infty}^{t} G\left(t-t^{\prime}\right) f\left(t^{\prime}\right) \Delta t^{\prime} . \tag{4.29}
\end{equation*}
$$

- see Fig. 2. The Green's function $G(\tau)$ thus describes the oscillator response to a unit pulse of force, measured at time $\tau=t-t^{\prime}$ after the pulse.


Fig. 4.2. Presentation of the force as a function of time as a sum of short pulses.

Mathematically, it is more convenient to go to the limit $d t t^{\prime} \rightarrow 0$ and describe the elementary, unit-area pulse by Dirac's $\delta$-function, ${ }^{9}$ thus returning to Eq. (27). This line of reasoning also gives a convenient way to calculate the Green's function. Indeed, for the particular case,

$$
\begin{equation*}
f(t)=\delta\left(t-t_{0}\right), \quad \text { with } t_{0}<t \tag{4.30}
\end{equation*}
$$

Eq. (27) yields $q(t)=G\left(t-t_{0}\right)$. In particular, if $t>0$, we may take $t_{0}=0$; then $q(t)=G(t)$. Hence the Green's function may be calculated as a solution of the differential equation of motion of the system, in our case, Eq. (13), with the $\delta$-functional right-hand part:

$$
\begin{equation*}
\frac{d^{2} G(\tau)}{d \tau^{2}}+2 \delta \frac{d G(\tau)}{d \tau}+\omega_{0}^{2} G(\tau)=\delta(\tau) \tag{4.31}
\end{equation*}
$$

[^44]and zero initial conditions:
\[

$$
\begin{equation*}
G(-0)=\frac{d G}{d \tau}(-0)=0 \tag{4.32}
\end{equation*}
$$

\]

where $t=-0$ means the instant immediately preceding $t=0$.
This calculation may be simplified even further. Let us integrate both sides of Eq. (31) over a infinitesimal interval including the origin, e.g. $[-d \tau / 2,+d \tau / 2]$, and then follow the limit $d \tau \rightarrow 0$. Since Green's function has to be continuous because of its physical sense as the (generalized) coordinate, all terms in the left hand part but the first one vanish, while the first term yields $d G /\left.d \tau\right|_{+0}-d G /\left.d \tau\right|_{-0}$. Due to the second of Eqs. (32), the last of these two terms equals zero, while the right-hand part yields 1. Thus, $G(\tau)$ may be calculated for $\tau>0$ (i.e. for all times when $G(\tau) \neq 0$ ) by solving the homogeneous version of system's equation of motion for $\tau>0$, with the following special initial conditions:

$$
\begin{equation*}
G(0)=0, \quad \frac{d G}{d \tau}(0)=1 \tag{4.33}
\end{equation*}
$$

This approach gives us a convenient way for calculation of Green's functions of linear systems. In particular for the oscillator with not very low damping ( $\delta>\omega_{0}$, i.e. $Q>1 / 2$ ), imposing boundary conditions (33) on the general free-oscillation solution (9), we immediately get ${ }^{10}$ function

$$
\begin{equation*}
G(\tau)=\frac{1}{\omega_{0}{ }^{\prime}} e^{-\delta \tau} \sin \omega_{0}{ }^{\prime} \tau \tag{4.34}
\end{equation*}
$$

Equations (27) and (34) provide a very convenient recipe for solving most forced oscillations problems. As a very simple example, let us calculate the transient process in an oscillator under the effect of a constant force being turned on at $t=0$ :

$$
f(t)=\left\{\begin{array}{cc}
0, & t<0  \tag{4.35}\\
f_{0}, & t>0
\end{array}\right.
$$

provided that at $t<0$ the oscillator was at rest, so that $q_{\text {free }}(t) \equiv 0$. Then the second form of Eq. (27) yields

$$
\begin{equation*}
q(t)=\int_{0}^{\infty} f(t-\tau) G(\tau) d \tau=f_{0} \int_{0}^{t} \frac{1}{\omega_{0}{ }^{\prime}} e^{-\delta \tau} \sin \omega_{0}{ }^{\prime} \tau d \tau \tag{4.36}
\end{equation*}
$$

The simplest way to work out such integrals is to present the sine function as the imaginary part of $\exp \left\{i \omega_{0}{ }^{\prime} t\right\}$, and merge the two exponents, getting

$$
\begin{equation*}
q(t)=f_{0} \frac{1}{\omega_{0}{ }^{\prime}} \operatorname{Im}\left[\frac{1}{\delta+i \omega_{0}{ }^{\prime}} e^{-\delta \tau-i \omega_{0}{ }^{\prime} \tau}\right]_{0}^{t}=\frac{F_{0}}{k}\left[1-e^{-\delta t}\left(\cos \omega_{0}{ }^{\prime} t+\frac{\delta}{\omega_{0}{ }^{\prime}} \sin \omega_{0}{ }^{\prime} t\right)\right] . \tag{4.37}
\end{equation*}
$$

This result, plotted in Fig. 3, is rather natural: it describes nothing more than the transient from the initial equilibrium position $q=0$ to the new equilibrium position $q_{0}=f_{0} / \omega_{0}{ }^{2}=F_{0} / \kappa$, accompanied by

[^45]decaying oscillations. For this particular simple function $f(t)$, the same result might be also obtained by introducing a new variable $\widetilde{q}(t) \equiv q(t)-q_{0}$ and solving the resulting homogeneous equation for $\widetilde{q}$ (with appropriate initial condition $\left.\widetilde{q}(0)=-q_{0}\right)$, but for more complicated functions $f(t)$ the Green's function approach is irreplaceable.


Fig. 4.3. Transient process in a linear oscillator, induced by a step-like force $f(t)$, for the particular case $\delta / \omega_{0}=0.1$ (i.e., $Q=5$ ).

Note that for any particular linear system, its Green's function should be calculated only once, and then may be repeatedly used in Eq. (27) to calculate the system response to various external forces either analytically or numerically. This property makes the Green's function approach very popular in many other fields of physics - with the corresponding generalization or re-definition of the function. ${ }^{11}$

### 4.2. Weakly nonlinear oscillations

In comparison with systems discussed in the last section, which are described by linear differential equations with constant coefficients and thus allow a complete and exact analytical solution, oscillations in nonlinear systems generally present a complex and, generally, analytically intractable problem. Let us start a discussion of such nonlinear oscillations ${ }^{12}$ from an important case that may be explored analytically. In many important 1D oscillators, higher terms in the potential expansion (3.10) cannot be neglected, but are small and may be accounted for approximately. If, in addition, damping is low (or negligible), the equation of motion may be presented as a slightly modified Eq. (13):

$$
\begin{equation*}
\ddot{q}+\omega^{2} q=f(t, q, \dot{q}, \ldots) \tag{4.38}
\end{equation*}
$$

Weakly nonlinear oscillator
where $\omega \approx \omega_{0}$ is the anticipated frequency of oscillations (whose choice is to a certain extent arbitrary see below), and the right-hand part $f$ is small (say, scales as some small dimensionless parameter $\varepsilon \ll$ $1)$, and may be considered as a perturbation.

Since at $\varepsilon=0$ this equation has the sinusoidal solution given by Eq. (3), one might naïvely think that at nonvanishing but small $\varepsilon$, the approximate solution to Eq. (38) should be sought in the form

$$
\begin{equation*}
q(t)=q^{(0)}+q^{(1)}+q^{(2)}+\ldots, \quad \text { where } q^{(n)} \propto \varepsilon^{n} \tag{4.39}
\end{equation*}
$$

with $q^{(0)}=A \cos \left(\omega_{0} t-\varphi\right) \propto \varepsilon^{0}$. This is a good example of an apparently impeccable mathematical reasoning that would lead to a very inefficient procedure. Indeed, let us apply it to the problem we

[^46]already know the exact solution for, namely the free oscillations in a linear but damped oscillator, for this occasion assuming the damping to be very low, $\delta / \omega_{0} \sim \varepsilon \ll 1$. The corresponding equation of motion, Eq. (6), may be presented in form (38) if we take $\omega=\omega_{0}$ and
\[

$$
\begin{equation*}
f=-2 \delta \dot{q}, \quad \delta \propto \varepsilon . \tag{4.40}
\end{equation*}
$$

\]

The naïve approach described above would allow us to find small corrections, of the order of $\delta$, to the free, non-decaying oscillations $A \cos \left(\omega_{0} t-\varphi\right.$ ). However, we already know from Eq. (9) that the main effect of damping is a gradual decrease of the free oscillation amplitude to zero, i.e. a very large change of the amplitude, though at low damping, $\delta \ll \omega_{0}$, this decay takes large time $t \sim \tau \gg 1 / \omega_{0}$. Hence, if we want our approximate method to be productive (i.e. to work at all time scales, in particular for forced oscillations with established, constant amplitude and phase), we need to account for the fact that the small right-hand part of Eq. (38) may eventually lead to essential changes of oscillation amplitude $A$ (and sometimes, as we will see below, also of oscillation phase $\varphi$ ) at large times, because of the slowly accumulating effects of the small perturbation. ${ }^{13}$

This goal may be achieved by the account of these slow changes already in the " 0 th approximation", i.e. the basic part of the solution in expansion (39):
$0^{\text {th }}$ order
RWA solution

$$
\begin{equation*}
q^{(0)}=A(t) \cos [\omega t-\varphi(t)], \quad \text { with } \dot{A}, \dot{\varphi} \rightarrow 0 \quad \text { at } \varepsilon \rightarrow 0 . \tag{4.41}
\end{equation*}
$$

The approximate methods based on Eqs. (39) and (41) have several varieties and several names, ${ }^{14}$ but their basic idea and the results in the most important approximation (41) are the same. Let me illustrate this approach on a particular, simple but representative example of a dissipative (but high- $Q$ ) pendulum driven by a weak sinusoidal external force with a nearly-resonant frequency:

$$
\begin{equation*}
\ddot{q}+2 \delta \dot{q}+\omega_{0}^{2} \sin q=f_{0} \cos \omega t \tag{4.42}
\end{equation*}
$$

with $\left|\omega-\omega_{0}\right|, \delta \ll \omega_{0}$, and the force amplitude $f_{0}$ so small that $|q| \ll 1$ at all times. From what we know about the forced oscillations from Sec. 1, it is natural to identify $\omega$ in the left-hand part of Eq. (38) with the force frequency. Expanding $\sin q$ into the Taylor series in small $q$, keeping only the first two terms of this expansion, and moving all the small terms to the right-hand part, we can bring Eq. (42) to the canonical form (38): ${ }^{15}$

$$
\begin{equation*}
\ddot{q}+\omega^{2} q=-2 \delta \dot{q}+2 \xi \omega q+\alpha q^{3}+f_{0} \cos \omega t \equiv f(t, q, \dot{q}) \tag{4.43}
\end{equation*}
$$

Here $\alpha=\omega_{0}{ }^{2} / 6$ in the case of the pendulum (though the calculations below will be valid for any $\alpha$ ), and the second term in the right-hand part was obtained using the approximation already employed in Sec. 1:

[^47]$\left(\omega^{2}-\omega_{0}^{2}\right) q \approx 2 \omega\left(\omega-\omega_{0}\right) q=2 \omega \xi q$, where $\xi \equiv \omega-\omega_{0}$ is the detuning parameter that was already used earlier - see Eq. (21).

Now, following the general recipe expressed by Eqs. (39) and (41), in the $1^{\text {st }}$ approximation in $f$ $\propto \varepsilon,{ }^{16}$ we may look for the solution to Eq. (43) in the form

$$
\begin{equation*}
q(t)=A \cos \Psi+q^{(1)}(t), \quad \text { where } \Psi \equiv \omega t-\varphi, \quad q^{(1)} \sim \varepsilon \tag{4.44}
\end{equation*}
$$

Let us plug this assumed solution into both parts of Eq. (43), leaving only the terms of the first order in $\varepsilon$. Thanks to our (smart :-) choice of $\omega$ in the left-hand part of that equation, the two zero-order terms in that part cancel each other. Moreover, since each term in the right-hand part of Eq. (43) is already of the order of $\varepsilon$, we may drop $q^{(1)} \propto \varepsilon$ from the substitution into that part at all, because this would give us only terms $O\left(\varepsilon^{2}\right)$ or higher. As a result, we get the following approximate equation:

$$
\begin{equation*}
\ddot{q}^{(1)}+\omega^{2} q^{(1)}=f^{(0)} \equiv-2 \delta \frac{d}{d t}(A \cos \Psi)+2 \xi \omega A \cos \Psi+\alpha(A \cos \Psi)^{3}+f_{0} \cos \omega t . \tag{4.45}
\end{equation*}
$$

According to Eq. (41), generally $A$ and $\varphi$ should be considered as (slow) functions of time. However, let us leave the analyses of transient process and system stability until the next section, and use Eq. (45) to find stationary oscillations in the system, that are established after the initial transient. For that limited task, we may take $A=$ const, $\varphi=$ const, so that $q^{(0)}$ presents sinusoidal oscillations of frequency $\omega$. Sorting the terms in the right-hand part according to their time dependence, ${ }^{17}$ we see that it has terms with frequencies $\omega$ and $3 \omega$.

$$
\begin{equation*}
f^{(0)}=\left(2 \xi \omega A+\frac{3}{4} \alpha A^{3}+f_{0} \cos \varphi\right) \cos \Psi+\left(2 \delta \omega A-f_{0} \sin \varphi\right) \sin \Psi+\frac{1}{4} \alpha A^{3} \cos 3 \Psi \tag{4.46}
\end{equation*}
$$

Now comes the main trick of the rotating-wave approximation: mathematically, Eq. (45) may be viewed as the equation of oscillations in a linear, dissipation-free harmonic oscillator of frequency $\omega$ (not $\omega_{0}!$ ) under the action of an external force represented by the right-hand part of the equation. In our particular case, it has three terms: two quadrature components at that very frequency $\omega$, and the third one at frequency $3 \omega$. As we know from our analysis of this problem in Sec. 1, if any of the first two components is nonvanishing, $q^{(1)}$ grows to infinity - see Eq. (19) with $\delta=0$. At the same time, by the very structure of the rotating-wave approximation, $q^{(1)}$ has to be finite - moreover, small! The only way out of this contradiction is to require that amplitudes of both quadrature components of $f^{(0)}$ with frequency $\omega$ are equal to zero:

$$
\begin{equation*}
2 \xi \omega A+\frac{3}{4} \alpha A^{3}+f_{0} \cos \varphi=0, \quad 2 \delta \omega A-f_{0} \sin \varphi=0 \tag{4.47}
\end{equation*}
$$

These two harmonic balance equations enable us to find both parameters of the forced oscillations: their amplitude $A$ and phase $\varphi$. In particular, the phase may be readily eliminated from this

[^48]system (most easily, by expressing $\sin \varphi$ and $\cos \varphi$ from the corresponding equations, and then requiring the sum $\sin ^{2} \varphi+\cos ^{2} \varphi$ to equal 1), and the solution for amplitude $A$ presented in the following implicit but convenient form:
\[

$$
\begin{equation*}
A^{2}=\frac{f_{0}^{2}}{4 \omega^{2}} \frac{1}{\xi^{2}(A)+\delta^{2}}, \quad \text { where } \quad \xi(A) \equiv \xi+\frac{3}{8} \frac{\alpha A^{2}}{\omega}=\omega-\left(\omega_{0}-\frac{3}{8} \frac{\alpha A^{2}}{\omega}\right) \tag{4.48}
\end{equation*}
$$

\]

This expression differs from Eq. (22) for the linear resonance in the low-damping limit only by the replacement of the detuning $\xi$ with its effective amplitude-dependent value $\xi(A)$ or, equivalently, of the eigenfrequency $\omega_{0}$ of the resonator with its effective, amplitude-dependent value

$$
\begin{equation*}
\omega_{0}(A)=\omega_{0}-\frac{3}{8} \frac{\alpha A^{2}}{\omega} . \tag{4.49}
\end{equation*}
$$

The physical meaning of $\omega_{0}(A)$ is simple: this is just the frequency of free oscillations of amplitude $A$ in a similar nonlinear system, but with zero damping. Indeed, for $\delta=0$ and $f_{0}=0$ we could repeat our calculations, assuming that $\omega$ is an amplitude-dependent eigenfrequency $\omega_{0}(A)$, to be found. Then the second of Eqs. (47) is trivially satisfied, while the second of them gives Eq. (49).

Expression (48) allows one to draw the curves of this nonlinear resonance just by bending the linear resonance plots (Fig. 1) according to the so-called skeleton curve expressed by Eq. (49). Figure 4 shows the result of this procedure. Note that at small amplitude, $\omega(A) \rightarrow \omega_{0}$, and we return to the usual, "linear" resonance (22).


Fig. 4.4. Nonlinear resonance in the Duffing oscillator, as described by the rotating-wave approximation result (48), for the particular case $\alpha=\omega_{0}^{2} / 6, \delta / \omega=0.01$ (i.e. $Q=50$ ), and seven values of parameter $f_{0} / \omega_{0}^{2}$, increased bv eaual stens from 0 to 0.035 .

To bring our solution to its logical completion, we should still find the first perturbation $q^{(1)}(t)$ from what is left of Eq. (45). Since the structure of this equation is similar to Eq. (13) with the force of frequency $3 \omega$ and zero damping, we may use Eqs. (16)-(17) to obtain

$$
\begin{equation*}
q^{(1)}(t)=-\frac{1}{32 \omega^{2}} \alpha A^{3} \cos 3(\omega t-\varphi) . \tag{4.50}
\end{equation*}
$$

Adding this perturbation (note the negative sign!) to the sinusoidal oscillation (41), we see that as the amplitude $A$ of oscillations in a system with $\alpha>0$ (e.g., a pendulum) grows, their waveform become a bit more "blunt" near the maximum deviations from the equilibrium.

Expression (50) also allows an estimate of the range of validity of the rotating-wave approximation: since it has been based on the assumption $\left|q^{(1)}\right| \ll\left|q^{(0)}\right| \leq A$, for this particular problem we have to require $\alpha A^{2} / 32 \omega^{2} \ll 1$. For a pendulum (with $\alpha=\omega_{0}^{2} / 6$ ), this condition becomes $A^{2} \ll 192$. Though numerical coefficients in such strong inequalities should be taken with a grain of salt, the large magnitude of this particular coefficient gives a good hint that the method should give very good results even for relatively large oscillations with $A \sim 1$. In Sec. 7 below, we will see that this is indeed the case.

From the mathematical viewpoint, the next step would be to calculate the next approximation

$$
\begin{equation*}
q(t)=A \cos \Psi+q^{(1)}(t)+q^{(2)}(t), \quad q^{(2)} \sim \varepsilon^{2}, \tag{4.51}
\end{equation*}
$$

and plug it into the Duffing equation (43), which (thanks to our special choice of $q^{(0)}$ and $q^{(1)}$ ) would retain only $\ddot{q}^{(2)}+\omega^{2} q^{(2)}$ in its left-hand part. Again, requiring that amplitudes of two quadrature components of frequency $\omega$ in the right-hand part to be zero, we may get the second-order corrections to $A$ and $\varphi$. Then we may use the remaining part of the equation to calculate $q^{(2)}$, and then go after the third-order terms, etc. However, for most purposes the sum $q^{(0)}+q^{(1)}$, and sometimes even just the crudest approximation $q^{(0)}$ alone, are completely sufficient. For example, according to Eq. (50), for a simple pendulum ( $\alpha=\omega_{0}{ }^{2} / 6$ ) swinging as much as between the opposite horizontal positions ( $A=\pi / 2$ ), the $1^{\text {st }}$ order correction $q^{(1)}$ is of the order of $0.5 \%$. (Soon beyond this value, completely new dynamic phenomena start - see Sec. 7 below, but these phenomena cannot be covered by the rotating-wave approximation, at least in our current form.) Due to this reason, higher approximations are rarely pursued either in physics or engineering.

### 4.3. RWA equations

A much more important issue is the stability of solutions described by Eq. (48). Indeed, Fig. 4 shows that within a certain range of parameters, these equations give three different values for the oscillation amplitude (and phase), and it is important to understand which of these solutions are stable. Since these solutions are not the fixed points in the sense discussed in the Sec. 3.2 (each point in Fig. 4 represents a nearly-sinusoidal oscillation), their stability analysis needs a more general approach that would be valid for oscillations with amplitude and phase slowly evolving in time. This approach will also enable the analysis of non-stationary (especially the initial transient) processes that are of key importance for some dynamic systems.

First of all, let us formalize the way the harmonic balance equations, such as Eqs. (47), are obtained for the general case (38) - rather than for the particular Eq. (43) considered in the last section. After plugging in the $0^{\text {th }}$ approximation (41) into the right-hand part of equation (38) we have to require the amplitudes of its both quadrature components of frequency $\omega$ to be zero. From the standard Fourier analysis we know that these requirements may be presented as

$$
\begin{equation*}
\overline{f^{(0)} \sin \Psi}=0, \quad \overline{f^{(0)} \cos \Psi}=0 \tag{4.52}
\end{equation*}
$$

where symbol $\ldots$ means time averaging - in our current case, over the period $2 \pi / \omega$ of the right-hand part of Eq. (52), with the arguments calculated in the $0^{\text {th }}$ approximation:

$$
\begin{equation*}
f^{(0)} \equiv f\left(t, q^{(0)}, \dot{q}^{(0)}, \ldots\right) \equiv f(t, A \cos \Psi,-A \omega \sin \Psi, \ldots), \quad \text { with } \Psi=\omega t-\varphi \tag{4.53}
\end{equation*}
$$

Now, for a transient process the contribution of $q^{(0)}$ to left-hand part of Eq. (38) is not zero any longer, because both amplitude and phase may be slow functions of time - see Eq. (41). Let us calculate this contribution. The exact result would be

$$
\begin{align*}
\ddot{q}^{(0)}+\omega^{2} q^{(0)} & \equiv\left(\frac{d^{2}}{d t^{2}}+\omega^{2}\right) A \cos (\omega t-\varphi)  \tag{4.54}\\
& =\left(\ddot{A}+2 \dot{\varphi} \omega A-\dot{\varphi}^{2} A\right) \cos (\omega t-\varphi)-2 \dot{A}(\omega-\dot{\varphi}) \sin (\omega t-\varphi)
\end{align*}
$$

However, in the first approximation in $\varepsilon$, we may neglect the second derivative of $A$, and also the squares and products of the first derivatives of $A$ and $\varphi$ (that are all of the second order in $\varepsilon$ ), so that Eq. (54) is reduced to

$$
\begin{equation*}
\ddot{q}^{(0)}+\omega^{2} q^{(0)} \approx 2 A \dot{\varphi} \omega \cos (\omega t-\varphi)-2 \dot{A} \omega \sin (\omega t-\varphi) \tag{4.55}
\end{equation*}
$$

In the right-hand part of Eq. (52), we can neglect the time derivatives of the amplitude and phase at all, because this part is already proportional to the small parameter. Hence, in the first order in $\varepsilon$, Eq. (38) becomes

$$
\begin{equation*}
\ddot{q}^{(1)}+\omega^{2} q^{(1)}=f_{\mathrm{ef}}^{(0)} \equiv f^{(0)}-(2 A \dot{\varphi} \omega \cos \Psi-2 \dot{A} \omega \sin \Psi) \tag{4.56}
\end{equation*}
$$

Now, applying Eqs. (52) to function $f_{\text {ef }}{ }^{(0)}$, and taking into account that the time averages of $\sin ^{2} \Psi$ and $\cos ^{2} \Psi$ are both equal to $1 / 2$, while the time average of the product $\sin \Psi \cos \Psi$ vanishes, we get a pair of so-called RWA equations (alternatively called "the reduced equations" or sometimes "the van der Pol equations") for the time evolution of the amplitude and phase:

$$
\begin{equation*}
\dot{A}=-\frac{1}{\omega} \overline{f^{(0)} \sin \Psi}, \quad \dot{\varphi}=\frac{1}{\omega A} \overline{f^{(0)} \cos \Psi} \tag{4.57a}
\end{equation*}
$$

Extending the definition (4) of the complex amplitude of oscillations to their slow evolution in time, $a(t)$ $\equiv A(t) \exp \{i \varphi(t)\}$, and differentiating this relation, we see that two equations (57a) may be also re-written in the form of either one equation for $a$ :

Alternative forms of RWA equations

$$
\begin{equation*}
\dot{a}=\frac{i}{\omega} \overline{f^{(0)} e^{i(\Psi+\varphi)}} \equiv \frac{i}{\omega} \overline{f^{(0)} e^{i \omega t}} \tag{4.57b}
\end{equation*}
$$

or two equations for the real and imaginary parts of $a(t)=u(t)+i v(t)$ :

$$
\begin{equation*}
\dot{u}=-\frac{1}{\omega} \overline{f^{(0)} \sin \omega t}, \quad \dot{v}=\frac{1}{\omega} \overline{f^{(0)} \cos \omega t} . \tag{4.57c}
\end{equation*}
$$

The first-order harmonic balance equations (52) are evidently just the particular case of the RWA equations (57) for stationary oscillations ( $\dot{A}=\dot{\varphi}=0$ ). ${ }^{18}$

Superficially, the system (57a) of two coupled, first-order differential equations may look more complex than the initial, second-order differential equation (38), but actually it is usually much simpler.

[^49]For example, let us spell them out for the easy case of free oscillations a linear oscillator with damping. For that, we may reuse the ready Eq. (46) with $\alpha=f_{0}=0$, turning Eqs. (4.57a) into

$$
\begin{align*}
& \dot{A}=-\frac{1}{\omega} \overline{f^{(0)} \sin \Psi}=-\frac{1}{\omega} \overline{(2 \xi \omega A \cos \Psi+2 \delta \omega A \sin \Psi) \sin \Psi}=-\delta A,  \tag{4.58a}\\
& \dot{\varphi}=\frac{1}{\omega A} \overline{f^{(0)} \cos \Psi}=\frac{1}{\omega A} \overline{(2 \xi \omega A \cos \Psi+2 \delta \omega A \sin \Psi) \cos \Psi}=\xi \tag{4.58b}
\end{align*}
$$

The solution of Eq. (58a) gives us the same "envelope" law $A(t)=A(0) e^{-\delta t}$ as the exact solution (10) of the initial differential equation, while the elementary integration of Eq. (58b) yields $\varphi(t)=\xi t+$ $\varphi(0)=\omega t-\omega_{0} t+\varphi(0)$. This means that our approximate solution,

$$
\begin{equation*}
q^{(0)}(t)=A(t) \cos [\omega t-\varphi(t)]=A(0) e^{-\delta t} \cos \left[\omega_{0} t-\varphi(0)\right] \tag{4.59}
\end{equation*}
$$

agrees with the exact Eq. (9), and misses only correction (8) to the oscillation frequency, that is of the second order in $\delta$, i.e. of the order of $\varepsilon^{2}$ - beyond the accuracy of our first approximation. It is remarkable how nicely do the RWA equations recover the proper frequency of free oscillations in this autonomous system - in which the very notion of $\omega$ is ambiguous.

The situation is different at forced oscillations. For example, for the (generally, nonlinear) Duffing oscillator described by Eq. (43) with $f_{0} \neq 0$, Eqs. (57a) yield the RWA equations,

$$
\begin{equation*}
\dot{A}=-\delta A+\frac{f_{0}}{2 \omega} \sin \varphi, \quad A \dot{\varphi}=\xi(A) A+\frac{f_{0}}{2 \omega} \cos \varphi \tag{4.60}
\end{equation*}
$$

which are valid for an arbitrary function $\xi(A)$, provided that the nonlinear detuning remains much smaller than the oscillation frequency. Here (after a transient), the amplitude and phase tend to the stationary states described by Eqs. (47). This means that $\varphi$ becomes a constant, so that $q^{(0)} \rightarrow A \cos (\omega t-$ const), i.e. the RWA equations again automatically recover the correct frequency of the solution, in this case equal to that of the external force.

Note that each stationary oscillation regime, with certain amplitude and phase, corresponds to a fixed point of the RWA equations, so that the stability of those fixed points determine that of the oscillations. In what follows, we will carry out such an analysis for several simple systems of key importance for physics and engineering.

### 4.4. Self-oscillations and phase locking

The rotating-wave approximation was pioneered by B. van der Pol in the late 1920s for analysis of one more type of oscillatory motion: self-oscillations. Several systems, e.g., electronic rf amplifiers with positive feedback, and optical media with quantum level population inversion, provide convenient means for the compensation, and even over-compensation of the intrinsic energy losses in oscillators. Phenomenologically, this effect may be described as the change of sign of the damping coefficient $\delta$ from positive to negative. Since for small oscillations the equation of motion is still linear, we may use Eq. (9) to describe its general solution. This equation shows that at $\delta<0$, even infinitesimal deviations from equilibrium (say, due to unavoidable fluctuations) lead to oscillations with exponentially growing amplitude. Of course, in any real system such growth cannot persist infinitely, and shall be limited by
this or that effect - e.g., in the above examples, respectively, by amplifier saturation or electron population exhaustion.

In many cases, the amplitude limitation may be described reasonably well by nonlinear damping:

$$
\begin{equation*}
2 \delta \dot{q} \rightarrow 2 \dot{q} \dot{q}+\beta \dot{q}^{3} \tag{4.61}
\end{equation*}
$$

with $\beta>0$. Let us analyze this phenomenon, applying the rotating-wave approximation to the corresponding homogeneous differential equation:

$$
\begin{equation*}
\ddot{q}+2 \delta \dot{q}+\beta \dot{q}^{3}+\omega_{0}^{2} q=0 \tag{4.62}
\end{equation*}
$$

Carrying out the dissipative and detuning terms to the right hand part as $f$, we can readily calculate the right-hand parts of the RWA equations (57a), getting ${ }^{19}$

$$
\begin{gather*}
\dot{A}=-\delta(A) A, \quad \text { where } \delta(A) \equiv \delta+\frac{3}{8} \beta \omega^{2} A^{2}  \tag{4.63a}\\
A \dot{\varphi}=\xi A \tag{4.63b}
\end{gather*}
$$

The second of these equations has exactly the same form as Eq. (58b) for the case of decaying oscillations and hence shows that the self-oscillations (if they happen, i.e. if $A \neq 0$ ) have frequency $\omega_{0}$ of the oscillator itself - see Eq. (59). Equation (63a) is more interesting. If the initial damping $\delta$ is positive, it has only the trivial fixed point, $A_{0}=0$ (that describes the oscillator at rest), but if $\delta$ is negative, there is also another fixed point,

$$
\begin{equation*}
A_{1}=\left(\frac{8|\delta|}{3 \beta \omega^{2}}\right)^{1 / 2} \tag{4.64}
\end{equation*}
$$

which describes steady self-oscillations with a non-zero amplitude.
Let us apply the general approach discussed in Sec. 3.2, the linearization of equations of motion, to this RWA equation. For the trivial fixed point $A_{0}=0$, the linearization of Eq. (63a) is reduced to discarding the nonlinear term in the definition of the amplitude-dependent damping $\delta(A)$. The resulting linear equation evidently shows that the system's equilibrium point, $A=A_{0}=0$, is stable at $\delta>0$ and unstable at $\delta<0$. (We have already discussed this self-excitation condition above.) The linearization of Eq. (63a) near the non-trivial fixed point $A_{1}$ requires a bit more math: in the first order in $\widetilde{A} \equiv A-A_{1} \rightarrow 0$, we get

$$
\begin{equation*}
\dot{\tilde{A}} \equiv \dot{A}=-\delta\left(A_{1}+\widetilde{A}\right)-\frac{3}{8} \beta \omega^{2}\left(A_{1}+\widetilde{A}\right)^{3} \approx-\delta \widetilde{A}-\frac{3}{8} \beta \omega^{2} 3 A_{1}^{2} \widetilde{A}=(-\delta+3 \delta) \widetilde{A}=2 \widetilde{\delta A} \tag{4.65}
\end{equation*}
$$

where Eq. (64) has been used to eliminate $A_{1}$. We see that fixed point $A_{1}$ (and hence the whole process) is stable as soon as it exists $(\delta<0)$ - similar to the situation in our "testbed problem" (Fig. 2.1).

Now let us consider another important problem: the effect of a external sinusoidal force on a self-excited oscillator. If the force is sufficiently small, its effects on the self-excitation condition and the oscillation amplitude are negligible. However, if frequency $\omega$ of such weak force is close to the

[^50]eigenfrequency $\omega_{0}$ of the oscillator, it may lead to a very important effect of phase-locking (also called "synchronization"). At this effect, oscillator's frequency deviates from $\omega_{0}$, and becomes exactly equal to the external force's frequency $\omega$, within a certain range
\[

$$
\begin{equation*}
-\Delta \leq \omega-\omega_{0}<+\Delta . \tag{4.66}
\end{equation*}
$$

\]

In order to prove this fact, and also to calculate the phase locking range width $2 \Delta$, we may repeat the calculation of the right-hand parts of the RWA equations (57a), adding term $f_{0} \cos \omega t$ to the righthand part of Eq. (62) - cf. Eqs. (42)-(43). This addition modifies Eqs. (63) as follows: ${ }^{20}$

$$
\begin{gather*}
\dot{A}=-\delta(A) A+\frac{f_{0}}{2 \omega} \sin \varphi,  \tag{4.67a}\\
A \dot{\varphi}=\xi A+\frac{f_{0}}{2 \omega} \cos \varphi . \tag{4.67b}
\end{gather*}
$$

If the system is self-excited, and the external force is weak, its effect on the oscillation amplitude is small, and in the first approximation in $f_{0}$ we can take $A$ to be constant and equal to the value $A_{1}$ given by Eq. (64). Plugging this approximation into Eq. (67b), we get a very simple equation ${ }^{21}$

$$
\begin{equation*}
\dot{\varphi}=\xi+\Delta \cos \varphi \tag{4.68}
\end{equation*}
$$

where in our current case

$$
\begin{equation*}
\Delta \equiv \frac{f_{0}}{2 \omega A_{1}} \tag{4.69}
\end{equation*}
$$

Within the range $-|\Delta|<\xi<+|\Delta|$, Eq. (68) has two fixed points on each $2 \pi$-segment of variable $\varphi$ :

$$
\begin{equation*}
\varphi_{ \pm}= \pm \cos ^{-1}\left(-\frac{\xi}{\Delta}\right)+2 \pi n . \tag{4.70}
\end{equation*}
$$

It is easy to linearize Eq. (68) near each point to analyze their stability in our usual way; however, let me this case to demonstrate another convenient way to do this in 1D systems, using the socalled phase plane - the plot of the right-hand part of Eq. (68) as a function of $\varphi$ - see Fig. 5.


Fig. 4.5. Phase plane of a phaselocked oscillator, for the particular case $\xi=\Delta / 2, f_{0}>0$.

[^51]Since the positive values of this function correspond to the growth of $\varphi$ in time, and vice versa, we may draw the arrows showing the direction of phase evolution. From this graphics, it is clear that one of these fixed points (for $f_{0}>0, \varphi_{+}$) is stable, while its counterpart is unstable. Hence the magnitude of $\Delta$ given by Eq. (69) is indeed the phase locking range (or rather it half) that we wanted to find. Note that the range is proportional to the amplitude of the phase locking signal - perhaps the most important feature of phase locking.

In order to complete our simple analysis, based on the assumption of fixed oscillation amplitude, we need to find the condition of validity of this assumption. For that, we may linearize Eq. (67a), for the stationary case, near value $A_{1}$, just as we have done in Eq. (65) for the transient process. The stationary result,

$$
\begin{equation*}
\widetilde{A} \equiv A-A_{1}=\frac{1}{2 \mid \delta} \frac{f_{0}}{2 \omega} \sin \varphi_{ \pm} \approx A_{1}\left|\frac{\Delta}{2 \delta}\right| \sin \varphi_{ \pm} \tag{4.71}
\end{equation*}
$$

shows that our assumption, $|\tilde{A}| \ll A_{1}$. and hence the final result (69), are valid if the phase locking range, $2 \Delta$, is much smaller than $4|\delta|$.

### 4.5. Parametric excitation

In both problems solved in the last section, the stability analysis was easy because it could be carried out for just one slow variable, either amplitude or phase. Generally, such analysis of the RWA equations involves both these variables. The classical example of such situation is provided by one important physical phenomenon - the parametric excitation of oscillations. An elementary example of such oscillations is given by a pendulum with an externally-changed parameter, for example length $l(t)$ see Fig. 6. Experiments (including those with playground swings :-) and numerical simulations show that if the length is changed (modulated) periodically, with frequency $2 \omega$ that is close to $2 \omega_{0}$ and a sufficiently large swing $\Delta l$, the equilibrium position of the pendulum becomes unstable, and it starts swinging with frequency $\omega$ equal exactly to the half of the length modulation frequency (and hence only approximately equal to the average eigenfrequency $\omega_{0}$ of the oscillator).


Fig. 4.6. Parametric excitation of pendulum oscillations.

For an elementary analysis of this effect we may consider the simplest case when the oscillations are small. At the lowest point $(\theta=0)$, where the pendulum moves with the highest velocity $v_{\max }$, string's tension $\tau$ is higher than $m g$ by the centripetal force: $\tau_{\max }=m g+m v_{\max }{ }^{2} / l$. On the contrary, at the maximum deviation of the pendulum from the equilibrium, the force is weakened by string's tilt: $\tau_{\min }$ $=m g \cos \theta_{\max }$. Using the energy conservation, $E=m v_{\max }^{2} / 2=m g l\left(1-\cos \theta_{\max }\right)$, we may express these values as $T_{\max }=m g+2 E / l$ and $T_{\min }=m g-E / l$. Now, if during each oscillation period the string is pulled
up sharply and slightly by $\Delta l(|\Delta l| \ll l)$ at each of its two passages through the lowest point, and is let to go down by the same amount at each of two points of the maximum deviation, the net work of the external force per period is positive:

$$
\begin{equation*}
W \approx 2\left(\tau_{\max }-\tau_{\min }\right) \Delta l \approx 6 \frac{\Delta l}{l} E, \tag{4.72}
\end{equation*}
$$

and hence results in an increase of the oscillator's energy. If the so-called modulation depth $\Delta l / 2 l$ is sufficient, this increase may be sufficient to overcompensate the energy drained out by damping. Quantitatively, Eq. (10) shows that low damping ( $\delta \ll \omega_{0}$ ) leads to the following energy decrease,

$$
\begin{equation*}
\Delta E \approx-4 \pi \frac{\delta}{\omega_{0}} E \tag{4.73}
\end{equation*}
$$

per oscillation period. Comparing Eqs. (72) and (73), we see that the net energy flow into the oscillations is positive, $W+\Delta E>0$, i.e. oscillation amplitude has to grow if ${ }^{22}$

$$
\begin{equation*}
\frac{\Delta l}{l}>\frac{2 \pi \delta}{3 \omega_{0}} \equiv \frac{\pi}{3 Q} . \tag{4.74}
\end{equation*}
$$

Since this result is independent on $E$, the growth of energy and amplitude is exponential (for sufficiently low $E$ ), so that Eq. (74) is the condition of parametric excitation - in this simple model.

However, this result does not account for the possible difference between the oscillation frequency $\omega$ and the eigenfrequency $\omega_{0}$, and also does not clarify whether the best phase shift between the parametric oscillations and parameter modulation, assumed in the above calculation, may be sustained automatically. In order to address these issues, we may apply the rotating-wave approximation to a simple but reasonable linear equation

$$
\begin{equation*}
\ddot{q}+2 \delta \dot{q}+\omega_{0}^{2}(1+\mu \cos 2 \omega t) q=0, \tag{4.75}
\end{equation*}
$$

describing the parametric excitation for a particular case of sinusoidal modulation of $\omega_{0}{ }^{2}(t)$. Rewriting this equation in the canonical form (38),

$$
\begin{equation*}
\ddot{q}+\omega^{2} q=f(t, q, \dot{q})=-2 \delta \dot{q}+2 \xi \omega q-\mu \omega_{0}^{2} q \cos 2 \omega t, \tag{4.76}
\end{equation*}
$$

and assuming that the dimensionless ratios $\delta / \omega$ and $\mid \xi / \omega$, and the modulation depth $\mu$ are all much less than 1, we may use general Eqs. (57a) to get the following RWA equations:

$$
\begin{align*}
& \dot{A}=-\delta A-\frac{\mu \omega}{4} A \sin 2 \varphi,  \tag{4.77}\\
& A \dot{\varphi}=A \xi-\frac{\mu \omega}{4} A \cos 2 \varphi .
\end{align*}
$$

These equations evidently have a fixed point $A_{0}=0$, but its stability analysis (though possible) is not absolutely straightforward, because phase $\varphi$ of oscillations is undetermined at that point. In order to

[^52]avoid this (technical rather than conceptual) difficulty, we may use, instead of the real amplitude and phase of oscillations, either their complex amplitude $a=A \exp \{i \varphi\}$, or its Cartesian components $u$ and $v$ - see Eqs. (4). Indeed, for our function $f$, Eq. (57b) gives
\[

$$
\begin{equation*}
\dot{a}=(-\delta+i \xi) a-i \frac{\mu \omega}{4} a^{*}, \tag{4.78}
\end{equation*}
$$

\]

while Eqs. (57c) yield

$$
\begin{align*}
\dot{u} & =-\delta u-\xi v-\frac{\mu \omega}{4} v  \tag{4.79}\\
\dot{v} & =-\delta v+\xi u-\frac{\mu \omega}{4} u
\end{align*}
$$

We see that in contrast to Eqs. (77), in Cartesian coordinates $\{u, v\}$ the trivial fixed point $a_{0}=0$ (i.e. $u_{0}=v_{0}=0$ ) is absolutely regular. Moreover, equations (78)-(79) are already linear, so they do not require any additional linearization. Thus we may use the same approach as was already used in Secs. 3.2 and 4.1, i.e. look for the solution of Eqs. (79) in the exponential form $\exp \{\lambda t\}$. However, now we are dealing with two variables, and should allow them to have, for each value of $\lambda$, a certain ratio $u / v$. For that, we should take the partial solution in the form

$$
\begin{equation*}
u=c_{u} e^{\lambda t}, \quad v=c_{v} e^{\lambda t} \tag{4.80}
\end{equation*}
$$

where constants $c_{u}$ and $c_{v}$ are frequently called the distribution coefficients. Plugging this solution into Eqs. (79), we get for them the following system of two linear algebraic equations:

$$
\begin{align*}
& (-\delta-\lambda) c_{u}+\left(-\xi-\frac{\mu \omega}{4}\right) c_{v}=0  \tag{4.81}\\
& \left(\xi-\frac{\mu \omega}{4}\right) c_{u}+(-\delta-\lambda) c_{v}=0
\end{align*}
$$

The characteristic equation of this system,

$$
\left|\begin{array}{cc}
-\delta-\lambda & -\xi-\frac{\mu \omega}{4}  \tag{4.82}\\
\xi-\frac{\mu \omega}{4} & -\delta-\lambda
\end{array}\right| \equiv \lambda^{2}+2 \delta \lambda+\delta^{2}+\xi^{2}-\left(\frac{\mu \omega}{4}\right)^{2}=0
$$

has two roots:

$$
\begin{equation*}
\lambda_{ \pm}=-\delta \pm\left[\left(\frac{\mu \omega}{4}\right)^{2}-\xi^{2}\right]^{1 / 2} \tag{4.83}
\end{equation*}
$$

Requiring the fixed point to be unstable, $\operatorname{Re} \lambda_{+}>0$, we get the parametric excitation condition

$$
\begin{equation*}
\frac{\mu \omega}{4}>\left(\delta^{2}+\xi^{2}\right)^{1 / 2} . \tag{4.84}
\end{equation*}
$$

Thus the parametric excitation may indeed happen without any artificial phase adjustment: the arising oscillations self-adjust their phase to pick up energy from the external source responsible for the parameter variation.

Our key result (84) may be compared with two other calculations. First, in the case of negligible damping ( $\delta=0$ ), Eq. (84) turns into condition $\mu \omega / 4>|\xi|$. This result may be compared with the welldeveloped theory of the so-called Mathieu equation whose canonical form is

$$
\begin{equation*}
\frac{d^{2} y}{d v^{2}}+(a-2 b \cos 2 v) y=0 . \tag{4.85}
\end{equation*}
$$

It is evident that with the substitutions $y \rightarrow q, v \rightarrow \omega t, a \rightarrow\left(\omega_{0} / \omega\right)^{2}, b \rightarrow-\mu / 2$, this equation is just a particular case of Eq. (75) for $\delta=0$. In terms of Eq. (85), the result of our approximate analysis may be re-written just as $b>|a-1|$, and is supposed to be valid for $b \ll 1$. This condition is shown in Fig. 7 together with the numerically calculated ${ }^{23}$ stability boundaries of the Mathieu equation.


Fig. 4.7. Stability boundaries of the Mathieu equation (85), as calculated: numerically (curves) and using the rotating-wave approximation (dashed straight lines). In the regions numbered by various $n$ the trivial solution $y=0$ of the equation is unstable, i.e. its general solution $y(v)$ includes an exponentially growing term.

One can see that the rotating-wave approximation works just fine within its applicability limit (and beyond :-), though it fails to predict some other important features of the Mathieu equation, such as the existence of higher, more narrow regions of parametric excitation (at $a \approx n^{2}$, i.e. $\omega_{0} \approx \omega / n$, for all integer $n$ ), and some spill-over of the stability region into the lower half-plane $a<0 .{ }^{24}$ The reason of these failures is the fact that, as can be seen in Fig. 7, these phenomena do not appear in the first approximation in the parameter modulation amplitude $\mu \propto q$, that is the RWA applicability realm.

In the opposite case of finite damping but exact tuning ( $\xi=0, \omega \approx \omega_{0}$ ), Eq. (84) gives

$$
\begin{equation*}
\mu>\frac{4 \delta}{\omega_{0}} \equiv \frac{2}{Q} . \tag{4.86}
\end{equation*}
$$

[^53]This condition may be compared with Eq. (74), taking $\Delta l / l=2 \mu$.. The comparison shows that though the structure of these conditions is similar, the numerical coefficients are different by a factor close to 2 . The first reason of this difference is that the instant parameter change at optimal moments of time is more efficient then the smooth, sinusoidal variation described by (75). Even more significantly, the change of pendulum's length modulates not only its eigenfrequency $\omega_{0}$, as Eq. (75) implies, but also its mechanical impedance $Z \equiv(g l)^{1 / 2}$ - the notion to be discussed in detail in the next chapter. (Due to the time restrictions, I have to leave the analysis of the general case of the simultaneous modulation of $\omega_{0}$ and $Z$ for reader's exercise.)

Before moving on, let me summarize the most important differences between the parametric and forced oscillations:
(i) Parametric oscillations completely disappear outside of their excitation range, while the forced oscillations have a non-zero amplitude for any frequency and amplitude of the external force see Eq. (18).
(ii) Parametric excitation may be described by a linear homogeneous equation - e.g., Eq. (75) which cannot predict any finite oscillation amplitude within the excitation range, even at finite damping. In order to describe stationary parametric oscillations, some nonlinear effect has to be taken into account. (Again, I am leaving analyses of such effects for reader's exercises.)

One more important feature of the parametric oscillations will be discussed in the end of the next section.

### 4.6. Fixed point classification

RWA equations (79) give us a good pretext for a brief discussion of fixed points of a dynamic system described by two time-independent, first-order differential equations. ${ }^{25}$ After their linearization near a fixed point, the equations for deviations can always be presented in the form similar to Eq. (79):

$$
\begin{align*}
& \dot{\tilde{q}}_{1}=M_{11} \widetilde{q}_{1}+M_{12} \widetilde{q}_{2},  \tag{4.87}\\
& \dot{\tilde{q}}_{2}=M_{21} \widetilde{q}_{1}+M_{22} \widetilde{q}_{2},
\end{align*}
$$

where $M_{j j}$ ' $($ with $j, j '=1,2)$ are some real scalars that may be understood as elements of a $2 \times 2$ matrix M . Looking for an exponential solution of the type (80),

$$
\begin{equation*}
\widetilde{q}_{1}=c_{1} e^{\lambda t}, \quad \widetilde{q}_{2}=c_{2} e^{\lambda t} \tag{4.88}
\end{equation*}
$$

we get a more general system of two linear equations for the distribution coefficients $c_{1,2}$ :

$$
\begin{align*}
& \left(M_{11}-\lambda\right) c_{1}+M_{12} c_{2}=0 \\
& M_{21} c_{1}+\left(M_{22}-\lambda\right) c_{2}=0 . \tag{4.89}
\end{align*}
$$

These equations are consistent if

[^54]\[

\left|$$
\begin{array}{cc}
M_{11}-\lambda & M_{12} \\
M_{21} & M_{22}-\lambda
\end{array}
$$\right|=0
\]

Characteristic equation of system (87)
giving us a quadratic characteristic equation

$$
\begin{equation*}
\lambda^{2}-\lambda\left(M_{11}+M_{22}\right)+\left(M_{11} M_{22}-M_{12} M_{21}\right)=0 \tag{4.91}
\end{equation*}
$$

Its solution, ${ }^{26}$

$$
\begin{equation*}
\lambda_{ \pm}=\frac{1}{2}\left(M_{11}+M_{22}\right) \pm \frac{1}{2}\left[\left(M_{11}-M_{22}\right)^{2}+4 M_{12} M_{21}\right]^{1 / 2} \tag{4.92}
\end{equation*}
$$

shows that the following situations are possible:
A. The expression under the square root, $\left(M_{11}-M_{22}\right)^{2}+4 M_{12} M_{21}$, is positive. In this case, both characteristic exponents $\lambda_{ \pm}$are real, and we can distinguish three sub-cases:
(i) Both $\lambda_{+}$and $\lambda_{\text {- }}$ are negative. In this case, the fixed point is evidently stable. Because of generally different magnitudes of exponents $\lambda_{ \pm}$, the process presented on the phase plane [ $\widetilde{q}_{1}, \widetilde{q}_{2}$ ] (Fig. 8a) may be seen as consisting of two stages: first, a faster (with rate $\left|\lambda_{-}\right|$) relaxation to a linear asymptote, ${ }^{27}$ and then a slower decline, with rate $\left|\lambda_{+}\right|$, along this line, i.e. at the virtually fixed ratio of the variables. Such fixed point is called the stable node.
(ii) Both $\lambda_{+}$and $\lambda_{\text {- }}$ are positive. This case (rarely met in actual physical systems) of the unstable node differs from the previous one only by the direction of motion along the phase plane trajectories (see dashed arrows in Fig. 8a). Here the variable ratio is also approaching a constant soon, but now the one corresponding to $\lambda_{+}>\lambda_{\text {. }}$
(iii) Finally, in the case of a saddle $\left(\lambda_{+}>0, \lambda_{-}<0\right)$ the system dynamics is different (Fig. $8 b)$ : after the rate- $\lambda_{-} \mid$relaxation to the $\lambda_{+}$-asymptote, the perturbation starts to grow, with the rate $\lambda_{+}$, along one of two opposite directions. (The direction is determined on which side of another straight line, called separatrix, the system has been initially.) It is evident that the saddle ${ }^{28}$ is an unstable fixed point.
B. The expression under the square root, $\left(M_{11}-M_{22}\right)^{2}+4 M_{12} M_{21}$, is negative. In this case the square root in Eq. (92) is imaginary, making the real parts of both roots equal, $\operatorname{Re} \lambda_{ \pm}=\left(M_{11}+M_{22}\right) / 2$, and their imaginary parts equal but sign-opposite. As a result, here there can be just two types of fixed points:
(i) Stable focus, at $\left(M_{11}+M_{22}\right)<0$. The phase plane trajectories are spirals going to the center (i.e. toward the fixed point) - see Fig. 8c with solid arrow.
(ii) Unstable focus, taking place at $\left(M_{11}+M_{22}\right)>0$, differs from the stable one only by the direction of motion along the phase trajectories - see the dashed arrow in Fig. 8c.

[^55]

Fig. 4.8. Typical trajectories on the phase plane $\left[\widetilde{q}_{1}, \widetilde{q}_{2}\right]$ near fixed points of various types: (a) node, (b) saddle, (c) focus, and (d) center. The particular values of the matrix M used in the first three panels correspond to the RWA equations (81) for parametric oscillators with $\xi=\delta$, and three different values of parameter $\mu \omega / 4 \delta$ : (a) 1.25 , (b) 1.6 and (c) 0.
C. Sometimes the border case, $M_{11}+M_{22}=0$, is also distinguished, and the corresponding fixed point is refereed to as the center (Fig. 8d). Considering centers a special category makes sense because such fixed points are typical for Hamiltonian systems whose first integral of motion may be frequently presented as the distance of the from a fixed point. For example, a harmonic oscillator without dissipation may be described by the system

$$
\begin{equation*}
\dot{q}=\frac{p}{m}, \quad \dot{p}=-m \omega_{0}^{2} q, \tag{4.94}
\end{equation*}
$$

that is evidently a particular case of Eq. (87) with $M_{11}=M_{22}=0, M_{12} M_{21}=-\omega_{0}{ }^{2}<0$, and hence ( $M_{11}$ $\left.M_{22}\right)^{2}+4 M_{12} M_{21}=-4 \omega_{0}^{2}<0$, and $M_{11}+M_{22}=0$. The phase plane of the system may be symmetrized by plotting $q$ vs. the properly normalized momentum $p / m \omega_{0}$. On the symmetrized plane, sinusoidal oscillations of amplitude $A$ are represented by a circle of radius $A$ about the center-type fixed point $A=$ 0 . Such a circular trajectory correspond to the conservation of the oscillator's energy

$$
\begin{equation*}
E=\frac{m \dot{q}^{2}}{2}+\frac{m \omega_{0}^{2} q^{2}}{2}=\frac{m \omega_{0}^{2}}{2}\left[\left(\frac{p}{m \omega_{0}}\right)^{2}+q^{2}\right] \tag{4.95}
\end{equation*}
$$

This is a convenient moment for a brief discussion of the so-called Poincaré (or "slow-variable", or "stroboscopic") plane. ${ }^{29}$ From the point of view of the rotating-wave approximation, sinusoidal oscillations $q(t)=A \cos (\omega t-\varphi)$, in particular those described by a circular trajectory on the real (or "fast") phase plane (Fig. 8c) correspond to a fixed point $\{A, \varphi\}$, which may conveniently presented by a steady geometrical point on a plane with these polar coordinates (Fig. 9a). (As follows from Eq. (4), the Cartesian coordinates on that plane are $u$ and $v$.) The quasi-sinusoidal process (41), with slowly changing $A$ and $\varphi$, may be represented by a slow motion of that point on this Poincaré plane.


Fig. 4.9. (a) Presentation of a sinusoidal oscillation (point) and a slow transient (line) on the Poincaré plane, and (b) transfer from the "fast" phase plane to the "slow" (Poincaré) plane.

Figure 9 b shows one possible way to visualize the relation between the "real" phase plane of an oscillator, with symmetrized Cartesian coordinates $q$ and $p / m \omega_{0}$, and the Poincaré plane with Cartesian coordinates $u$ and $v$ : the latter reference frame rotates relative to the former one about the origin clockwise, with angular velocity $\omega .{ }^{30}$ Another, "stroboscopic" way to generate the Poincaré plane pattern is to have a fast glance at the "real" phase plane just once during the oscillation period $T=2 \pi / \omega$.

In many cases, such presentation is more convenient than that on the "real" phase plane. In particular, we have already seen that the RWA equations for such important phenomena as phase locking and parametric oscillations, whose original differential equations include time explicitly, are time-independent - cf., e.g., (75) and (79) describing the latter effect. This simplification brings the

[^56]equations into the category considered in this section, and enables the classification of their fixed points, which may shed additional light on their dynamic properties.

In particular, Fig. 10 shows the classification of the trivial fixed point of a parametric oscillator, which follows from Eq. (83). As the parameter modulation depth $\mu$ is increased, the type of the trivial fixed point $A_{1}=0$ on the Poincaré plane changes from a stable focus (typical for a simple oscillator with damping) to a stable node and then to a saddle describing the parametric excitation. In the last case, the two directions of the perturbation growth, so prominently featured in Fig. 8b, correspond to the two possible values of the oscillation phase $\varphi$, with the phase choice determined by initial conditions.


Fig. 4.10. Types of the trivial fixed point of a parametric oscillator.

This double degeneracy of the parametric oscillation's phase could already be noticed from Eqs. (77), because they are evidently invariant with respect to replacement $\varphi \rightarrow \varphi+\pi$. Moreover, the degeneracy is not an artifact of the rotating-wave approximation, because the initial Eq. (75) is already invariant with respect to the corresponding replacement $q(t) \rightarrow q(t-\pi / \omega)$. This invariance means that all other characteristics (e.g., the amplitude) of the parametric oscillations excited with either of two phases are absolutely similar. At the dawn of the computer age (in the late 1950s and early 1960s), there were substantial attempts, especially in Japan, to use this property for storage and processing digital information coded in the phase-binary form.

### 4.7. Numerical approach

If the amplitude of oscillations, by whatever reason, becomes so large that the nonlinear terms in the equation describing a system are comparable to its linear terms, numerical methods are virtually the only avenue available for their study. In Hamiltonian 1D systems, such methods may be applied directly to integral (3.26), but dissipative and/or parametric systems typically lack first integrals of motion similar to Eq. (3.24), so that the initial differential equation has to be solved.

Let us discuss the general idea of such methods on the example of what mathematicians call the Cauchy problem (finding the solution for all moments of time, starting from known initial conditions) for first-order differential equation

$$
\begin{equation*}
\dot{q}=f(t, q) . \tag{4.96}
\end{equation*}
$$

(The generalization to a set of several such equations is straightforward.) Breaking the time axis into small, equal steps $h$ (Fig. 11) we can reduce the equation integration problem to finding the function value in the next time point, $q_{n+1} \equiv q\left(t_{n+1}\right)=q\left(t_{n}+h\right)$ from the previously found value $q_{n}=q\left(t_{n}\right)$ - and, if
necessary, the values of $q$ at other previous time steps. In the generic approach (called the Euler method), $q_{n+1}$ is found using the following formula:

$$
\begin{align*}
& q_{n+1}=q_{n}+k  \tag{4.97}\\
& k \equiv h f\left(t_{n}, q_{n}\right) .
\end{align*}
$$

It is evident that this approximation is equivalent to the replacement of the genuine function $q(t)$, on the segment $\left[t_{n}, t_{n+1}\right]$, with the two first terms of its Taylor expansion in point $t_{n}$ :

$$
\begin{equation*}
q\left(t_{n}+h\right) \approx q\left(t_{n}\right)+\dot{q}\left(t_{n}\right) h \equiv q\left(t_{n}\right)+h f\left(t_{n}, q_{n}\right) . \tag{4.98}
\end{equation*}
$$



Fig. 4.11. The basic notions used at numerical integration of ordinary differential equations.

Such approximation has an error proportional to $h^{2}$. One could argue that making the step $h$ sufficiently small the Euler's method error might be done arbitrary small, but even with the numbercrunching power of modern computers, the computation time necessary to reach sufficient accuracy may be too high for large problems. ${ }^{31}$ Besides that, the increase of the number of time steps, which is necessary at $h \rightarrow 0$, increases the total rounding errors, and eventually may cause an increase, rather than the reduction of the overall error of the computed result.

A more efficient way is to modify Eq. (97) to include the terms of the second order in $h$. There are several ways to do this, for example using the $2^{\text {nd }}$-order Runge-Kutta method:

$$
\begin{align*}
& q_{n+1}=q_{n}+k_{2} \\
& k_{2} \equiv h f\left(t_{n}+\frac{h}{2}, q_{n}+\frac{k_{1}}{2}\right), \quad k_{1} \equiv h f\left(t_{n}, q_{n}\right) . \tag{4.99}
\end{align*}
$$

One can readily check that this method gives the exact result if function $q(t)$ is a quadratic polynomial, and hence in the general case its errors are of the order of $h^{3}$. We see that the main idea here is to first break the segment $\left[t_{n}, t_{n+1}\right]$ in half (Fig. 11), then evaluate the right-hand part of the differential equation (96) at the point intermediate (in both $t$ and $q$ ) between points $n$ and $(n+1)$, and then use this information to predict $q_{n+1}$.

The advantage of the Runge-Kutta approach is that it can be readily extended to the $4^{\text {th }}$ order, without an additional breaking of the interval $\left[t_{n}, t_{n+1}\right]$.:

[^57]\[

$$
\begin{align*}
& q_{n+1}=q_{n}+\frac{1}{6}\left(k_{1}+2 k_{2}+2 k_{3}+k_{4}\right)  \tag{4.100}\\
& k_{4} \equiv h f\left(t_{n}+h, q_{n}+k_{3}\right), k_{3} \equiv h f\left(t_{n}+\frac{h}{2}, q_{n}+\frac{k_{2}}{2}\right), k_{2} \equiv h f\left(t_{n}+\frac{h}{2}, q_{n}+\frac{k_{1}}{2}\right), k_{1} \equiv h f\left(t_{n}, q_{n}\right)
\end{align*}
$$
\]

This method reaches much lower error, $O\left(h^{5}\right)$, without being not too cumbersome. These features have made the $4^{\text {th }}$-order Runge-Kutta the default method in most numerical libraries. Its extension to higher orders is possible but requires more complex formulas and is justified only for some special cases, e.g., very abrupt functions $q(t) .{ }^{32}$ The most frequent enhancement of the method is the automatic adjustment of step $h$ to reach the specified accuracy.

Figure 12 shows a typical example of application of that method to the very simple problem of a damped linear oscillator, for two values of fixed time step $h$ (expressed in terms of the number $N$ of such steps per oscillation period). Black lines connect the points obtained by the $4^{\text {th }}$-order Runge-Kutta method, while the points connected by green straight lines present the exact analytical solution (22). A few-percent errors start to appear only at as few as $\sim 10$ time steps per period, so that the method is indeed very efficient. I will illustrate the convenience and handicaps of the numerical approach to the solution of dynamics problems on the discussion of the following topic.


Fig. 4.12. Results of the fixed-point Runge-Kutta solution to the equation of linear oscillator with damping (with $\delta / \omega_{0}=0.03$ ) for: (a) 30 and (b) 6 points per oscillation period. The results are shown by points; lines are only the guide for the eye.

### 4.8. Higher harmonic and subharmonic oscillations

Figure 13 shows the numerically calculated ${ }^{33}$ transient process and stationary oscillations in a linear oscillator and a very representative nonlinear system, the pendulum described by Eq. (42), both with the same resonance frequency $\omega_{0}$ for small oscillations. Both systems are driven by a sinusoidal

[^58]external force of the same amplitude and frequency - in this illustration, equal to the small-oscillation eigenfrequency $\omega_{0}$ of both systems. The plots show that despite a very substantial amplitude of the pendulum oscillations (an angle amplitude of about one radian) their waveform remains almost exactly sinusoidal. ${ }^{34}$ On the other hand, the nonlinearity affects the oscillation amplitude very substantially. These results illustrate that the validity of the small-parameter method and its RWA extension far exceeds what might be expected from the formal requirement $|q| \ll 1$.


Fig. 4.13. Oscillations induced by a similar sinusoidal external force (turned on at $t=0$ ) in two systems with the same small-oscillation frequency $\omega_{0}$ and low damping - a linear oscillator (two top panels) and a pendulum (two bottom panels). $\delta / \omega_{0}=0.03, f_{0}=0.1$, and $\omega=\omega_{0}$.

The higher harmonic contents in the oscillation waveform may be sharply increased ${ }^{35}$ by reducing the external force frequency to $\sim \omega_{0} / n$, where integer $n$ is the number of the desirable harmonic. For example, Fig. 14a shows oscillations in a pendulum described by the same Eq. (42), but driven at frequency $\omega_{0} / 3$. One can see that the $3^{\text {rd }}$ harmonic amplitude may be comparable with that of the basic harmonic, especially if the external frequency is additionally lowered (Fig. 14b) to accommodate for the deviation of the effective frequency $\omega_{0}(a)$ of own oscillations from its small-oscillation value $\omega_{0}$ - see Eq. (49), Fig. 4 and their discussion in Sec. 2 above.

Generally, the higher harmonic generation by nonlinear systems might be readily anticipated. Indeed, the Fourier theorem tells us that any non-sinusoidal periodic function of time, e.g., an initially sinusoidal waveform of frequency $\omega$, distorted by nonlinearity, may be presented as a sum of its basic harmonic and higher harmonics with frequencies $n \omega$. Note that an effective generation of higher

[^59]harmonics is only possible with adequate nonlinearity of the system. For example, consider the nonlinear term $\alpha q^{3}$ used in equations explored in Secs. 2 and 3. If the waveform $q(t)$ is approximately sinusoidal, such term can create only the basic and $3^{\text {rd }}$ harmonics. The "pendulum nonlinearity" $\sin q$ cannot produce, without a constant component is process $q(t)$, any even (e.g., the $2^{\text {nd }}$ ) harmonic. The most efficient generation of harmonics may be achieved using systems with the sharpest nonlinearities e.g., semiconductor diodes whose current may follow an exponential dependence on the applied voltage through several orders of magnitude.


Fig. 4.14. Oscillations induced in a pendulum with damping $\delta / \omega_{0}=0.03$, driven by a sinusoidal external force of amplitude $f_{0}=0.75$, and frequency $\omega_{0} / 3$ (top panel) and $0.8 \omega_{0} / 3$ (bottom panel).

However, numerical modeling of nonlinear oscillators, as well as experiments with their physical implementations, bring more surprises. For example, the bottom panel of Fig. 15 shows oscillations in a pendulum under effect of a strong sinusoidal force with a frequency close to $3 \omega_{0}$. One can see that at some parameter values and initial conditions the system's oscillation spectrum is heavily contributed (almost dominated) by the $3^{\text {rd }}$ subharmonic, i.e. a component that is synchronous with the driving force of frequency $3 \omega$, but has the frequency $\omega$ that is close to the eigenfrequency $\omega_{0}$ of the system.

This counter-intuitive phenomenon may be explained as follows. Let us assume that the subharmonic oscillations of frequency $\omega \approx \omega_{0}$ have somehow appeared, and coexist with the forced oscillations of frequency $3 \omega$ :

$$
\begin{equation*}
q(t) \approx A \cos \Psi+A_{\mathrm{sub}} \cos \Psi_{\mathrm{sub}}, \quad \text { where } \Psi \equiv 3 \omega t-\varphi, \quad \Psi_{\mathrm{sub}} \equiv \omega t-\varphi_{\mathrm{sub}} . \tag{4.101}
\end{equation*}
$$

Then, the first nonlinear term $\alpha q^{3}$ of the Taylor expansion of pendulum's nonlinearity $\sin q$ yields

$$
\begin{align*}
q^{3} & =\left(A \cos \Psi+A_{\text {sub }} \cos \Psi_{\text {sub }}\right)^{3}  \tag{4.102}\\
& =A^{3} \cos ^{3} \Psi+3 A^{2} A_{\text {sub }} \cos ^{2} \Psi \cos \Psi_{\text {sub }}+3 A A_{\text {sub }}^{2} \cos \Psi \cos ^{2} \Psi_{\text {sub }}+A_{\text {sub }}^{3} \cos ^{3} \Psi_{\text {sub }}
\end{align*}
$$

While the first and the last terms of this expression depend only of amplitudes of the individual components of oscillations, the two middle terms are more interesting because they produce so-called combinational frequencies of the two components. For our case, the third term,

$$
\begin{equation*}
3 A A_{\text {sub }}^{2} \cos \Psi \cos ^{2} \Psi_{\text {sub }}=\frac{3}{4} A A_{\text {sub }}^{2} \cos \left(\Psi-2 \Psi_{\text {sub }}\right)+\ldots \tag{4.103}
\end{equation*}
$$

of a special importance, because it produces, besides other combinational frequencies, the subharmonic component with the total phase

$$
\begin{equation*}
\Psi-2 \Psi_{\text {sub }}=\omega t-\varphi+2 \varphi_{\mathrm{sub}} . \tag{4.104}
\end{equation*}
$$

Thus, within a certain range of the mutual phase shift between the Fourier components, this nonlinear contribution is synchronous with the subharmonic oscillations, and describes the interaction that can deliver to it the energy from the external force, so that the oscillations may be self-sustained. Note, however, that the amplitude of the term (103) describing this energy exchange is proportional to the square of $A_{\text {sub }}$, and vanishes at the linearization of the equations of motion near the trivial fixed point. This means that the point is always stable, i.e., the $3^{\text {rd }}$ subharmonic cannot be self-excited and always need an initial "kick-off" - compare the two panels of Fig. 15. The same is evidently true for higher subharmonics.


Fig. 4.15. Oscillations induced in a pendulum with $\delta / \omega_{0}=0.03$ by a sinusoidal external force of amplitude $f_{0}=3$ and frequency $3 \omega_{0} \times 0.8$, with initial conditions $q(0)=0$ (the top row) and $q(0)=1$ (the bottom row).

Only the second subharmonic presents a special case. Indeed, let us make a calculation similar to Eq. (102), by replacing Eq. (101) with

$$
\begin{equation*}
q(t) \approx A \cos \Psi+A_{\mathrm{sub}} \cos \Psi_{\mathrm{sub}}, \quad \text { where } \Psi \equiv 2 \omega t-\varphi, \quad \Psi_{\mathrm{sub}} \equiv \omega t-\varphi_{\mathrm{sub}} \tag{4.105}
\end{equation*}
$$

for a nonlinear term proportional to $q^{2}$ :

$$
\begin{equation*}
q^{2}=\left(A \cos \Psi+A_{\mathrm{sub}} \cos \Psi_{\mathrm{sub}}\right)^{2}=A^{2} \cos ^{2} \Psi+2 A A_{\mathrm{sub}} \cos \Psi \cos \Psi_{\mathrm{sub}}+A_{\mathrm{sub}}^{2} \cos ^{2} \Psi_{\mathrm{sub}} \tag{4.106}
\end{equation*}
$$

Here the combinational-frequency term capable of supporting the $2^{\text {nd }}$ subharmonic,

$$
\begin{equation*}
2 A A_{\text {sub }} \cos \Psi \cos \Psi_{\text {sub }}=A A_{\text {sub }} \cos \left(\Psi-\Psi_{\text {sub }}\right)=A A_{\text {sub }} \cos \left(\omega t-\varphi+\varphi_{\text {sub }}\right)+\ldots \tag{4.107}
\end{equation*}
$$

is linear in the subharmonic amplitude, i.e. survives the equation linearization near the trivial fixed point. This mean that the second subharmonic may arise spontaneously, from infinitesimal fluctuations.

Moreover, such excitation of the second subharmonic is very similar to the parametric excitation that was discussed in detail in Sec. 5, and this similarity is not coincidental. Indeed, let us redo expansion (4.106) at a somewhat different assumption that the oscillations are a sum of the forced oscillations at the external force frequency $2 \omega$, and an arbitrary but weak perturbation:

$$
\begin{equation*}
q(t)=A \cos (2 \omega t-\varphi)+\widetilde{q}(t), \quad|\widetilde{q}| \ll A . \tag{4.108}
\end{equation*}
$$

Then, neglecting the small term proportional to $\widetilde{q}^{2}$, we get

$$
\begin{equation*}
q^{2} \approx A^{2} \cos ^{2}(2 \omega t-\varphi)+2 \widetilde{q}(t) A \cos (2 \omega t-\varphi) . \tag{4.109}
\end{equation*}
$$

Besides the inconsequential phase $\varphi$, the second term in the last formula is exactly similar to the term describing the parametric effects in Eq. (75). This fact means that for a weak perturbation, a system with a quadratic nonlinearity in the presence of a strong "pumping" signal of frequency $2 \omega$ is equivalent to a system with parameters changing in time with frequency $2 \omega$. This fact is broadly used for the parametric excitation at high (e.g., optical) frequencies where the mechanical means of parameter modulation (see, e.g., Fig. 5) are not practicable. The necessary quadratic nonlinearity at optical frequencies may be provided by a noncentrosymmetric nonlinear crystal, e.g., the $\beta$-phase barium borate $\left(\mathrm{BaB}_{2} \mathrm{O}_{4}\right)$.

Before finishing this chapter, let me elaborate a bit on a general topic: the relation between the numerical and analytical approaches to problems of dynamics (and physics as a whole). We have just seen that sometimes numerical solutions, like those shown in Fig. 15b, may give vital clues for previously unanticipated phenomena such as the excitation of subharmonics. (The phenomenon of deterministic chaos, which will be discussed in Chapter 9 below, presents another example of such "numerical discoveries".) One might also argue that in the absence of exact analytical solutions, numerical simulations may be the main theoretical tool for the study of such phenomena. These hopes are, however, muted by the problem that is frequently called the curse of dimensionality, ${ }^{36}$ in which the last word refers to the number of input parameters of the problem to be solved. ${ }^{37}$

Indeed, let us have another look at Fig. 15. OK, we have been lucky to find a new phenomenon, the $3^{\text {rd }}$ subharmonic generation, for a particular set of parameters - in that case, five of them: $\delta / \omega_{0}=$ $0.03,3 \omega / \omega_{0}=2.4, f_{0}=3, q(0)=1$, and $d q / d t(0)=0$. Could we tell anything about how common this effect is? Are subharmonics with different $n$ possible in the system? The only way to address these

[^60]questions computationally is to carry out similar numerical simulations in many points of the $d$ dimensional (in this case, $d=5$ ) space of parameters. Say, we have decided that breaking the reasonable range of each parameter to $N=100$ points is sufficient. (For many problems, even more points are necessary - see, e.g., Sec. 9.1.) Then the total number of numerical experiments to carry out is $N^{d}=$ $\left(10^{2}\right)^{5}=10^{10}-$ not a simple task even for the powerful modern computing facilities. (Besides the pure number of required CPU cycles, consider storage and analysis of the results.) For many important problems of nonlinear dynamics, e.g., turbulence, the parameter dimensionality $d$ is substantially larger, and the computer resources necessary for one numerical experiment, are much greater.

In the view of the curse of dimensionality concerns, approximate analytical considerations, like those outlined above for the subharmonic excitation, are invaluable. More generally, physics used to stand on two legs, experiment and (analytical) theory. The enormous progress of computer performance during a few last decades has provided it with one more point of support (a tail? :-) - numerical simulation. This does not mean we can afford to cut and throw away any of the legs we are standing on.

### 4.9. Exercise problems

4.1.* Prove Eq. (26) for the response function given by Eq. (17).

Hint: You may like to use the Cauchy integral theorem for analytical functions of complex variable. ${ }^{38}$
4.2. A square-wave pulse of force (see Fig. on the right) is exerted on a linear oscillator with eigenfrequency $\omega_{0}$ (no damping), initially at rest. Calculate the law of motion $q(t)$, sketch it, and interpret the result.
4.3. At $t=0$, a sinusoidal external force $F(t)=F_{0} \cos \omega t$, with constant $A$
 and $\omega$, is applied to a linear oscillator with eigenfrequency $\omega_{0}$ and damping $\delta$, which was at rest at $t \leq 0$.
(i) Calculate the general expression for the time evolution of the oscillator's coordinate, and interpret the result.
(ii) Spell out your result for the case of the resonance $\left(\omega=\omega_{0}\right)$ in a system with low damping ( $\delta$ $\ll \omega_{0}$ ), and, in particular, explore the limit $\delta \rightarrow 0$.
4.4. A pulse of external force $F(t)$, with a finite duration $T$, is exerted on a harmonic oscillator, initially at rest in the equilibrium position. Neglecting dissipation, calculate the change of oscillator's energy, using two different methods, and compare the results.
4.5.* For a system with the following Lagrangian function:

$$
L=\frac{m}{2} \dot{q}^{2}-\frac{\kappa}{2} q^{2}+\frac{\varepsilon}{2} \dot{q}^{2} q^{2},
$$

calculate the frequency of free oscillations as a function of their amplitude $A$, at $A \rightarrow 0$, using two different approaches.

[^61]4.6. For a system with the Lagrangian function
$$
L=\frac{m}{2} \dot{q}^{2}-\frac{\kappa}{2} q^{2}+\varepsilon \dot{q}^{4},
$$
with small parameter $\varepsilon$, use the rotating-wave approximation to find the frequency of free oscillations as a function of their amplitude.
4.7. Find the regions of real, time-independent parameters $a_{1}$ and $a_{2}$, in which the fixed point of the following system of equations,
\[

$$
\begin{aligned}
& \dot{q}_{1}=a_{1}\left(q_{2}-q_{1}\right), \\
& \dot{q}_{2}=a_{2} q_{1}-q_{2},
\end{aligned}
$$
\]

is unstable. On the $\left[a_{1}, a_{2}\right]$ plane, sketch the regions of each fixed point type - stable and unstable nodes, focuses, etc.
4.8. Solve Problem 4.3(ii) using the rotating-wave approximation, and compare the result with the exact solution.
4.9. Use the rotating-wave approximation to analyze forced oscillations in an oscillator with weak nonlinear damping, described by equation

$$
\ddot{q}+2 \delta \dot{q}+\omega_{0}^{2} q+\beta \dot{q}^{3}=f_{0} \cos \omega t,
$$

with $\omega \approx \omega_{0} ; \beta, \delta>0$; and $\beta \omega A^{2} \ll 1$. In particular, find the stationary amplitude of forced oscillations and analyze their stability. Discuss the effect(s) of the nonlinear term on the resonance.
4.10.* Analyze stability of the forced nonlinear oscillations described by Eq. (43). Relate the result to the slope of resonance curves (Fig. 4).
4.11. Use the rotating-wave approximation to analyze parametric excitation of an oscillator with weak nonlinear damping, described by equation

$$
\ddot{q}+2 \delta \dot{q}+\beta \dot{q}^{3}+\omega_{0}^{2}(1+\mu \cos 2 \omega t) q=0
$$

with $\omega \approx \omega_{0} ; \beta, \delta>0$; and $\mu, \beta \omega A^{2} \ll 1$. In particular, find the amplitude of stationary oscillations and analyze their stability.
4.12. Adding nonlinear term $\alpha q^{3}$ to the left-hand part of Eq. (76),
(i) find the corresponding addition to the RWA equations,
(ii) find the stationary amplitude $A$ of parametric oscillations,
(iii) sketch and discuss the $A(\xi)$ dependence,
(iv) find the type and stability of each fixed point of the RWA equations,
(v) sketch the Poincaré phase plane of the system in main parameter regions.
4.13. Use the rotating-wave approximation to find the conditions of parametric excitation in an oscillator with weak modulation of both the effective mass $m(t)=m_{0}\left(1+\mu_{m} \cos 2 \omega t\right)$ and spring constant $\kappa(t)=\kappa_{0}\left[1+\mu_{k} \cos (2 \omega t-\psi)\right]$, with the same frequency $2 \omega \approx 2 \omega_{0}$, but arbitrary modulation depths ratio
$\mu_{m} / \mu_{k}$ and phase shift $\psi$. Interpret the result in terms of modulation of the instantaneous frequency $\omega(t) \equiv$ $[\kappa(t) / m(t)]^{1 / 2}$ and mechanical impedance $Z(t) \equiv[\kappa(t) m(t)]^{1 / 2}$ of the oscillator.
4.14.* Find the condition of parametric excitation of a nonlinear oscillator described by equation

$$
\ddot{q}+2 \delta \dot{q}+\omega_{0}^{2} q+\gamma q^{2}=f_{0} \cos 2 \omega t
$$

with sufficiently small $\delta, \gamma, f_{0}$, and $\xi \equiv \omega-\omega_{0}$.

## Chapter 5. From Oscillations to Waves

In this chapter, the discussion of oscillations is extended to systems with two and more degrees of freedom. This extension naturally leads to another key notion - waves. The discussion of waves (at this stage, in $1 D$ systems) is focused at such key phenomena as their dispersion and reflection from interfaces/boundaries.

### 5.1. Two coupled oscillators

Let us move on to discuss oscillations in systems with more than one degree of freedom, starting from the simplest case of two linear, dissipation-free oscillators. If the Lagrangian of the system may be presented as a sum of those for two harmonic oscillators,

$$
\begin{equation*}
L=L_{1}+L_{2}, \quad L_{1,2}=T_{1,2}-U_{1,2}=\frac{m_{1,2}}{2} \dot{q}_{1,2}^{2}-\frac{\kappa_{1,2}}{2} q_{1,2}^{2}, \tag{5.1}
\end{equation*}
$$

(plus arbitrary, inconsequential constants if you like), then according to Eq. (2.19), the equations of motion of the oscillators are independent of each other, and each one is similar to Eq. (1.1), with its partial frequency $\Omega_{1,2}$ equal to

$$
\begin{equation*}
\Omega_{1,2}^{2}=\frac{\kappa_{1,2}}{m_{1,2}} . \tag{5.2}
\end{equation*}
$$

This means that in this simplest case, the arbitrary motion of the system is just a sum of independent sinusoidal oscillations at two frequencies equal to the partial frequencies (2).

Hence, in order to describe the oscillator coupling (i.e. interaction), the full Lagrangian $L$ should contain an additional mixed term $L_{\text {int }}$ depending on both generalized coordinates $q_{1}$ and $q_{2}$ and/or generalized velocities. The simplest, and most frequently met type of such interaction term is the following bilinear form $U_{\mathrm{int}}=-\kappa q_{1} q_{2}$, where $\kappa$ is a constant, giving $L_{\mathrm{int}}=-U_{\mathrm{int}}=\kappa q_{1} q_{2}$. Figure 1 shows the simplest example of system with such interaction. ${ }^{1}$ In it, three springs, keeping two massive particles between two stiff walls, have generally different spring constants.


Fig. 5.1. Simple system of two coupled harmonic oscillators.

Indeed, in this case the kinetic energy is still separable, $T=T_{1}+T_{2}$, but the total potential energy, consisting of elastic energies of three springs, is not:

$$
\begin{equation*}
U=\frac{\kappa_{L}}{2} q_{1}^{2}+\frac{\kappa_{M}}{2}\left(q_{1}-q_{2}\right)^{2}+\frac{\kappa_{R}}{2} q_{2}^{2}, \tag{5.3a}
\end{equation*}
$$

[^62]where $q_{1.2}$ are the horizontal displacements of particles from their equilibrium positions. It is convenient to rewrite this expression as
\[

$$
\begin{equation*}
U=\frac{\kappa_{1}}{2} q_{1}^{2}+\frac{\kappa_{2}}{2} q_{2}^{2}-\kappa q_{1} q_{2}, \quad \text { where } \kappa_{1} \equiv \kappa_{L}+\kappa_{M}, \quad \kappa_{2} \equiv \kappa_{R}+\kappa_{M}, \quad \kappa \equiv \kappa_{M} \tag{5.3b}
\end{equation*}
$$

\]

showing that the Lagrangian $L=T-U$ of this system indeed contains a bilinear interaction term:

$$
\begin{equation*}
L=L_{1}+L_{2}+L_{\mathrm{int}}, \quad L_{\mathrm{int}}=\kappa q_{1} q_{2} \tag{5.4}
\end{equation*}
$$

The resulting Lagrange equations of motion are

$$
\begin{align*}
& m_{1} \ddot{q}_{1}+m_{1} \Omega_{1}^{2} q_{1}=\kappa q_{2},  \tag{5.5}\\
& m_{2} \ddot{q}_{2}+m_{2} \Omega_{2}^{2} q_{2}=\kappa q_{1} .
\end{align*}
$$

Linearly coupled oscillators

Thus the interaction energy describes effective generalized force $\kappa q_{2}$ exerted on subsystem 1 by subsystem 2, and the reciprocal effective force $\kappa q_{1}$. Note that in contrast to real physical forces (such as $F_{12}=-F_{21}=\kappa_{M}\left(q_{2}-q_{1}\right)$ for the system shown in Fig. 1) the effective forces in the right-hand part of Eqs. (5) do not obey the $3^{\text {rd }}$ Newton law. Note also that they are proportional to the same coefficient $\kappa$, this feature is a result of the general bilinear structure (4) of the interaction energy rather than of any special symmetry.

We already know how to solve Eqs. (5), because it is still a system of linear and homogeneous differential equations, so that its general solution is a sum of particular solutions of the form similar to Eqs. (4.88),

$$
\begin{equation*}
q_{1}=c_{1} e^{\lambda t}, \quad q_{2}=c_{2} e^{\lambda t} \tag{5.6}
\end{equation*}
$$

for all possible values of $\lambda$. These values may be found by plugging Eq. (6) into Eqs. (5), and requiring the resulting system of two linear algebraic equations for the distribution coefficients $c_{1,2}$,

$$
\begin{align*}
& m_{1} \lambda^{2} c_{1}+m_{1} \Omega_{1}^{2} c_{1}=\kappa c_{2}  \tag{5.7}\\
& m_{2} \lambda^{2} c_{2}+m_{2} \Omega_{2}^{2} c_{2}=\kappa c_{1}
\end{align*}
$$

to be self-consistent. In our particular case, we get a characteristic equation,

$$
\left|\begin{array}{cc}
m_{1}\left(\lambda^{2}+\Omega_{1}^{2}\right) & -\kappa  \tag{5.8}\\
-\kappa & m_{2}\left(\lambda^{2}+\Omega_{2}^{2}\right)
\end{array}\right|=0
$$

that is quadratic in $\lambda^{2}$, and thus allows a simple solution:

$$
\begin{align*}
\left(\lambda^{2}\right)_{ \pm} & =-\frac{1}{2}\left(\Omega_{1}^{2}+\Omega_{2}^{2}\right) \mp\left[\frac{1}{4}\left(\Omega_{1}^{2}+\Omega_{2}^{2}\right)^{2}-\Omega_{1}^{2} \Omega_{2}^{2}+\frac{\kappa^{2}}{m_{1} m_{2}}\right]^{1 / 2}  \tag{5.9}\\
& =-\frac{1}{2}\left(\Omega_{1}^{2}+\Omega_{2}^{2}\right) \mp\left[\frac{1}{4}\left(\Omega_{1}^{2}-\Omega_{2}^{2}\right)^{2}+\frac{\kappa^{2}}{m_{1} m_{2}}\right]^{1 / 2} .
\end{align*}
$$

According to Eqs. (2) and (3b), for any positive values of spring constants, product $\Omega_{1} \Omega_{2}=\left(\kappa_{L}+\kappa_{M}\right)\left(\kappa_{R}\right.$ $\left.+\kappa_{M}\right) /\left(m_{1} m_{2}\right)^{1 / 2}$ is always larger than $\kappa /\left(m_{1} m_{2}\right)^{1 / 2}=\kappa_{M} /\left(m_{1} m_{2}\right)^{1 / 2}$, so that the square root in Eq. (9) is always less than $\left(\Omega_{1}{ }^{2}+\Omega_{2}{ }^{2}\right) / 2$. As a result, both values of $\lambda^{2}$ are negative, i.e. the general solution to Eq.
(5) is a sum of four terms, each proportional to $\exp \left\{ \pm i \omega_{ \pm} t\right\}$, where both eigenfrequencies $\omega_{ \pm} \equiv i \lambda_{ \pm}$are real:

$$
\begin{equation*}
\omega_{ \pm}^{2} \equiv-\lambda_{ \pm}^{2}=\frac{1}{2}\left(\Omega_{1}^{2}+\Omega_{2}^{2}\right) \pm\left[\frac{1}{4}\left(\Omega_{1}^{2}-\Omega_{2}^{2}\right)^{2}+\frac{\kappa^{2}}{m_{1} m_{2}}\right]^{1 / 2} \tag{5.10}
\end{equation*}
$$

A plot of these eigenfrequencies as a function of one of the partial frequencies $\Omega$ (say, $\Omega_{1}$ ), with the other partial frequency fixed, gives the famous anticrossing (also called "avoided crossing" or noncrossing") diagram (Fig. 2). One can see that at weak coupling, frequencies $\omega_{ \pm}$are close to the partial frequencies everywhere besides a narrow range near the anticrossing point $\Omega_{1}=\Omega_{2}$. Most remarkably, at passing through this region, $\omega_{+}$smoothly "switches" from following $\Omega_{2}$ to following $\Omega_{1}$ and vice versa.


Fig. 5.2. Anticrossing diagram for two values of the oscillator coupling strength $K /\left(m_{1} m_{2}\right)^{1 / 2} \Omega_{2}{ }^{2}$ : 0.3 (red lines) and 0.1 (blue lines). In this plot, $\Omega_{1}$ is assumed to be changed by varying $\kappa_{1}$ rather than $m_{1}$, but in the opposite case the diagram is qualitatively similar.

The reason for this counterintuitive behavior may be found by examining the distribution coefficients $c_{1,2}$ corresponding to each branch of the diagram, which may be obtained by plugging the corresponding value of $\lambda_{ \pm}=-i \omega_{ \pm}$back into Eqs. (7). For example, at the anticrossing point $\Omega_{1}=\Omega_{2} \equiv \Omega$, Eq. (10) is reduced to

$$
\begin{equation*}
\omega_{ \pm}^{2}=\Omega^{2} \pm \frac{\kappa}{\left(m_{1} m_{2}\right)^{1 / 2}}=\Omega^{2}\left(1 \pm \frac{\kappa}{\left(\kappa_{1} \kappa_{2}\right)^{1 / 2}}\right) . \tag{5.11}
\end{equation*}
$$

Plugging this expression back into any of Eqs. (7), we see that for the two branches of the anticrossing diagram, the distribution coefficient ratio is the same by magnitude but opposite by sign: ${ }^{2}$

$$
\begin{equation*}
\left(\frac{c_{1}}{c_{2}}\right)_{ \pm}=\mp\left(\frac{m_{2}}{m_{1}}\right)^{1 / 2}, \quad \text { at } \Omega_{1}=\Omega_{2} \tag{5.12}
\end{equation*}
$$

In particular, if the system is symmetric ( $m_{1}=m_{2}, \kappa_{L}=\kappa_{R}$ ), then at the upper branch, corresponding to $\omega_{+}>\omega_{-}, c_{1}=-c_{2}$. This means that in this hard mode, ${ }^{3}$ masses oscillate in anti-phase: $q_{1}(t) \equiv-q_{2}(t)$. The

[^63]resulting substantial extension/compression of the middle spring yields additional returning force which increases the oscillation frequency. On the contrary, on the lower branch, corresponding to $\omega$, the particle oscillations are in phase: $c_{1}=c_{2}, q_{1}(t) \equiv q_{2}(t)$, so that the middle spring is never stretched at all. As a result, the soft mode oscillation frequency $\omega_{\text {- }}$ is lower than $\omega_{+}$and does not depend on $\kappa$.
\[

$$
\begin{equation*}
\omega_{-}^{2}=\Omega^{2}-\frac{\kappa}{m}=\frac{\kappa_{L}}{m}=\frac{\kappa_{R}}{m} . \tag{5.13}
\end{equation*}
$$

\]

Note that for both modes, the oscillations equally engage both particles.
Far from the anticrossing point, the situation is completely different. Indeed, an absolutely similar calculation of $c_{1,2}$ shows that on each branch of the diagram, one of the distribution coefficients is much larger (by magnitude) than its counterpart. Hence, in this limit any particular mode of oscillations involves virtually only one particle. A slow change of system parameters, bringing it through the anticrossing, results, first, in a maximal delocalization of each mode, and then in the restoration of the localization, but in a different partial degree of freedom.

We could readily carry out similar calculations for the case when the systems are coupled via their velocities, $L_{\text {int }}=m \dot{q}_{1} \dot{q}_{2}$, where $m$ is a coupling coefficient - not necessarily a certain physical mass. (In mechanics, with $q_{1,2}$ standing for actual particle displacements, such coupling is hard to implement, but there are many dynamic systems of non-mechanical nature in which such coupling is the most natural one.) The results are generally similar to those discussed above, again with the maximum level splitting at $\Omega_{1}=\Omega_{2} \equiv \Omega$ :

$$
\begin{equation*}
\omega_{ \pm}^{2}=\frac{\Omega^{2}}{1 \mp|m| /\left(m_{1} m_{2}\right)^{1 / 2}} \approx \Omega^{2}\left(1 \pm \frac{|m|}{\left(m_{1} m_{2}\right)^{1 / 2}}\right), \tag{5.14}
\end{equation*}
$$

the last relation being valid for weak coupling. The generalization to the case of both coordinate and velocity coupling is also straightforward - see the next section.

The anticrossing diagram shown in Fig. 2 may be met not only in classical mechanics. It is even more ubiquitous quantum mechanics, because, due to the time-oscillatory character of the Schrödinger equation solutions, weak coupling of any two quantum states leads to a qualitatively similar behavior of eigenfrequencies $\omega_{ \pm}$and hence of the eigenenergies ("energy levels") $E_{ \pm}=\hbar \omega_{ \pm} .{ }^{4}$

## 5.2. $N$ coupled oscillators

The calculations of the previous section may be readily generalized to the case of arbitrary number (say, $N$ ) coupled harmonic oscillators, with arbitrary type of coupling. It is evident that in this case Eq. (4) should be replaced with

[^64]\[

$$
\begin{equation*}
L=\sum_{j=1}^{N} L_{j}+\sum_{j, j^{\prime}=1}^{N} L_{i j^{\prime}} \tag{5.15}
\end{equation*}
$$

\]

Moreover, we can generalize the above relations for the mixed terms $L_{i j}$, taking into account their possible dependence not only on the generalized coordinates, but on the generalized velocities, in a bilinear form similar to Eq. (4). The resulting Lagrangian may be presented in a compact form,

$$
\begin{equation*}
L=\sum_{j, j^{\prime}=1}^{N}\left(\frac{m_{i j^{\prime}}}{2} \dot{q}_{j} \dot{q}_{j^{\prime}}-\frac{\kappa_{i j^{\prime}}}{2} q_{j} q_{j^{\prime}}\right) \tag{5.16}
\end{equation*}
$$

where the off-diagonal terms are index-symmetric: $m_{j j^{\prime}}=m_{j^{\prime} j^{\prime}}, \kappa_{j j^{\prime}}=\kappa_{j^{\prime} j}$, and the factors $1 / 2$ compensate the double counting of each term with $j \neq j^{\prime}$, taking place at the summation over two independently running indices. One may argue that Eq. (16) is quite general if we still want the equations of motion to be linear - as they have to be if the oscillations are small enough.

Plugging Eq. (16) into the general form (2.19) of the Lagrange equation, we get $N$ equations of motion of the system, one for each value of index $j^{\prime}=1,2, \ldots, N$ :

$$
\begin{equation*}
\sum_{j=1}^{N}\left(m_{i j} \ddot{q}_{j}+\kappa_{j j} q_{j}\right)=0 \tag{5.17}
\end{equation*}
$$

Just as in the previous section, let us look for a particular solution to this system in the form

$$
\begin{equation*}
q_{j}=c_{j} e^{\lambda t} \tag{5.18}
\end{equation*}
$$

As a result, we are getting a system of $N$ linear, homogeneous algebraic equations,

$$
\begin{equation*}
\sum_{j=1}^{N}\left(m_{i j j^{\prime}} \lambda^{2}+\kappa_{i j^{\prime}}\right) c_{j}=0 \tag{5.19}
\end{equation*}
$$

for the set of $N$ distribution coefficients $c_{j}$. The condition that this system is self-consistent is that the determinant of its matrix equals zero:

$$
\begin{equation*}
\operatorname{Det}\left(m_{j j} \cdot \lambda^{2}+\kappa_{j j^{\prime}}\right)=0 \tag{5.20}
\end{equation*}
$$

This characteristic equation is an algebraic equation of degree $N$ for $\lambda^{2}$, and so has $N$ roots $\left(\lambda^{2}\right)_{n}$. For any Hamiltonian system with stable equilibrium, matrices $m_{j j}$, and $\kappa_{j j}$, ensure that all these roots are real and negative. As a result, the general solution to Eq. (17) is the sum of $2 N$ terms proportional to $\exp \left\{ \pm i \omega_{n} t\right\}$, $n=1,2, \ldots, N$, where all $N$ eigenfrequencies $\omega_{n}$ are real.

Plugging each of these $2 N$ values of $\lambda= \pm i \omega_{n}$ back into the set of linear equations (17), one can find the corresponding set of distribution coefficients $c_{j \pm}$. Generally, the coefficients are complex, but in order to keep $q_{\mathrm{j}}(t)$ real, the coefficients $c_{j+}$ corresponding to $\lambda=+i \omega_{n}$ and $c_{j \text { - }}$ corresponding to $\lambda=-i \omega_{n}$ have to be complex conjugate of each other. Since the sets of the distribution coefficients may be different for each $\lambda_{n}$, they should be marked with two indices, $j$ and $n$. Thus, at general initial conditions, the time evolution of $j$-th coordinate may be presented as

$$
\begin{equation*}
q_{j}=\frac{1}{2} \sum_{n=1}^{N}\left(c_{j n} \exp \left\{+i \omega_{n} t\right\}+c_{j n}^{*} \exp \left\{-i \omega_{n} t\right\}\right)=\operatorname{Re} \sum_{n=1}^{N} c_{j n} \exp \left\{i \omega_{n} t\right\} . \tag{5.21}
\end{equation*}
$$

This formula shows very clearly again the physical sense of the distribution coefficients $c_{j n}$ : a set of these coefficients, with different values of index $j$ but the same $n$, gives the complex amplitudes of oscillations of the coordinates for the special choice of initial conditions, that ensures purely sinusoidal motion of the system, with frequency $\omega_{n}$. Moreover, these coefficients show how exactly such special initial conditions should be selected - within a common constant factor.

Calculation of the eigenfrequencies and distribution coefficients of a coupled system with many degrees of freedom from Eq. (20) is a task that frequently may be only done numerically. ${ }^{5}$ Let us discuss just two particular but very important cases. First, let all the coupling coefficients be small $\left(\left|m_{j j}\right| \ll m_{j}\right.$ $\equiv m_{j j}$ and $\left|\kappa_{j j^{\prime}}\right| \ll \kappa_{j} \equiv \kappa_{j j}$, for all $j \neq j$ ), and all partial frequencies $\Omega_{j} \equiv\left(\kappa_{j} / m_{j}\right)^{1 / 2}$ be not too close to each other:

$$
\begin{equation*}
\frac{\left|\Omega_{j}^{2}-\Omega_{j^{\prime}}^{2}\right|}{\Omega_{j}^{2}} \gg \frac{\left|\kappa_{i j^{\prime}}\right|}{\kappa_{j}}, \frac{\left|m_{j j^{\prime}}\right|}{m_{j}}, \quad \text { for all } j \neq j^{\prime} \tag{5.22}
\end{equation*}
$$

(Such situation frequently happens if parameters of the system are "random" in the sense that they do not follow any special, simple rule.) Results of the previous section imply that in this case the coupling does not produce a noticeable change of oscillation frequencies: $\left\{\omega_{n}\right\} \approx\left\{\Omega_{j}\right\}$. In this situation, oscillations at each eigenfrequency are heavily concentrated in one degree of freedom, i.e. in each set of the distribution coefficients $c_{j n}$ (for a given $n$ ), one coefficient's magnitude is much larger than all others.

Now let the conditions (22) be valid for all but one pair of partial frequencies, say $\Omega_{1}$ and $\Omega_{2}$, while these two frequencies are so close that coupling of the corresponding partial oscillators becomes essential. In this case the approximation $\left\{\omega_{n}\right\} \approx\left\{\Omega_{j}\right\}$ is still valid for all other degrees of freedom, and the corresponding terms may be neglected in Eqs. (19) for $j=1$ and 2. As a result, we return to Eqs. (7) (perhaps generalized for velocity coupling) and hence to the anticrossing diagram (Fig. 2) discussed in the previous section. As a result, an extended change of only one partial frequency (say, $\Omega_{1}$ ) of a weakly coupled system produces a series of eigenfrequency anticrossings - see Fig. 3.


Fig. 5.3. Level anticrossing in a system of $N$ weakly coupled oscillators - schematically.

[^65]
### 5.3. 1D waves in periodic systems

For coupled systems with considerable degree of symmetry, the general results of the last section may be simplified, some with very profound implications. Perhaps the most important of them are waves. Figure 4 shows a classical example of a wave-supporting system - a long 1D chain of massive particles, with the elastic next-neighbor coupling.


Fig. 5.4. Uniform 1D chain of elastically coupled particles.

Let us start from the case when the system is so long (formally, infinite) that the boundary effects may be neglected; then its Lagrangian may be represented by an infinite sum of similar terms, each including the kinetic energy of $j$-th particle, and the potential energy of the spring on one (say, right) side of it:

$$
\begin{equation*}
L=\sum_{j}\left[\frac{m}{2} \dot{q}_{j}^{2}-\frac{\kappa}{2}\left(q_{j+1}-q_{j}\right)^{2}\right] . \tag{5.23}
\end{equation*}
$$

From here, the Lagrange equations of motion (2.19) have the same form for each particle:

$$
\begin{equation*}
m \ddot{q}_{j}-\kappa\left(q_{j+1}-q_{j}\right)+\kappa\left(q_{j}-q_{j-1}\right)=0 . \tag{5.24}
\end{equation*}
$$

Apart from the (formally) infinite size of the system, this is evidently just a particular case of Eq. (17), and thus its particular solution may be looked in the form (18), with $\lambda^{2} \rightarrow-\omega^{2}<0$. With this substitution, Eq. (24) gives the following simple form of the general system (17) for the distribution coefficients $c_{j}$ :

$$
\begin{equation*}
\left(-m \omega^{2}+2 \kappa\right) c_{j}-\kappa c_{j+1}-\kappa c_{j-1}=0 \tag{5.25}
\end{equation*}
$$

Now comes the most important conceptual step toward the wave theory: the translational symmetry of Eq. (23), i.e. its invariance to the replacement $j \rightarrow j+1$, allows it to have a particular solution of the following form:

$$
\begin{equation*}
c_{j}=a e^{i \alpha j} \tag{5.26}
\end{equation*}
$$

where coefficient $\alpha$ may depend on $\omega$ (and system's parameters), but not on the particle number $j$. Indeed, plugging Eq. (26) into Eq. (25) and cancelling the common factor $e^{i \alpha j}$, we see that it is identically satisfied, if $\alpha$ obeys the following algebraic equation:

$$
\begin{equation*}
\left(-m \omega^{2}+2 \kappa\right)-\kappa e^{+i \alpha}-\kappa e^{-i \alpha}=0 . \tag{5.27}
\end{equation*}
$$

The physical sense of solution (26) becomes clear if we use it and Eq. (18) with $\lambda=\mp i \omega$ to write

$$
\begin{equation*}
q_{j}(t)=\operatorname{Re}\left[a e^{i\left(k z_{j} \mp \omega t\right)}\right]=\operatorname{Re}\left[a e^{i k\left(z_{j} \mp v_{\mathrm{ph}} t\right)}\right], \tag{5.28}
\end{equation*}
$$

where wave number $k$ is defined as $k \equiv \alpha / d$, and $z_{j}=j d$ is the equilibrium position of $j$-th particle - the notion that should not be confused with particle's displacement $q_{j}$ from that equilibrium position - see Fig. 4. Relation (28) describes nothing else than a sinusoidal traveling wave of particle displacements (and hence of spring extensions/constrictions), that propagates, depending on the sign before $v_{\mathrm{ph}}$, to the right or to the left along the particle chain with phase velocity

$$
\begin{equation*}
v_{\mathrm{ph}} \equiv \frac{\omega}{k} . \tag{5.29}
\end{equation*}
$$

Perhaps the most important characteristic of a wave is the so-called dispersion relation, i.e. the relation between its frequency $\omega$ and wave number $k$ - essentially between the temporal and spatial frequencies of the wave. For our current system, this relation is given by Eq. (27) with $\alpha \equiv k d$. Taking into account that $\left(2-e^{+i \alpha}-e^{-i \alpha}\right)=2(1-\cos \alpha)=4 \sin ^{2}(\alpha / 2)$, it may be rewritten in a simpler form:

$$
\begin{equation*}
\omega= \pm \omega_{0} \sin \frac{\alpha}{2}= \pm \omega_{0} \sin \frac{k d}{2}, \quad \text { where } \omega_{0} \equiv 2\left(\frac{\kappa}{m}\right)^{1 / 2} \tag{5.30}
\end{equation*}
$$

This result, frequently called the Debye dispersion relation, ${ }^{6}$ is sketched in Fig. 5, and is rather remarkable in several aspects.


Fig. 5.5. The Debye dispersion relation.

First, if the wavelength $\lambda \equiv 2 \pi||k|$ is much larger than the spatial period a of the structure, i.e. if $|k d| \ll 1$ (so that $|\omega| \ll \omega_{0}$ ), the dispersion relation is approximately linear:

$$
\begin{equation*}
\omega= \pm \omega_{0} \frac{k d}{2}= \pm v k \tag{5.31}
\end{equation*}
$$

where parameter $v$ is frequency-independent:

$$
\begin{equation*}
v \equiv \frac{\omega_{0} d}{2}=\left(\frac{\kappa}{m}\right)^{1 / 2} d \tag{5.32}
\end{equation*}
$$

Comparison of Eq. (31) with Eq. (28) shows that this constant plays, in the low-frequency region, the role of phase velocity for any frequency component of a waveform created in the system - say, by initial conditions. As a result, low-frequency waves of arbitrary form can propagate in the system without

[^66]deformation (called dispersion). Such waves are called acoustic, ${ }^{7}$ and are the general property of any elastic continuous medium.

Indeed, the limit $|k d| \ll 1$ means that distance $d$ between adjacent particles is much smaller than wavelength $\lambda=2 \pi /|k|$, i.e. that the differences $q_{j+1}(t)-q_{j}(t)$ and $q_{j}(t)-q_{j-1}(t)$, participating in Eq. (24), are relatively small and may be approximated with $\partial q / \partial j=\partial q / \partial(z / d)=d(\partial q / \partial z)$, with the derivatives taken at middle points between the particles: respectively, $z_{+} \equiv\left(z_{j+1}-z_{j}\right) / 2$ and $z_{-} \equiv\left(z_{j}-z_{j-1}\right) / 2$. Here $z$ in now considered as a continuous argument (and hence the system, as a 1 D continuum), and $q(z, t)$, as a continuous function of space and time. In this approximation, the sum of the last two terms of Eq. (24) is equal to $-\kappa d\left[\partial q / \partial z\left(z_{+}\right)-\partial q / \partial z\left(z_{-}\right)\right]$, and may be similarly approximated by $-\kappa d^{2}\left(\partial^{2} q / \partial z^{2}\right)$, with the second derivative taken at point $\left(z_{+}-z_{-}\right) / 2=z_{j}$, i.e. exactly at the same point as the time derivative. As the result, the ordinary differential equation (24) is reduced to a partial differential equation

$$
\begin{equation*}
m \frac{\partial^{2} q}{\partial t^{2}}-\kappa d^{2} \frac{\partial^{2} q}{\partial z^{2}}=0 \tag{5.33a}
\end{equation*}
$$

Using Eqs. (30) and (32), we may present this equation in a more general form

1D wave equation

$$
\begin{equation*}
\left(\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}-\frac{\partial^{2}}{\partial z^{2}}\right) q(z, t)=0 \tag{5.33b}
\end{equation*}
$$

which describes a scalar acoustic wave (of any physical nature) in a 1D linear, dispersion-free continuum - cf. Eq. (1.2). In our current simple model (Fig. 4), direction $z$ of the wave propagation coincides with the direction of particle displacements $q$; such acoustic waves are called longitudinal. However, in Chapter 7 we will see that 3D elastic media may also support different, transverse waves that also obey Eq. (33b), but with a different acoustic velocity $v$.

Second, when the wavelength is comparable with the structure period $d$ (i.e. the product $k d$ is not small), the dispersion relation is not linear, and the system is dispersive. This means that as a wave, whose Fourier spectrum has several essential components with frequencies of the order of $\omega_{0}$, travels along the structure, its waveform (which may be defined as the shape of a snapshot of all $q_{j}$, at the same time) changes. ${ }^{8}$ This effect may be analyzed by presenting the general solution of Eq. (24) as the sum (more generally, an integral) of components (28) with different complex amplitudes $a$ :

$$
\begin{equation*}
q_{j}(t)=\operatorname{Re} \int_{-\infty}^{+\infty} a_{k} e^{i\left[k z_{j}-\omega(k) t\right]} d k \tag{5.34}
\end{equation*}
$$

This notation emphasizes the dependence of the partial wave amplitudes $a_{k}$ and frequencies on the wave number $k$. While the latter dependence is given by the dispersion relation, in our current case by Eq. (30), function $a_{k}$ is determined by the initial conditions. For applications, the case when $a_{k}$ is substantially different from zero only is a narrow interval, of width $\Delta k \ll k_{0}$ around some central value $k_{0}$, is of special importance. (The Fourier transform reciprocal to Eq. (34) shows that this is true, in particular for a so-called wave packet - a sinusoidal wave modulated by an envelope with a large width

[^67]$\Delta z \sim 1 / \Delta k \gg 1 / k_{0}-$ see Fig. 6.) Using that strong inequality, the wave packet propagation may be analyzed by expending the dispersion relation $\omega(k)$ into the Taylor series at point $k_{0}$, and, in the first approximation in $\Delta k / k_{0}$, restricting the expansion by its first two terms:
\[

$$
\begin{equation*}
\omega(k) \approx \omega_{0}+\left.\frac{d \omega}{d k}\right|_{k=k_{0}} \widetilde{k}, \quad \text { where } \omega_{0} \equiv \omega\left(k_{0}\right), \text { and } \tilde{k} \equiv k-k_{0} . \tag{5.35}
\end{equation*}
$$

\]

In this approximation, Eq. (34) yields

$$
\begin{align*}
q_{j}(t) & \approx \operatorname{Re} \int_{-\infty}^{+\infty} a_{k} \exp \left\{i\left[\left(k_{0}+\widetilde{k}\right) z_{j}-\left(\left.\omega_{0}+\frac{d \omega}{d k} \right\rvert\, k=k_{0} \tilde{k}\right) t\right]\right\} d k \\
& =\operatorname{Re}\left[\exp \left\{i\left(k_{0} z_{j}-\omega_{0} t\right)\right\} \int_{-\infty}^{+\infty} a_{k} \exp \left\{i \tilde{k}\left(\left.z_{j}-\frac{d \omega}{d k} \right\rvert\, k=k_{0} t\right)\right\} d k\right] . \tag{5.36}
\end{align*}
$$

Comparing this expression with the initial form of the wave packet,

$$
\begin{equation*}
q_{j}(0)=\operatorname{Re} \int_{-\infty}^{+\infty} a_{k} e^{i k z_{j}} d k=\operatorname{Re}\left[\exp \left\{i k_{0} z_{j} \int_{-\infty}^{+\infty} \int_{k} \exp \left\{i \widetilde{k} z_{j}\right\} d k\right]\right. \tag{5.37}
\end{equation*}
$$

and taking into account that the phase factors before the integrals in the last forms of Eqs. (36) and (37) do not affect its envelope, we see that in this approximation ${ }^{9}$ the envelope sustains its initial form and propagates along the system with the so-called group velocity

$$
\begin{equation*}
\left.v_{\mathrm{gr}} \equiv \frac{d \omega}{d k}\right|_{k=k_{0}} \tag{5.38}
\end{equation*}
$$

Note that, with the exception of the acoustic wave limit (31), this velocity (that characterizes the propagation of waveform's envelope), is different from the phase velocity (28) that describes the propagation of the "carrier" sine wave - for example, one of its zeros - see Fig. 6.


Fig. 5.6. Phase and group velocities of a wave packet.

Next, at the Debye dispersion law (30), the difference between $v_{\mathrm{ph}}$ and $v_{\mathrm{gr}}$ increases as the average frequency $\omega$ approaches $\omega_{0}$, with the group velocity tending to zero, while the phase velocity staying virtually constant. The existence of such a maximum for the wave propagation frequency

[^68]presents one more remarkable feature of this system. It physics may be readily understood by noticing that according to Eq. (30), at $\omega=\omega_{0}$, the wave number $k$ equals $n \pi / d$, where $n$ is an odd integer, and hence the phase shift $\alpha \equiv k d$ is an odd multiple of $\pi$. Plugging this value into Eq. (28), we see that at the Debye frequency, oscillations of two adjacent particles are in anti-phase, for example:
\[

$$
\begin{equation*}
q_{0}(t)=a \exp \{-i \omega t\}, \quad q_{1}(t)=a \exp \{i(\pi-\omega t)\}=-a \exp \{-i \omega t\}=-q_{0}(t) \tag{5.39}
\end{equation*}
$$

\]

It is clear from Fig. 4 that at such phase shift, all the springs are maximally stretched/compressed (just as in the hard mode of the two coupled oscillators analyzed in Sec. 1), so that it is natural that this mode has the highest frequency.

This invites a natural question what happens with the system if it is excited at a frequency $\omega>$ $\omega_{0}$, say by an external force applied at the system's boundary. While the boundary phenomena will be considered in the next section, the most essential part of the answer may be obtained immediately from Eqs. (26) and (30). Indeed, reviewing the calculations that have led to these results, we see that they are valid not only for real but also any complex values of $\alpha$. In particular, at $\omega>\omega_{0}$ the dispersion relation (30) gives

$$
\begin{equation*}
\alpha=n \pi \pm i \frac{d}{\Lambda}, \quad \text { where } \Lambda \equiv \frac{d}{2 \cosh ^{-1}\left(\omega / \omega_{0}\right)} \tag{5.40}
\end{equation*}
$$

Plugging this relation into Eq. (26), we see that the wave's amplitude becomes an exponential function of position:

$$
\begin{equation*}
\left|q_{j}\right|=|a| e^{ \pm j \operatorname{Im} \alpha} \propto e^{ \pm z_{j} / \Lambda} . \tag{5.41}
\end{equation*}
$$

Physically this means that the wave decays penetrating into the structure (from the excitation point), dropping by a factor of $e \approx 3$ on the so-called penetration depth $\Lambda$. (According to Eq. (40), this depth decreases with frequency, but rather slowly, always remaining of the order of the distance between the adjacent particles.) Such a limited penetration is a very common property of various waves, including the electromagnetic waves in plasmas and superconductors, and quantum-mechanical "de Broglie waves" (wavefunctions) in the classically-forbidden regions. Note that this effect of "wave expulsion" from the media they cannot propagate in does not require any energy dissipation.

Finally, one more fascinating feature of the dispersion relation (30) is that if it is satisfied by some wave number $k_{0}(\omega)$, it is also satisfied at any $k_{n}(\omega)=k_{0}(\omega)+2 \pi n / d$, where $n$ is any integer. This property is independent of the particular dynamics of the system: it follows already from Eq. (27), before its substitution into Eq. (25), because such a wave number translation by $2 \pi / d$, i.e. the addition of $2 \pi$ to phase shift $\alpha$, is equivalent to the multiplication of $q_{j}(t)$ by $\exp \{i 2 \pi\}=1$. Thus, such $(2 \pi / d)$ periodicity in the wave number space is a common property of all systems that are $d$-periodic in the usual ("direct") space. ${ }^{10}$

Besides dispersion, one more key characteristic of any wave-supporting system is its wave impedance - the notion strangely missing from many physics (but not engineering) textbooks. It may be

[^69]revealed by calculating the forces in the sinusoidal wave (28). For example, the force exerted by $j$-th particle on its right neighbor, given by the second term in Eq. (24), equals
\[

$$
\begin{equation*}
F_{j+}(t)=\kappa\left[q_{j}(t)-q_{j+1}(t)\right]=\operatorname{Re}\left[\kappa\left(1-e^{i k d}\right) a e^{i\left(k z_{j} \mp \omega t\right)}\right] \rightarrow \operatorname{Re}\left[-i k d \kappa a e^{i\left(k z_{j} \mp \omega t\right)}\right], \tag{5.42}
\end{equation*}
$$

\]

where the last form is valid in the most important acoustic wave limit, $k d \rightarrow 0$. Let us compare this expression for the wave of forces with that for the corresponding wave of particle velocities:

$$
\begin{equation*}
\dot{q}_{j}(t)=\operatorname{Re}\left[\mp i \omega a e^{i\left(k z_{j} \mp \omega t\right)}\right] . \tag{5.43}
\end{equation*}
$$

We see that these two waves have the same phase, and hence their ratio does not depend on either time or the particle number. Moreover, this ratio,

$$
\begin{equation*}
\frac{F_{+}}{\dot{q}}= \pm \frac{k d \kappa}{\omega}= \pm \frac{d \kappa}{v}= \pm Z \tag{5.44}
\end{equation*}
$$

is a real constant independent even on wave's frequency. Its magnitude is called the wave impedance:

$$
\begin{equation*}
Z \equiv \frac{d \kappa}{v}=(\kappa m)^{1 / 2} \tag{5.45}
\end{equation*}
$$

and characterizes the dynamic "stiffness" of the system for the propagating waves.
In particular, the impedance scales the power carried by the wave. Indeed, the direct time averaging of the instantaneous power $\mathcal{P}_{j}(t) \equiv F_{j}(t) d q_{j} / d t$ transferred through particle $j$ to the subsystem on the right of it, using Eqs. (42)-(43), yields a position-independent result

$$
\begin{equation*}
\overline{P_{j}} \equiv \overline{\left[F_{j}(t) \dot{q}_{j}(t)\right]_{ \pm}}= \pm \frac{\omega^{2} Z}{2} a a^{*} \equiv \pm \frac{\omega^{2} Z}{2} A^{2} \tag{5.46}
\end{equation*}
$$

where $A \equiv|a|$ is the real amplitude of the wave, and, as before, the positive sign corresponds to the wave propagating to the right (and vice versa). Note that $\mathcal{P}$ is the power flow in the acoustic wave, and its spatial and temporal independence means that wave's energy is conserved - as could be expected from our Hamiltonian system we are considering. ${ }^{11}$ Hence, the wave impedance $Z$ characterizes the energy transfer along the system rather than its dissipation.

### 5.4. Interfaces and boundaries

The importance of the wave impedance notion becomes even more evident when we consider waves in non-uniform and finite-size systems. Indeed, our previous analysis assumed that the 1D system supporting the waves (Fig. 4) is exactly periodic, i.e. macroscopically uniform, and extends all the way from $-\infty$ to $+\infty$. Now let us examine what happens when this is not true. The simplest (and very important) example of such nonuniform systems is an interface, i.e. a point at which system parameters experience a change. Figure 7 shows a simple and representative example of such a sharp interface, for the same 1D wave system that was analyzed in the last section.

[^70]

Fig. 5.7. 1D system with a sharp interface at $z=0$, and the wave components at the partial reflection of a wave incident from the left.

Since the parameters $\kappa$ and $m$ are still constant on each side of the interface (put, for convenience, at $z_{j}=0$ ), equations of motion (24) are is still valid for $j<0$ and $j>0$ (in the latter case, with the primed parameters), and show that at a fixed frequency $\omega$, they can sustain sinusoidal waves of the type (28). However, the final jump of parameters at the interface ( $m^{\prime} \neq m, \kappa^{\prime} \neq \kappa$ ) leads to a partial reflection of the incident wave from the interface, so that at least on the side of incidence (say, $z_{j} \leq 0$ ), we need to assume two such waves, one describing the incident wave and another, the reflected wave:

$$
q_{j}(t)=\operatorname{Re} \begin{cases}a_{\rightarrow} e^{i\left(k z_{j}-\omega t\right)}+a_{\leftarrow} e^{i\left(-k z_{j}-\omega t\right)}, & \text { for } j \leq 0,  \tag{5.47}\\ a_{\rightarrow}^{\prime} e^{i\left(k^{\prime} z_{j}-\omega t\right)}, & \text { for } j \geq 0 .\end{cases}
$$

In order to obtain boundary conditions for "stitching" these waves (i.e. getting relations between their complex amplitudes) at $j=0$, i.e. $z_{j}=0$, we need to take into account, first, that displacement $q_{0}(t)$ of the interface particle has to be the same whether it is considered a part of the left or right sub-system, and hence participates in Eqs. (24) for both $j \leq 0$ and $j \geq 0$. This gives us the first boundary condition,

$$
\begin{equation*}
a_{\rightarrow}+a_{\leftarrow}=a_{\rightarrow}^{\prime} . \tag{5.48}
\end{equation*}
$$

Second, writing the equation of motion for the special particle with $j=0$,

$$
\begin{equation*}
m_{0} \ddot{q}_{0}-\kappa^{\prime}\left(q_{1}-q_{0}\right)+\kappa\left(q_{0}-q_{-1}\right)=0 . \tag{5.49}
\end{equation*}
$$

and plugging into it the solution (47), we get the second boundary condition

$$
\begin{equation*}
-\omega^{2} m_{0} a_{\rightarrow}^{\prime}-\kappa^{\prime} a_{\rightarrow}^{\prime}\left(e^{i k^{\prime} d}-1\right)+\kappa\left[a_{\rightarrow}\left(1-e^{-i k d}\right)+a_{\leftarrow}\left(1-e^{i k d}\right)\right]=0 . \tag{5.50}
\end{equation*}
$$

The system of two linear equations (48) and (50) allows one to express both $a_{\leftarrow}$ and $a^{\prime}{ }_{\rightarrow}$ via amplitude $a_{\rightarrow}$ of the incident wave, and hence find the reflection $(R)$ and transmission $(T)$ coefficients of the interface: ${ }^{12}$

$$
\begin{equation*}
R \equiv \frac{a_{\leftarrow}}{a_{\rightarrow}}, \quad T \equiv \frac{a_{\rightarrow}^{\prime}}{a_{\rightarrow}} . \tag{5.51}
\end{equation*}
$$

The general result for $R$ and $T$ is a bit bulky, but may be simplified in the most important acoustic wave limit: $k^{\prime} d, k d \rightarrow 0$. Indeed, in this limit all three parentheses participating in Eq. (50) may be approximated by the first terms of their Taylor expansions, e.g., $\exp \{i k ' d\}-1 \approx i k ' d$, etc. Moreover, in this limit, the first term of Eq. (50) is of the second order in small parameter $\omega / \omega_{0} \sim k a \ll 1$ (unless the

[^71]interface particle mass $m_{0}$ is much larger than both $m$ and $m$ '), and hence may be neglected. As a result, Eq. (50) takes a very simple form ${ }^{13}$
\[

$$
\begin{equation*}
\kappa k\left(a_{\rightarrow}-a_{\leftarrow}\right)=\kappa^{\prime} k^{\prime} a_{\rightarrow}^{\prime} . \tag{5.52a}
\end{equation*}
$$

\]

According to Eqs. (31), (32) and (45), in the acoustic limit the ratio of factors $\kappa k$ of the waves (with the same frequency $\omega$ !) propagating at $z<0$ and $z>0$ is equal to that of the wave impedances $Z$ of the corresponding parts of the system, so that Eq. (52a) may be rewritten as

$$
\begin{equation*}
Z\left(a_{\rightarrow}-a_{\leftarrow}\right)=Z^{\prime} a_{\rightarrow}^{\prime} . \tag{5.52b}
\end{equation*}
$$

Now, solving the simple system of linear equations (48) and (52a), we get very important formulas,

$$
\begin{equation*}
R=\frac{Z-Z^{\prime}}{Z+Z^{\prime}}, \quad T=\frac{2 Z}{Z+Z^{\prime}}, \tag{5.53}
\end{equation*}
$$

which are valid for any waves in 1D continua - with the corresponding re-definition of impedance. ${ }^{14}$ Note that coefficients $R$ and $T$ characterize the ratios of wave amplitudes rather than their power. Using Eq. (46), for the time-averaged power flows we get relations

$$
\begin{equation*}
\frac{\mathcal{P}_{\leftarrow}}{\mathcal{P}_{\rightarrow}}=\left(\frac{Z-Z^{\prime}}{Z+Z^{\prime}}\right)^{2}, \quad \frac{P_{\rightarrow}^{\prime}}{\mathcal{P}_{\rightarrow}}=\frac{4 Z Z^{\prime}}{\left(Z+Z^{\prime}\right)^{2}} . \tag{5.54}
\end{equation*}
$$

(Note that $\mathcal{P}_{\leftarrow}+\mathcal{P}_{\rightarrow}^{\prime}{ }_{\rightarrow}=\mathcal{P}_{\rightarrow}$, again reflecting the energy conservation.)
The first important result of this calculation that wave is fully transmitted through the interface if the so-called impedance matching condition $Z^{\prime}=Z$ is satisfied, even if the wave velocities $v(32)$ are different on the left and the right sides of the interface. On the contrary, the equality of the acoustic velocities in two media does not guarantee the full transmission of their interface. Again, this is a very general result.

Now let us consider the two limits in which Eq. (53) predicts a total wave reflection, $\mathcal{P}_{\leftarrow} / \mathcal{P}_{\rightarrow} \rightarrow$ $0: Z^{\prime} / Z \rightarrow \infty$ (when $R=-1$ ) and $Z^{\prime} / Z \rightarrow 0$ (when $R=1$ ). According to Eq. (45), the former limit corresponds to the infinite product $\kappa^{\prime} m^{\prime}$, so that particles on the right side of the interface cannot move at all. This means that this particular case also describes a perfectly rigid boundary (Fig. 8a) for arbitrary $\omega$, i.e. not necessarily in the acoustic wave limit. The negative sign of $R$ in the relation $R=-1$ means that in the reflected wave, the phase of particle oscillations is shifted by $\pi$ relative to the initial wave, $a=a_{\leftarrow}$ $=-a_{\rightarrow}$, so that the sum of these two traveling waves may be also viewed as a single standing wave

$$
\begin{equation*}
q_{j \leq 0}(t)=\operatorname{Re}\left[a e^{i\left(k z_{j}-\omega t\right)}-a e^{i\left(-k z_{j}-\omega t\right)}\right]=\operatorname{Re}\left[2 i a e^{-i \omega t} \sin k z_{j}\right]=2 A \sin (\omega t-\varphi) \sin k z_{j} \tag{5.55}
\end{equation*}
$$

where $a \equiv a_{\rightarrow}=A e^{i \varphi}$. At the boundary $\left(z_{j}=0\right)$ this expression yields $q_{0}(t) \equiv 0$, i.e., a node of particle displacements. On the contrary, the corresponding standing wave of spring forces, described by Eq. (42), has a maximum at $z=0$.

[^72]A similar standing wave forms in the opposite limit $Z^{\prime} / Z \rightarrow 0$, that describes an "open" boundary shown in Fig. 8b. However, in this limit (with $R=+1$ ), the standing wave of displacements has a maximum at $z_{j}=0$,

$$
\begin{equation*}
q_{j \leq 0}(t)=\operatorname{Re}\left[a e^{i\left(k z_{j}-\omega t\right)}+a e^{i\left(-k z_{j}-\omega t\right)}\right]=\operatorname{Re}\left[2 a e^{-i \omega t} \cos k z_{j}\right]=2 A \cos (\omega t-\varphi) \cos k z_{j} \tag{5.56}
\end{equation*}
$$

while the corresponding wave of forces has a node at that point. Most importantly, for both boundaries shown in Fig. 8, the standing waves are formed at any ratio $\omega / \omega_{0}$.

(a)

Fig. 5.8. (a) Rigid and (b) open
(b) boundaries of a 1D chain.

If the opposite boundary of a finite-length chain also provides a total wave reflection, the system may only support standing waves with certain wave numbers $k_{n}$, and hence certain eigenfrequencies $\omega_{n}$ that may be found from the set of $k_{n}$ and the dispersion relation $\omega_{n} \equiv \omega\left(k_{n}\right)$, in our case given by Eq. (30). For example, if both boundaries of a chain with length $L$ are rigid (Fig. 8a), then the standing wave (54) should have nodes at them both, giving the wave number quantization condition ${ }^{15}$

$$
\begin{equation*}
\sin k_{n} L=0, \quad \text { i.e. } k_{n}=\frac{\pi n}{L}, \tag{5.57a}
\end{equation*}
$$

where $n$ is an integer. In order to count the number of different modes in a chain with a finite number $N$ of oscillating particles, let us take into account, first, that adding one period $\Delta k=2 \pi / d$ of the dispersion relation to any $k_{n}$ leads to the same mode. Moreover, changing the sign of $k_{n}$ in standing wave (55) is equivalent to changing the sign of its amplitude. Hence, there are only $N$ different modes, for example with

$$
\begin{equation*}
n=1,2, \ldots, N, \quad \text { i.e. } k_{n}=\frac{\pi}{L}, 2 \frac{\pi}{L}, \ldots, N \frac{\pi}{L} . \tag{5.57b}
\end{equation*}
$$

This fact is of course just a particular case of the general result obtained in Sec. 2.
According to Eq. (56), if both boundaries are open (Fig. 8b), the oscillation modes are different, but their wave numbers form the same set (57). Finally, if the types of boundary conditions on the chain's ends are opposite, the wave number set is somewhat different,

$$
\begin{equation*}
k_{n}=\frac{\pi}{L}\left(n-\frac{1}{2}\right) \tag{5.58}
\end{equation*}
$$

15 This result should be very familiar to the reader from freshmen-level "guitar string"-type problems. Note, however, that Eqs. (54)-(56) are valid not only for continuous 1D systems like a string, but also for (uniform) chains with a finite and arbitrary number $N$ of particles - the fact we will use below.
but since the distance between the adjacent values of $k_{n}$ is still the same $(\pi / N d)$, the system still has exactly $N$ such values within each period $2 \pi / d$ of the dispersion law, and hence, again, exactly $N$ different oscillation modes.

This insensitivity of the number of modes and their equal spacing (called equidistance) on the $k$ axis, enables the following useful (and very popular) trick. In many applications, it is preferable to speak about the number of different traveling, rather than standing waves in a system of a large but finite size, with coordinates $z_{0}$ and $z_{N}$ describing the same particle. One can plausibly argue that the local dynamics of the chain of $N \gg 1$ particles should not be affected if it is gradually bent into a large closed loop of length $L=N d \gg d$. Such a loop may sustain traveling waves, if they satisfy the following periodic Born-Karman condition: $q_{0}(t) \equiv q_{N}(t)$. (A popular vivid image is that the wave "catches its own tail with its teeth".) According to Eq. (27), this condition is equivalent to

$$
\begin{equation*}
e^{i k_{n} L}=1, \quad \text { i.e. } k_{n}=\frac{2 \pi}{L} n \tag{5.59}
\end{equation*}
$$

This equation gives a set of wave numbers twice more sparse than that described by Eqs. (57). However, now we can use $N$ values of $n$, giving $k_{n}$, for example, from $-N$ to $+N$ (strictly speaking, excluding one of the boundary values to avoid double counting of the identical modes with $n= \pm N$ ), because traveling waves (28) with equal but opposite values of $k_{n}$ propagate in opposite directions and hence present different modes. As a result, the total number of different traveling-wave modes is the same $(N)$ as that of different standing-wave modes, and they are similarly (uniformly) distributed along the wave number axis. Since for $N \gg 1$ the exact values of $k_{n}$ are not important, the Born-Carman boundary conditions and the resulting set (59) of wave numbers are frequently used even for multidimensional systems whose bending into a ring along each axis is hardly physically plausible.

### 5.5. Dissipative, parametric, and nonlinear phenomena

In conclusion, let us discuss more complex effects in oscillatory systems with more than one degree of freedom. Starting from linear systems, energy dissipation may be readily introduced, just as for a single oscillator, by adding terms proportional to $\eta_{j} \dot{q}_{j}$, to the equations of motion such as Eqs. (5), (17), or (24). In arbitrary case, viscosity coefficients $\eta_{j}$ are different for different particles; however, in many uniform systems like that shown in Fig. 4, the coefficients are naturally equal, turning Eq. (24) into

$$
\begin{equation*}
m \ddot{q}_{j}+\eta \dot{q}_{j}-\kappa\left(q_{j+1}-q_{j}\right)+\kappa\left(q_{j}-q_{j-1}\right)=0 . \tag{5.60}
\end{equation*}
$$

In the most important limit of acoustic waves, we may now repeat the arguments that have led to the wave equation (33) to get its generalization

$$
\begin{equation*}
\left(\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}+\frac{2 \delta}{v^{2}} \frac{\partial}{\partial t}-\frac{\partial^{2}}{\partial z^{2}}\right) q(z, t)=0, \quad \text { with } \delta \equiv \frac{\eta}{2 m} . \tag{5.61}
\end{equation*}
$$

Such dissipative equation may describe two major particular effects. First, it describes the decay in time of the standing waves in an autonomous wave system (say, of a finite length $L$ ) that have been caused by some initial push, described by non-trivial initial conditions, say, $q(z, 0) \neq 0$. In order to analyze these decaying oscillations, one may look for the solution of Eq. (61) in the form of a sum of standing wave modes (that satisfy the given boundary conditions), each with its own, time-dependent


amplitude $A_{n}(t)$. For example, for rigid boundary conditions $(q=0)$ at $z=0$ and $z=L$, we can use Eq. (55) as a hint to write

$$
\begin{equation*}
q(z, t)=\sum_{n=1}^{N} A_{n}(t) \sin k_{n} z, \tag{5.62}
\end{equation*}
$$

where the set of $q_{n}$ is given by Eq. (57). Plugging this solution into Eq. (61), ${ }^{16}$ we get

$$
\begin{equation*}
\frac{1}{v^{2}} \sum_{n=1}^{N}\left(\ddot{A}_{n}+2 \delta \dot{A}_{n}+\omega_{n}^{2} A_{n}\right) \sin k_{n} z=0, \quad \text { with } k_{n}=\frac{\pi}{L} n . \tag{5.63}
\end{equation*}
$$

Since functions $\sin k_{n} z$ are mutually orthogonal, Eq. (63) may be only satisfied if all $N$ expressions in parentheses are equal to zero. As the result, the amplitude of each mode satisfies an ordinary differential equation absolutely similar to that studied in Sec. 4.1, with a similar solution describing the free oscillation decay with the relaxation constant (4.23). Here the wave character of the system gives nothing new, besides that different modes have different $Q$-factors: $Q_{n}=\omega_{n} / 2 \delta$.

More wave-specific is a different situation when the waves are due to their persisting excitation by some actuator at one of the ends (say, $z=0$ ) of a very long structure. In this case, an initial transient process settles to a wave with a time-independent waveform limited by certain envelope $A(z)$ that decays at $z \rightarrow \infty$. In order to find the envelope, for the simplest case of sinusoidal excitation of frequency $\omega$, one may look for a particular solution to Eq. (61) in a form very different from Eq. (60):

$$
\begin{equation*}
q(z, t)=\operatorname{Re}\left[a(z) e^{-i \omega t}\right] \tag{5.64}
\end{equation*}
$$

generally with complex $a(z)$. Plugging this solution into Eq. (61), we see that this is indeed a valid solution, provided that $q(0, t)=a(0) \exp \{-i \omega t\}$ satisfies the boundary condition (now describing the wave excitation), and $a(z)$ obeys an following ordinary differential equation that describes wave's evolution in space rather than in time: ${ }^{17}$

$$
\begin{equation*}
\left(\frac{d^{2}}{d z^{2}}+k^{2}\right) a=0, \quad \text { with } k^{2} \equiv\left(\frac{\omega}{v}\right)^{2}+2 i \frac{\delta \omega}{v^{2}} . \tag{5.65}
\end{equation*}
$$

The general solution to such differential equation is

$$
\begin{equation*}
a(x)=a_{+} e^{i k z}+a_{-} e^{-i k z} \tag{5.66}
\end{equation*}
$$

with $k$ now having both real and imaginary parts, $k=k^{\prime}+i k^{\prime \prime}$, so that the wave (64) is

$$
\begin{equation*}
q(z, t)=a_{+} e^{i\left(k^{\prime} z-\omega t\right)} e^{-k^{\prime \prime} z}+a_{-} e^{i\left(-k^{\prime} z-\omega t\right)} e^{k^{\prime \prime} z} . \tag{5.67}
\end{equation*}
$$

If our boundary conditions correspond to the wave propagating to the right, we have to keep only the first term of this expression, with positive $k$ ". The first exponent of that term describes the wave propagating from the boundary into the system (at low damping, with velocity virtually equal to $v$ ), while the second exponent describes an exponential decay of the wave's amplitude in space:

[^73]\[

$$
\begin{equation*}
A(z) \equiv|a(z)|=A(0) e^{-\alpha z / 2}, \quad \frac{\alpha}{2} \equiv-k^{\prime \prime} \approx \frac{\delta}{v} \tag{5.68}
\end{equation*}
$$

\]

where the last, approximate relation is valid in the weak damping limit ( $\delta \ll \omega$, i.e. $\delta / v \ll k^{\prime}$ ). Constant $\alpha$ is called the attenuation coefficient, and in more general wave systems may depend on frequency $\omega$. Physically, $2 / \alpha$ is the scale of wave penetration into a dissipative system. ${ }^{18}$ Note that our simple solution (68) is only valid if the system length $L$ is much larger than $2 / \alpha$; otherwise we would need to use the second term in Eq. (67) to describe wave reflection from the second end.

Now let me discuss (because of the lack of time, on a semi-quantitative level only), nonlinear and parametric phenomena in oscillatory systems with more than one degree of freedom. One important new effect here is the mutual phase locking of (two or more) weakly coupled self-excited oscillators with close frequencies: if the eigenfrequencies of the oscillators are sufficiently close, their oscillation frequencies "stick together" to become exactly equal. Though its dynamics of this process is very close to that of the phase locking of a single oscillator by external signal, that was discussed in Sec. 4.4, it is rather counter-intuitive in the view of the results of Sec. 1, and in particular the anticrossing diagram shown in Fig. 2. The analysis of the effect using the rotating-wave approximation (that is highly recommend to the reader) shows that the origin of the difference is oscillator's nonlinearity, which makes oscillation amplitude virtually independent of phase evolution - see Eq. (4.68) and its discussion.

One more new effect is the so-called non-degenerate parametric excitation. It may be illustrated of the example of just two coupled oscillators - see Sec. 1 above. Let us assume that the coupling constant $\kappa$, participating in Eqs. (5), is not constant, but oscillates in time - say with frequency $\omega_{p}$. In this case the forces acting on each oscillator from its counterpart, described by the right-hand parts of Eqs. (5), will be proportional to $\kappa q_{2,1}\left(1+\mu \cos \omega_{p} t\right)$. Assuming that oscillations of $q_{1}$ and $q_{2}$ are close to sinusoidal, with frequencies $\omega_{1,2}$, we see that the force acting on each oscillator will contain the socalled combinational frequencies

$$
\begin{equation*}
\omega_{p} \pm \omega_{2,1} \cdot \tag{5.69}
\end{equation*}
$$

If one of these frequencies in the right-hand part of each equation coincides with its own oscillation frequency, we can expect a substantial parametric interaction between the oscillators (on the top of the constant coupling effects discussed in Sec. 1). According to Eq. (69), this may happen in two cases:

$$
\begin{equation*}
\omega_{p}=\omega_{1} \pm \omega_{2} \tag{5.70}
\end{equation*}
$$

The quantitative analysis (also highly recommended for reader's exercise) shows that in the positive sign case, the parameter modulation indeed leads to energy "pumping" into oscillations. As a result, sufficiently large $\mu$, at sufficiently low damping coefficients $\delta_{1,2}$ and effective detuning

$$
\begin{equation*}
\xi \equiv \omega_{p}-\left(\Omega_{1}+\Omega_{2}\right), \tag{5.71}
\end{equation*}
$$

may lead to the simultaneous excitation of two frequency components $\omega_{1,2}$. These frequencies, while being close to corresponding eigenfrequencies of the system, are related to the pumping frequency $\omega_{p}$ by exact relation (70), but otherwise are arbitrary, e.g., incommensurate (Fig. 9a), thus justifying the term

[^74]non-degenerate parametric excitation. (The parametric excitation of a single oscillator, that was analyzed in Sec. 4.5, is a particular, degenerate case of such excitation, with $\omega_{1}=\omega_{2}=\omega_{p} / 2$.) On the other hand, for the case described by Eq. (70) with the negative sign, parameter modulation always pumps energy from the oscillations, effectively increasing system's damping.

Somewhat counter-intuitively, this difference between two cases (70) may be simpler interpreted using the notions of quantum mechanics. Namely, equality $\omega_{p}=\omega_{1}+\omega_{2}$ enables a decay of an external photon of energy $\hbar \omega_{p}$ into two photons of energies $\hbar \omega_{1}$ and $\hbar \omega_{2}$ going into the oscillatory system. (The complementary relation, $\omega_{1}=\omega_{p}+\omega_{2}$, results in the oscillation photon decay.)
(a)



Fig. 5.9. Spectra of oscillations at (a) the non-degenerate parametric excitation, and (b) fourwave mixing. The arrow directions symbolize the power flows into and out of the system.

Proceeding to nonlinear phenomena, let us note, first of all, that the simple reasoning, that accompanied Eq. (4.109), is also valid in the case when oscillations consist of two (or more) sinusoidal components with incommensurate frequencies. Replacing notation $2 \omega$ for $\omega_{p}$, we see that nondegenerate parametric excitation of the type (70a) is possible to implement in a system of two coupled oscillators with a quadratic nonlinearity (of the type $\gamma q^{2}$ ), "pumped" by an intensive external signal at frequency $\omega_{p} \approx \Omega_{1}+\Omega_{2}$. In optics, it is often more convenient to have all signals within the same, relatively narrow frequency range. A simple calculation, similar to the one made in Eqs. (4.108)-(4.109), shows that this may be done using the cubic nonlinearity ${ }^{19}$ of the type $\alpha q^{3}$, which allows the similar parametric energy exchange at frequency relation (Fig. 9b)

Four-
wave mixing

$$
\begin{equation*}
2 \omega=\omega_{1}+\omega_{2}, \quad \text { with } \omega \approx \omega_{1} \approx \omega_{2} \tag{5.72a}
\end{equation*}
$$

This process is often called the four-wave mixing (FWM), because it may be interpreted quantum-mechanically as the transformation of two externally-delivered photons, each with energy $\hbar \omega_{p}$, into two other photons of energies $\hbar \omega_{1}$ and $\hbar \omega_{2}$. Word "wave" in this term stems from the fact that at optical frequencies, it is hard to couple a sufficient volume of a nonlinear medium with lumped-type resonators. It is easier to implement the parametric excitation of light (as well as other nonlinear phenomena like the higher harmonic generation) in distributed systems of a linear size much larger than the involved wavelengths. In such systems, the energy transfer from the incoming wave of frequency $\omega$ to generated waves of frequencies $\omega_{1}$ and $\omega_{2}$ is gradually accumulated at their joint propagation along the system. From the analogy between Eq. (65) (describing the evolution of wave's amplitude in space), and the usual equation of the harmonic oscillator (describing its evolution in time), it is clear that this

[^75]energy transfer accumulation requires not only the frequencies $\omega$, but also wave numbers $k$ be in similar relations. For example, the four-wave mixing requires that not only the frequency balance (72a), but also a similar relation
\[

$$
\begin{equation*}
2 k=k_{1}+k_{2}, \tag{5.72b}
\end{equation*}
$$

\]

to be exactly fulfilled. Since all three frequencies are close, this is easy to arrange if the dispersion relation $\omega(k)$ of the media is not too steep. Unfortunately, due to the lack of time/space, for more discussion of this interesting subject, nonlinear optics, I have to refer the reader to special literature. ${ }^{20}$

Note that even if the frequencies $\omega_{1}$ and $\omega_{2}$ of the parametrically excited oscillations are incommensurate, the oscillations are highly correlated. Indeed, the quantum mechanical theory of this effect ${ }^{21}$ shows that the generated photons are entangled. This fact makes the parametric excitation very popular for a broad class of experiments in several currently active fields including quantum computation and encryption, and Bell inequality / local reality studies. ${ }^{22}$

It may look like a dispersion-free media, with $\omega / k=v=$ const, is the perfect solution for arranging the parametric interaction of waves, because in such media, for example, Eq. (72b) automatically follows from Eq. (72a). However, in such media not only the desirable three parametrically interacting waves, but also all their harmonics, have the same velocity. At these conditions, energy transfer rates between all harmonics are of the same order. Perhaps the most important result of such multi-harmonic interaction is that intensive waves, interacting with nonlinear media, may develop sharply non-sinusoidal waveforms, in particular those with an almost instant change of the field at a certain moment. Such shock waves, especially those of mechanical nature, present large interest for certain applications - some not quite innocent, e.g., the explosion of usual and nuclear bombs. I will only briefly return to shock waves in Sec. 8.5. ${ }^{23}$

### 5.6. Exercise problems

5.1. For the system of two elastically coupled pendula, confined to a vertical plane, with the parameters shown in Fig. on the right (cf. Problem 1.3), find possible frequencies of small sinusoidal oscillations and the corresponding distribution coefficients. Sketch the oscillation modes.

5.2. The same task as in Problem 1, for the double pendulum, confined to the vertical plane containing the support point (considered in Problem 2.1), with $m^{\prime}=m$ and $l=l^{\prime}$ - see Fig. on the right.


[^76]5.3.* The same tasks as in Problem 5.1, for the triple pendulum shown in Fig. on the right, with the motion confined to a vertical plane containing the support point.

Hint: You may use any (e.g., numerical) method to calculate the characteristic equation roots.
5.4. ${ }^{*}$

(i) Explore an approximate way to analyze waves in a continuous 1D system with parameters slowly varying along its length. ${ }^{24}$
(ii) Apply this method to calculate eigenfrequencies of transverse standing waves on a freely hanging heavy rope of length $L$, with constant mass per unit length - see Fig. on the right.
(iii) For three lowest standing wave modes, compare the results with those obtained in the solution of Problem 5.3 for the triple pendulum.

5.5. The same tasks as in Problem 1, for a linear, symmetric system of 3 particles, shown in Fig. on the right. Assume that the connections between the particles not only act as usual elastic springs (as described by their potential energies $U=\kappa \widetilde{l}^{2} / 2$ ), but also resist system's bending, giving an additional potential energy $U^{\prime}=\kappa^{\prime} l^{2} \theta^{2} / 2$, where $\theta$ is the (small) bending angle. ${ }^{25}$
5.6. Three similar beads, which may slide along a circle of radius $R$ without friction, are connected with similar springs with elastic constants $\kappa$ and equilibrium lengths $l_{0}$ - see Fig. on the right. Analyze stability of the symmetric stationary state of the system, and calculate the frequencies and modes of its small oscillations about this state.

5.7. An external force $F(t)$ is applied to the right particle of system of shown in Fig. 5.1 of the lecture notes, with $\kappa_{L}=\kappa_{R}=\kappa^{\prime}$ and $m_{1}=m_{2} \equiv m$ (see Fig. on the right), and the response $q_{1}(t)$ of the left particle to this force is being measured.

5.8. Calculate the spatial distributions of the kinetic and potential energies in a standing, sinusoidal, 1D acoustic wave, and analyze its evolution in time.

[^77]5.9. Calculate the dispersion law $\omega(k)$ and the maximum frequency of small longitudinal waves in an infinite line of similar, spring-coupled pendula - see Fig. on the right.

5.10. Calculate and analyze the dispersion relation $\omega(k)$ for longitudinal waves in an infinite 1D chain of coupled oscillators with alternating masses - see Fig. on the right. In particular, find and discuss dispersion relation's period $\Delta k$.

5.11. Calculate the longitudinal wave reflection from a "point inhomogeneity": a single particle with a different mass $m_{0} \neq m$, in an otherwise uniform 1D chain see Fig. on the right. Analyze the result.

5.12.* Use the rotating-wave approximation to analyze the mutual phase locking of two weakly coupled self-oscillators with the dissipative nonlinearity, for the cases of:
(i) direct coordinate coupling, described by Eq. (5.5) of the lecture notes, and
(ii) linear but otherwise arbitrary coupling of two similar oscillators.
5.13.* Extend the second task of the previous problem to the mutual phase locking of $N$ similar oscillators. In particular, explore the in-phase mode's stability for the case of the so-called global coupling via a single force $F$ contributed equally by all oscillators.
5.14.* Find the condition of non-degenerate parametric excitation in a system of two coupled oscillators, described by Eqs. (5) with time-dependent coupling: $\kappa \rightarrow \kappa\left(1+\mu \cos \omega_{p} t\right)$, with $\omega_{p} \approx \Omega_{1}+$ $\Omega_{2}$, and $\Omega_{2}-\Omega_{1} \gg k / m$.

Hint: Assuming the modulation depth $\mu$, static coupling $\kappa$, and detuning $\xi \equiv \omega_{p}-\left(\Omega_{1}+\Omega_{2}\right)$ sufficiently small, use the rotating-wave approximation for each of the coupled oscillators.
5.15. Show that the cubic nonlinearity of the type $\alpha q^{3}$ indeed enables the parametric interaction ("four-wave mixing") of oscillations with incommensurate frequencies related by Eq. (72a).

## Chapter 6. Rigid Body Motion

This chapter discusses the motion of rigid bodies, with a focus on their rotation. Some byproduct results of this analysis will enable us to discuss, in the end of the chapter, the description of motion of point particles in non-inertial reference frames.

### 6.1. Angular velocity vector

Our study of 1D waves in the past chapter has prepared us to for a discussion of 3D systems of particles. We will start it with a (relatively :-) simple limit when the changes of distances $r_{k k^{\prime}} \equiv\left|\mathbf{r}_{\mathrm{k}}-\mathbf{r}_{\mathrm{k}^{\prime}}\right|$ between particles of the system are negligibly small. Such an abstraction is called the (absolutely) rigid body, and is a reasonable approximation in many practical problems, including the motion of solids. In this model we neglect deformations - that will be the subject of the next two chapters.

The rigid body approximation reduces the number of degrees of freedom of the system from 3 N to just 6 - for example, 3 Cartesian coordinates of one point (say, $O$ ), and 3 angles of the system rotation about 3 mutually perpendicular axes passing through this point. (An alternative way to arrive at the same number 6 is to consider 3 points of the body, which uniquely define its position. If movable independently, the points would have 9 degrees of freedom, but since 3 distances $r_{k k}$, between them are now fixed, the resulting 3 constraints reduce the number of degrees of freedom to 6 .)

Let us show that an arbitrary elementary displacement of such a rigid body may be always considered as a sum of a translational motion and a rotation. Consider a "moving" reference frame, firmly bound to the body, and an arbitrary vector $\mathbf{A}$ - see Fig. 1.


Fig. 6.1. Deriving Eq. (8).

The vector may be represented by its Cartesian components $A_{j}$ in that reference frame:

$$
\begin{equation*}
\mathbf{A}=\sum_{j=1}^{3} A_{j} \mathbf{n}_{j} \tag{6.1}
\end{equation*}
$$

Let us calculate its time derivative in an arbitrary, possibly different ("lab") frame, taking into account that if the body rotates relative to this frame, then the directions of the unit vectors $\mathbf{n}_{j}$ change in time. Hence, we have to differentiate both operands in each product contributing to sum (1):

$$
\begin{equation*}
\left.\frac{d \mathbf{A}}{d t}\right|_{\text {in lab }}=\sum_{j=1}^{3} \frac{d A_{j}}{d t} \mathbf{n}_{j}+\sum_{j=1}^{3} A_{j} \frac{d \mathbf{n}_{j}}{d t} . \tag{6.2}
\end{equation*}
$$

In this expression, the first sum evidently describes the change of vector $\mathbf{A}$ as observed from the moving frame. Each of the infinitesimal vectors $d \mathbf{n}_{j}$ participating in the second sum may be presented by its Cartesian components in the moving frame:

$$
\begin{equation*}
d \mathbf{n}_{j}=\sum_{j^{\prime}=1}^{3} d \varphi_{i j} \mathbf{n}_{j^{\prime}} . \tag{6.3}
\end{equation*}
$$

In order to find more about the set of scalar coefficients $d \varphi_{j j}$, let us scalar-multiply each part of this relation by an arbitrary unit vector $\mathbf{n}_{j}$ ", and take into account the evident orthogonality condition:

$$
\begin{equation*}
\mathbf{n}_{j^{\prime}} \cdot \mathbf{n}_{j^{\prime \prime}}=\delta_{j j^{\prime \prime}} \tag{6.4}
\end{equation*}
$$

As a result, we get

$$
\begin{equation*}
d \varphi_{j j^{\prime \prime}}=d \mathbf{n}_{j} \cdot \mathbf{n}_{j^{\prime \prime}} \tag{6.5}
\end{equation*}
$$

Now let us use Eq. (5) to calculate the first differential of Eq. (4):

$$
\begin{equation*}
d \mathbf{n}_{j^{\prime}} \cdot \mathbf{n}_{j^{\prime \prime}}+\mathbf{n}_{j^{\prime}} \cdot d \mathbf{n}_{j^{\prime \prime}}=d \varphi_{j^{\prime \prime}}+d \varphi_{j^{\prime \prime} j^{\prime}}=0 ; \quad \text { in particular, } 2 d \mathbf{n}_{j} \cdot \mathbf{n}_{j}=2 d \varphi_{j j}=0 \tag{6.6}
\end{equation*}
$$

These relations, valid for any choice of indices $j, j$, and $j$ " of the set $\{1,2,3\}$, mean that the matrix of elements $d \varphi_{i j}$ is antisymmetric; in other words, there are not 9 , but just 3 independent coefficients $d \varphi_{j j}$, all with $j \neq j^{\prime}$. Hence it is natural to renumber them in a simpler way: $d \varphi_{j j}{ }^{\prime}=-d \varphi_{j}{ }^{\prime} \equiv d \varphi_{j^{\prime \prime}}$, where indices $j, j$ ', and $j$ " follow in a "correct" order - either $\{1,2,3\}$, or $\{2,3,1\}$, or $\{3,1,2\}$. Now it is easy to check (say, just by a component-by-component comparison) that in this new notation, Eq. (3) may be presented just as a vector product:

$$
\begin{equation*}
d \mathbf{n}_{j}=d \boldsymbol{\varphi} \times \mathbf{n}_{j}, \tag{6.7}
\end{equation*}
$$

Elementary rotation
where $d \varphi$ is the infinitesimal vector defined by its Cartesian components $d \varphi_{j}$ (in the moving frame).
Relation (7) is the basis of all rotation kinematics. Using it, Eq. (2) may be rewritten as

$$
\begin{equation*}
\left.\frac{d \mathbf{A}}{d t}\right|_{\text {in lab }}=\left.\frac{d \mathbf{A}}{d t}\right|_{\text {in mov }}+\sum_{j=1}^{3} A_{j} \frac{d \boldsymbol{\varphi}}{d t} \times \mathbf{n}_{j}=\left.\frac{d \mathbf{A}}{d t}\right|_{\text {in mov }}+\boldsymbol{\omega} \times \mathbf{A}, \quad \text { where } \boldsymbol{\omega} \equiv \frac{d \boldsymbol{\varphi}}{d t} . \tag{6.8}
\end{equation*}
$$

In order to interpret the physical sense of vector $\omega$, let us apply Eq. (8) to the particular case when $\mathbf{A}$ is the radius-vector $\mathbf{r}$ of a point of the body, and the lab frame is selected in a special way: its origin moves with the same velocity as that of the moving frame in the particular instant under consideration. In this case the first term in the right-hand part of Eq. (8) is zero, and we get

$$
\begin{equation*}
\left.\frac{d \mathbf{r}}{d t}\right|_{\text {in special lab frame }}=\boldsymbol{\omega} \times \mathbf{r}, \tag{6.9}
\end{equation*}
$$

were vector $\mathbf{r}$ is the same in both frames. According to the vector product definition, the particle velocity described by this formula has a direction perpendicular to vectors $\omega$ and $\mathbf{r}$ (Fig. 2), and magnitude $\omega r \sin \theta$. As Fig. 2 shows, this expression may be rewritten as $\omega \rho$, where $\rho=r \sin \theta$ is the distance from the line that is parallel to vector $\omega$ and passes through point $O$. This is of course just the pure rotation about that line (called the instantaneous axis of rotation), with angular velocity $\omega$. Since, according to Eqs. (3) and (8), the angular velocity vector $\omega$ is defined by the time evolution of the moving frame alone, it is the same for all points $\mathbf{r}$, i.e. for the rigid body as a whole. Note that nothing in
our calculations forbids not only the magnitude but also the direction of vector $\omega$, and thus of the instantaneous axis of rotation, to change in time (and in many cases it does); hence the name.


Fig. 6.2. Instantaneous axis of rotation.

Now let us generalize our result a step further, considering two laboratory reference frames that do not rotate versus each other: one arbitrary, and another one selected in the special way described above, so that for it Eq. (9) is valid in it. Since their relative motion of these two reference frames is purely translational, we can use the simple velocity addition rule given by Eq. (1.8) to write

$$
\begin{equation*}
\left.\mathbf{v}\right|_{\left.\right|_{\text {in lab }}}=\left.\mathbf{v}_{o}\right|_{\text {in lab }}+\left.\mathbf{v}\right|_{\text {in special lab frame }}=\left.\mathbf{v}_{o}\right|_{\text {in lab }}+\boldsymbol{\omega} \times \mathbf{r}, \tag{6.10}
\end{equation*}
$$

where $\mathbf{r}$ is the radius-vector of a point is measured in the body-bound ("moving") frame $O$.

### 6.2. Inertia tensor

Since the dynamics of each point of a rigid body is strongly constrained by conditions $r_{k k}=$ const, this is one of the most important fields of application of the Lagrangian formalism that was discussed in Chapter 2. The first thing we need to know for using this approach is the kinetic energy of the body in an inertial reference frame. It is just the sum of kinetic energies of all its points, so that we can use Eq. (10) to write: ${ }^{1}$

$$
\begin{equation*}
T=\sum \frac{m}{2} \mathbf{v}^{2}=\sum \frac{m}{2}\left(\mathbf{v}_{O}+\boldsymbol{\omega} \times \mathbf{r}\right)^{2}=\sum \frac{m}{2} v_{O}^{2}+\sum m \mathbf{v}_{O} \cdot(\boldsymbol{\omega} \times \mathbf{r})+\sum \frac{m}{2}(\boldsymbol{\omega} \times \mathbf{r})^{2} . \tag{6.11}
\end{equation*}
$$

Let us apply to the right-hand part of Eq. (11) two general vector analysis formulas, listed in the Math Appendix: the operand rotation rule MA Eq. (7.6) to the second term, and MA Eq. (7.7b) to the third term. The result is

$$
\begin{equation*}
T=\sum \frac{m}{2} v_{O}^{2}+\sum m \mathbf{r} \cdot\left(\mathbf{v}_{O} \times \boldsymbol{\omega}\right)+\sum \frac{m}{2}\left[\omega^{2} r^{2}-(\boldsymbol{\omega} \cdot \mathbf{r})^{2}\right] . \tag{6.12}
\end{equation*}
$$

This expression may be further simplified by making a specific choice of point $O$ (from the radiusvectors $\mathbf{r}$ of all particles are measured), namely if we use for this point the center of mass of the body. As was already mentioned in Sec. 3.4, radius-vector $\mathbf{R}$ of this point is defined as

$$
\begin{equation*}
M \mathbf{R} \equiv \sum m \mathbf{r}, \quad M \equiv \sum m, \tag{6.13}
\end{equation*}
$$

[^78]where $M$ is just the total mass of the body. In the reference frame centered as that point, $\mathbf{R}=0$, so that in that frame the second sum in Eq. (12) vanishes, so that the kinetic energy is a sum of two terms:
\[

$$
\begin{equation*}
T=T_{\text {tran }}+T_{\mathrm{rot}}, \quad T_{\text {tran }} \equiv \frac{M}{2} V^{2}, \quad T_{\mathrm{rot}} \equiv \sum \frac{m}{2}\left[\omega^{2} r^{2}-(\boldsymbol{\omega} \cdot \mathbf{r})^{2}\right], \tag{6.14}
\end{equation*}
$$

\]

where $\mathbf{V} \equiv d \mathbf{R} / d t$ is the center-of-mass velocity in our inertial reference frame, and all particle positions $\mathbf{r}$ have to be measured in the center-of-mass frame. Since the angular velocity vector $\omega$ is common for all points of a rigid body, it is more convenient to rewrite the rotational energy in a form in which the summation over the components of this vector is clearly separated from the summation over the points of the body:

$$
\begin{equation*}
T_{\mathrm{rot}}=\frac{1}{2} \sum_{j, j^{\prime}=1}^{3} I_{i j} \omega_{j} \omega_{j^{\prime}}, \tag{6.15}
\end{equation*}
$$

where the $3 \times 3$ matrix with elements

$$
\begin{equation*}
I_{i j j^{\prime}} \equiv \sum m\left(r^{2} \delta_{j j^{\prime}}-r_{j} r_{j^{\prime}}\right) \tag{6.16}
\end{equation*}
$$

## Inertia

 tensoris called the inertia tensor of the body.
Actually, the term "tensor" for the matrix has to be justified, because in physics this name implies a certain reference-frame-independent notion, so that its elements have to obey certain rules at the transfer between reference frames. In order to show that the inertia tensor deserves its title, let us calculate another key quantity, the total angular momentum $\mathbf{L}$ of the same body. ${ }^{2}$ Summing up the angular momenta of each particle, defined by Eq. (1.31), and using Eq. (10) again, in our inertial reference frame we get

$$
\begin{equation*}
\mathbf{L} \equiv \sum \mathbf{r} \times \mathbf{p}=\sum m \mathbf{r} \times \mathbf{v}=\sum m \mathbf{r} \times\left(\mathbf{v}_{O}+\boldsymbol{\omega} \times \mathbf{r}\right)=\sum m \mathbf{r} \times \mathbf{v}_{O}+\sum m \mathbf{r} \times(\boldsymbol{\omega} \times \mathbf{r}) . \tag{6.17}
\end{equation*}
$$

We see that the momentum may be presented as a sum of two terms. The first one,

$$
\begin{equation*}
\mathbf{L}_{O} \equiv \sum m \mathbf{r} \times \mathbf{v}_{O}=M \mathbf{R} \times \mathbf{v}_{O} \tag{6.18}
\end{equation*}
$$

describes possible rotation of the center of mass about the inertial frame origin. This term evidently vanishes if the moving reference frame's origin $O$ is positioned at the center of mass. In this case we are left with only the second term, which describes the rotation of the body about its center of mass:

$$
\begin{equation*}
\mathbf{L}=\mathbf{L}_{\mathrm{rot}} \equiv \sum m \mathbf{r} \times(\boldsymbol{\omega} \times \mathbf{r}) \tag{6.19}
\end{equation*}
$$

Using one more vector algebra formula, the "bac minis cab" rule, ${ }^{3}$ we may rewrite this expression as

$$
\begin{equation*}
\mathbf{L}=\sum m\left[\omega r^{2}-\mathbf{r}(\mathbf{r} \cdot \boldsymbol{\omega})\right] \tag{6.20}
\end{equation*}
$$

Let us spell out an arbitrary Cartesian component of this vector:

[^79]\[

$$
\begin{equation*}
L_{j}=\sum m\left[\omega_{j} r^{2}-r_{j} \sum_{j^{\prime}=1}^{3} r_{j^{\prime}} \omega_{j^{\prime}}\right]=\sum m \sum_{j^{\prime}=1}^{3} \omega_{j^{\prime}}\left(r^{2} \delta_{j j^{\prime}}-r_{j} r_{j^{\prime}}\right) . \tag{6.21}
\end{equation*}
$$

\]

Changing the order of summations, and comparing the result with Eq. (16), we see that the angular momentum may be conveniently expressed via the same matrix elements $I_{j j}$, as the rotational kinetic energy:

Angular momentum

$$
\begin{equation*}
L_{j}=\sum_{j^{\prime}=1}^{3} I_{i j j^{\prime}} \omega_{j^{\prime}} \tag{6.22}
\end{equation*}
$$

Since $\mathbf{L}$ and $\omega$ are both legitimate vectors (meaning that they describe physical vectors independent on the reference frame choice), their connection, the matrix of elements $I_{j j^{\prime}}$, is a legitimate tensor. This fact, and the symmetry of the tensor $\left(I_{j j^{\prime}}=I_{j^{\prime} j}\right)$, which is evident from its definition (16), allow the tensor to be further simplified. In particular, mathematics tells us that by a certain choice of the axis orientation, any symmetric tensor may be reduced to a diagonal form

$$
\begin{equation*}
I_{i j j^{\prime}}=I_{j} \delta_{i j j^{\prime}}, \tag{6.23}
\end{equation*}
$$

where, in our case

Principal moments of inertia

Rotational energy and angular momentum in principal axes

$$
\begin{equation*}
I_{j}=\sum m\left(r^{2}-r_{j}^{2}\right)=\sum m\left(r_{j^{\prime}}^{2}+r_{j^{\prime \prime}}^{2}\right)=\sum m \rho_{j}^{2} \tag{6.24}
\end{equation*}
$$

$\rho_{j}$ being the distance of the particle from the $j$-th axis, i.e. the length of the perpendicular dropped from the point to that axis. The axes of such special coordinate system are called the principal axes, while the diagonal elements $I_{j}$ given by Eq. (24), the principal moments of inertia of the body. In such a special reference frame, Eqs. (15) and (22) are reduced to very simple forms:

$$
\begin{gather*}
T_{\mathrm{rot}}=\sum_{j=1}^{3} \frac{I_{j}}{2} \omega_{j}^{2},  \tag{6.25}\\
L_{j}=I_{j} \omega_{j} . \tag{6.26}
\end{gather*}
$$

Both these results remind the corresponding relations for the translational motion, $T_{\text {tran }}=M V^{2} / 2$ and $\mathbf{P}=$ $M V$, with the angular velocity $\omega$ replacing the "linear" velocity $\mathbf{V}$, and the tensor of inertia playing the role of scalar mass $M$. However, let me emphasize that even in the specially selected coordinate system, with axes pointing in principal directions, the analogy is incomplete, and rotation is generally more complex than translation, because the measures of inertia, $I_{j}$, are generally different for each principal axis.

Let me illustrate this fact on a simple but instructive system of three similar massive particles fixed in the vertices of an equilateral triangle (Fig. 3).


Fig. 6.3. Principal moments of inertia: a simple case study.

Due to symmetry of the configuration, one of the principal axes has to pass through the center of mass $O$, perpendicular to the plane of the triangle. For the corresponding principal moment of inertia, Eq. (24) readily yields $I_{3}=3 m \rho^{2}$. If we want to express the result in terms of the triangle side $a$, we may notice that due to system's symmetry, the angle marked in Fig. 3 equals $\pi / 6$, and from the corresponding right triangle, $a / 2=\rho \cos (\pi / 6) \equiv \rho \sqrt{ } 3 / 2$, giving $\rho=a / \sqrt{ } 3$, so that, finally, $I_{3}=m a^{2}$.

Another way to get the same result is to use the following general axis shift theorem, which may be rather useful - especially for more complex cases. Let us relate the inertia tensor components $I_{j j}$, and $I^{\prime}{ }_{j j}$, , calculated in two reference frames - one in the center of mass $O$, and another one displaced by a certain vector $\mathbf{d}$ (Fig. 4a), so that for an arbitrary point, $\mathbf{r}^{\prime}=\mathbf{r}+\mathbf{d}$. Plugging this relation into Eq. (16), we get

$$
\begin{align*}
I_{j j^{\prime}}^{\prime} & =\sum m\left[(\mathbf{r}+\mathbf{d})^{2} \delta_{i j^{\prime}}-\left(r_{j}+d_{j}\right)\left(r_{j^{\prime}}+d_{j^{\prime}}\right)\right] \\
& =\sum m\left[\left(r^{2}+2 \mathbf{r} \cdot \mathbf{d}+d^{2}\right) \delta_{j j^{\prime}}\left(r_{j} r_{j^{\prime}}+r_{j} d_{j^{\prime}}+r_{j^{\prime}} d_{j}+d_{j} d_{j^{\prime}}\right)\right] . \tag{6.27}
\end{align*}
$$

Since in the center-of-mass frame, all sums $\sum m r_{j}$ equal zero, we may use Eq. (16) to finally obtain

$$
\begin{equation*}
I_{j j^{\prime}}^{\prime}=I_{j j^{\prime}}+M\left(\delta_{j j^{\prime}} d^{2}-d_{j} d_{j^{\prime}}\right) \tag{6.28}
\end{equation*}
$$

Rotation
axis
shift

In particular, this equation shows that if the shift vector $\mathbf{d}$ is perpendicular to one (say, $j$-th) of the principal axes (Fig. 4b), i.e. $d_{j}=0$, then Eq. (28) is reduced to a very simple formula:

$$
\begin{equation*}
I_{j}^{\prime}=I_{j}+M d^{2} \tag{6.29}
\end{equation*}
$$


(a)
(b)


Fig. 6.4. (a) General reference frame shift from the center of mass, and (b) a shift perpendicular to one of the principal axes.

Returning to the system shown in Fig. 3, let us perform such a shift so that the new ("primed") axis passes through the location of one of the particles, still perpendicular to particles' plane. Then the contribution of that particular mass to the primed moment of inertia vanishes, and $I_{3}=2 \mathrm{ma}^{2}$. Now, returning to the center of mass and applying Eq. (29), we get $I_{3}=I_{3}-M \rho^{2}=2 m a^{2}-(3 m)(a / \sqrt{ } 3)^{2}=m a^{2}$, i.e. the same result as above.

The symmetry situation inside the triangle plane is somewhat less evident, so let us start with calculating the moments of inertia for the axes shown vertical and horizontal in Fig. 3. From Eq. (24) we readily get:

$$
\begin{equation*}
I_{1}=2 m h^{2}+m \rho^{2}=m\left[2\left(\frac{a}{2 \sqrt{3}}\right)^{2}+\left(\frac{a}{\sqrt{3}}\right)^{2}\right]=\frac{m a^{2}}{2}, \quad I_{2}=2 m\left(\frac{a}{2}\right)^{2}=\frac{m a^{2}}{2} \tag{6.30}
\end{equation*}
$$

where I have taken into account the fact that the distance $h$ from the center of mass and any side of the triangle is $h=\rho \sin (\pi / 6)=\rho / 2=a / 2 \sqrt{3}$. We see that $I_{1}=I_{2}$, and mathematics tells us that in this case any in-plane axis (passing through the center of mass $O$ ) may be considered as principal, and has the same moment of inertia. A rigid body with this property, $I_{1}=I_{2} \neq I_{3}$, is called the symmetric top. (The last direction is called the main principal axis of the system.)

Despite the name, the situation may be even more symmetric in the so-called spherical tops, i.e. highly symmetric systems whose principal moments of inertia are all equal,

$$
\begin{equation*}
I_{1}=I_{2}=I_{3} \equiv I \tag{6.31}
\end{equation*}
$$

Spherical
top:
definition
and description

Mathematics says that in this case the moment of inertia for rotation about any axis (but still passing through the center of mass) is equal to the same $I$. Hence Eqs. (25) and (26) are further simplified for any direction of vector $\omega$ :

$$
\begin{equation*}
T_{\mathrm{rot}}=\frac{I}{2} \omega^{2}, \quad \mathbf{L}=I \omega \tag{6.32}
\end{equation*}
$$

thus making the analogy of rotation and translation complete. (As will be discussed in the next section, the analogy is also complete if the rotation axis is fixed by external constraints.)

An evident example of a spherical top is a uniform sphere or spherical shell; a less obvious example is a uniform cube - with masses either concentrated in vertices, or uniformly spread over the faces, or uniformly distributed over the volume. Again, in this case any axis passing through the center of mass is principal, and has the same principal moment of inertia. For a sphere, this is natural; for a cube, rather surprising - but may be confirmed by a direct calculation.

### 6.3. Fixed-axis rotation

Now we are well equipped for a discussion of rigid body's rotational dynamics. The general equation of this dynamics is given by Eq. (1.38), which is valid for dynamics of any system of particles - either rigidly connected or not:

$$
\begin{equation*}
\dot{\mathbf{L}}=\boldsymbol{\tau} \tag{6.33}
\end{equation*}
$$

where $\tau$ is the net torque of external forces. Let us start exploring this equation from the simplest case when the axis of rotation, i.e. the direction of vector $\omega$, is fixed by some external constraints. Let us direct axis $z$ along this vector; then $\omega_{x}=\omega_{y}=0$. According to Eq. (22), in this case, the $z$-component of the angular momentum,

$$
\begin{equation*}
L_{z}=I_{z z} \omega_{z}, \tag{6.34}
\end{equation*}
$$

where $I_{z z}$, though not necessarily one of the principal momenta of inertia, still may be calculated using Eq. (24):

$$
\begin{equation*}
I_{z z}=\sum m \rho_{z}^{2}=\sum m\left(x^{2}+y^{2}\right) \tag{6.35}
\end{equation*}
$$

with $\rho_{z}$ being the distance of each particle from the rotation axis z. According to Eq. (15), the rotational kinetic energy in this case is just

$$
\begin{equation*}
T_{\text {rot }}=\frac{I_{z z}}{2} \omega_{z}^{2} . \tag{6.36}
\end{equation*}
$$

Moreover, it is straightforward to use Eqs. (12), (17), and (28) to show that if the rotation axis is fixed, Eqs. (34)-(36) are valid even if the axis does not pass through the center of mass - if only distances $\rho_{z}$ are now measured from that axis. (The proof is left for reader's exercise.)

As a result, we may not care about other components of vector $\mathbf{L},{ }^{4}$ and use just one component of Eq. (33),

$$
\begin{equation*}
\dot{L}_{z}=\tau_{z}, \tag{6.37}
\end{equation*}
$$

because it, when combined with Eq. (34), completely determines the dynamics of rotation:

$$
\begin{equation*}
I_{z z} \dot{\omega}_{z}=\tau_{z}, \text { i.e. } I_{z z} \ddot{\theta}_{z}=\tau_{z}, \tag{6.38}
\end{equation*}
$$

where $\theta_{z}$ is the angle of rotation about the axis, so that $\omega_{z}=\dot{\theta}$. Scalar relations (34), (36) and (38), describing rotation about a fixed axis, are completely similar to the corresponding formulas of 1D motion of a single particle, with $\omega_{z}$ corresponding to the usual ("linear") velocity, the angular momentum component $L_{z}$ - to the linear momentum, and $I_{z}$ - to particle's mass.

The resulting motion about the axis is also frequently similar to that of a single particle. As a simple example, let us consider what is called the physical pendulum (Fig. 5) - a rigid body free to rotate about a fixed horizontal axis $A$ that does not pass through the center of mass $O$, in the uniform gravity field $\mathbf{g}$.


Fig. 6.5. Physical pendulum. The fixed (horizontal) rotation axis $A$ is perpendicular to the plane of drawing.

Let us drop a perpendicular from point $O$ to the rotation axis, and call the corresponding vector $\mathbf{I}$ (Fig. 5). Then the torque (relative to axis $A$ ) of the forces exerted by the axis constraint is zero, and the only contribution to the net torque is due to gravity alone:

$$
\begin{equation*}
\left.\left.\boldsymbol{\tau}\right|_{\text {in } A} \equiv \sum \mathbf{r}\right|_{\text {in } A} \times \mathbf{F}=\sum\left(\mathbf{l}+\left.\mathbf{r}\right|_{\text {in } O}\right) \times m \mathbf{g}=\sum m(\mathbf{l} \times \mathbf{g})+\left.\sum m \mathbf{r}\right|_{\text {in } O} \times \mathbf{g}=M \mathbf{l} \times \mathbf{g} . \tag{6.39}
\end{equation*}
$$

(For the last transition, I have used the facts that point $O$ is the center of mass, and that vectors $\mathbf{I}$ and $\mathbf{g}$ are the same for all particles of the body.) This result shows that the torque is directed along the rotation

[^80]axis, and its (only) component $\tau_{z}$ is equal to $-M g l \sin \theta$, where $\theta$ is the angle between vectors $\mathbf{l}$ and $\mathbf{g}$, i.e. the angular deviation of the pendulum from the position of equilibrium. As a result, Eq. (38) takes the form,
\[

$$
\begin{equation*}
I_{A} \ddot{\theta}=-M g l \sin \theta, \tag{6.40}
\end{equation*}
$$

\]

where, $I_{A}$ is the moment of inertia for rotation about axis $A$ rather about the center of mass. This equation is identical to that of the point-mass (sometimes called "mathematical") pendulum, with the small-oscillation frequency

Physical pendulum's frequency

$$
\begin{equation*}
\Omega=\left(\frac{M g l}{I_{A}}\right)^{1 / 2} \tag{6.41}
\end{equation*}
$$

As a sanity check, in the simplest case when the linear size of the body is much smaller than the suspension length $l$, Eq. (35) yields $I_{A}=M l^{2}$, and Eq. (41) reduces to the well-familiar formula $\Omega=$ $(g / l)^{1 / 2}$ for the mathematical pendulum.

Now let us discuss the situations when a body not only rotates, but also moves as the whole. As we already know from our introductory chapter, the total momentum of the body,

$$
\begin{equation*}
\mathbf{P} \equiv \sum m \mathbf{v}=\sum m \dot{\mathbf{r}}=\frac{d}{d t} \sum m \mathbf{r} \tag{6.42}
\end{equation*}
$$

satisfies the $2^{\text {nd }}$ Newton law in the form (1.30). Using the definition (13) of the center of mass, the momentum may be presented as

$$
\begin{equation*}
\mathbf{P}=M \dot{\mathbf{R}}=M \mathbf{V} \tag{6.43}
\end{equation*}
$$

so Eq. (1.30) may be rewritten as
C.o.m.'s law of motion

$$
\square-2+
$$

where $\mathbf{F}$ is the vector sum of all external forces. This equation shows that the center of mass of the body moves exactly as a point particle of mass $M$, under the effect of the net force $\mathbf{F}$. In many cases this fact makes the translational dynamics of a rigid body absolutely similar to that of a point particle.

The situation becomes more complex if some of the forces contributing to the vector sum $\mathbf{F}$ depend on rotation of the same body, i.e. if its rotational and translational motions are coupled. Analysis of such coupled motion is rather straightforward if the direction of the rotation axis does not change in time, and hence Eqs. (35)-(36) are still valid. Possibly the simplest example is a round cylinder (say, a wheel) rolling on a surface without slippage (Fig. 6).

(b)

Fig. 6.6. Round cylinder rolling over (a) plane surface and (b) concave surface.

The no-slippage condition may be presented as the requirement of zero net velocity of the particular wheel point $A$ that touches the surface - in the reference frame connected to the surface. For the simplest case of plane surface (Fig. 6a), the application of Eq. (10) shows that this requirement gives the following relation between the angular velocity $\omega$ of the wheel and the linear velocity $V$ of its center:

$$
\begin{equation*}
V+r \omega=0 \tag{6.45}
\end{equation*}
$$

Such kinematic relations are essentially holonomic constraints, which reduce the number of degrees of freedom of the system. For example, without condition (45) the wheel on a plane surface has to be considered as a system with two degrees of freedom, so that its total kinetic energy (14) is a function of two independent generalized velocities, say $V$ and $\omega$ :

$$
\begin{equation*}
T=T_{\text {tran }}+T_{\mathrm{rot}}=\frac{M}{2} V^{2}+\frac{I}{2} \omega^{2} \tag{6.46}
\end{equation*}
$$

Using Eq. (45) we may eliminate, for example, the linear velocity and reduce Eq. (46) to

$$
\begin{equation*}
T=\frac{M}{2}(\omega r)^{2}+\frac{I}{2} \omega^{2}=\frac{I_{\mathrm{ef}}}{2} \omega^{2}, \quad \text { where } \quad I_{\mathrm{ef}} \equiv I+M r^{2} \tag{6.47}
\end{equation*}
$$

This result may be interpreted as the kinetic energy of pure rotation of the wheel about the instantaneous axis $A$, with $I_{\text {ef }}$ being the moment of inertia about that axis, satisfying Eq. (29).

Kinematic relations are not always as simple as Eq. (45). For example, if the wheel is rolling on a concave surface (Fig. 6b), we need relate the angular velocities of the wheel rotation about its axis $O$ (denoted $\omega$ ) and that of its axis' rotation about the center $O^{\prime}$ of curvature of the surface ( $\Omega$ ). A popular error here is to write $\Omega=-(r / R) \omega$ [WRONG!]. A prudent way to get the correct relation is to note that Eq. (45) holds for this situation as well, and on the other hand the same linear velocity of wheel's center may be expressed as $V=(R-r) \Omega$. Combining these equations, we get a (not quite evident) relation

$$
\begin{equation*}
\Omega=-\frac{r}{R-r} \omega \tag{6.48}
\end{equation*}
$$

Another famous example of the relation between the translational and rotational motion is given by the "sliding ladder" problem (Fig. 7). Let us analyze it for the simplest case of negligible friction, and ladder's thickness small in comparison with its length $l$.


Fig. 6.7. Sliding ladder problem.

In order to use the Lagrangian formalism, we may write the kinetic energy of the ladder as the sum (14) of the translational and rotational parts:

$$
\begin{equation*}
T=\frac{M}{2}\left(\dot{X}^{2}+\dot{Y}^{2}\right)+\frac{I}{2} \dot{\alpha}^{2}, \tag{6.49}
\end{equation*}
$$

where $X$ and $Y$ are the Cartesian coordinates of its center of mass in an inertial reference frame, and $I$ is the moment of inertia for rotation about the $z$-axis passing through the center of mass. (For the uniformly-distributed mass, an elementary integration of Eq. (35) yields $I=M l^{2} / 12$ ). In the reference frame with the center in the corner $O$, both $X$ and $Y$ may be simply expressed via angle $\alpha$ :

$$
\begin{equation*}
X=\frac{l}{2} \cos \alpha, \quad Y=\frac{l}{2} \sin \alpha \tag{6.50}
\end{equation*}
$$

(The easiest way to obtain these relations is to notice that the dashed line in Fig. 7 has slope $\alpha$ and length $l / 2$.) Plugging these expressions into Eq. (49), we get

$$
\begin{equation*}
T=\frac{I_{\mathrm{ef}}}{2} \dot{\alpha}^{2}, \quad I_{\mathrm{ef}} \equiv I+M\left(\frac{l}{2}\right)^{2}=\frac{1}{3} M l^{2} . \tag{6.51}
\end{equation*}
$$

Since the potential energy of the ladder in the gravity field may be also expressed via the same angle,

$$
\begin{equation*}
U=M g Y=M g \frac{l}{2} \sin \alpha \tag{6.52}
\end{equation*}
$$

$\alpha$ may be conveniently used as the (only) generalized coordinate of the system. Even without writing the Lagrangian equation of motion for that coordinate explicitly, we may notice that since the Lagrangian function $(T-U)$ does not depend on time explicitly, and the kinetic energy (51) is a quadratichomogeneous function of the generalized velocity $\dot{\alpha}$, the full mechanical energy,

$$
\begin{equation*}
E \equiv T+U=\frac{I_{\mathrm{ef}}}{2} \dot{\alpha}^{2}+M g \frac{l}{2} \sin \alpha=\frac{M g l}{2}\left(\frac{l \dot{\alpha}^{2}}{3 g}+\sin \alpha\right), \tag{6.53}
\end{equation*}
$$

is conserved and gives us the first integral of motion. Moreover, Eq. (53) shows that the system's energy (and hence dynamics) is identical to that of a physical pendulum with an unstable fixed point $\alpha_{1}=\pi / 2$, stable fixed point at $\alpha_{2}=-\pi / 2$, and frequency

$$
\begin{equation*}
\Omega=\left(\frac{3 g}{2 l}\right)^{1 / 2} \tag{6.54}
\end{equation*}
$$

of small oscillations near the latter point. (Of course, that fixed point cannot be reached in the simple geometry shown in Fig. 7, where ladder's hitting the floor would change its equations of motion).

### 6.4. Free rotation

Now let us proceed to more complex case when the rotation axis is not fixed. A good illustration of the complexity arising is this case comes from the simplest case of a rigid body left alone, i.e. not subjected to external forces and hence its potential energy $U$ is constant. Since in this case, according to Eq. (44), the center of mass moves (as measured from any inertial reference frame) with a constant velocity, we can always use an convenient inertial reference frame with the center at that point. From the point of view of such frame, the body's motion is a pure rotation, and $T_{\text {tran }}=0$. Hence, the system's Lagrangian equals just the rotational energy (15), which is, first, a quadratic-homogeneous function of
components $\omega_{j}$ (that may be taken for generalized velocities), and, second, does not depend on time explicitly. As we know from Chapter 2, in this case the energy is conserved. For the components of vector $\omega$ in the principal axes, this means

$$
\begin{equation*}
T_{\mathrm{rot}}=\sum_{j=1}^{3} \frac{I_{j}}{2} \omega_{j}^{2}=\mathrm{const} . \tag{6.55}
\end{equation*}
$$

Next, as Eq. (33) shows, in the absence of external forces the angular momentum $\mathbf{L}$ of the body is conserved as well. However, though we can certainly use Eq. (26) to present this fact as

$$
\begin{equation*}
\mathbf{L}=\sum_{j=1}^{3} I_{j} \omega_{j} \mathbf{n}_{j}=\text { const } \tag{6.56}
\end{equation*}
$$

Rotational energy's conservation
where $\mathbf{n}_{j}$ are the principal axes of inertia, this does not mean that components $\omega_{j}$ of the angular velocity vector $\omega$ are constant, because the principal axes are fixed relative to the rigid body, and hence may rotate with it.

Before going after these complications, let us briefly mention two conceptually trivial, but practically very important, particular cases. The first is a spherical top $\left(I_{1}=I_{2}=I_{3}=I\right)$. In this case Eqs. (55) and (56) imply that all components of vector $\omega=\mathbf{L} / I$, i.e. both the magnitude and the direction of the angular velocity are conserved, for any initial spin. In other words, the body conserves its rotation speed and axis direction, as measured in an inertial frame.

The most obvious example is a spherical planet. For example, our Mother Earth, rotating about its axis with angular velocity $\omega=2 \pi /(1$ day $) \approx 7.3 \times 10^{-5} \mathrm{~s}^{-1}$, keeps its axis at a nearly constant angle of $23^{\circ} 27^{\prime}$ to the ecliptic pole, i.e. the axis normal to the plane of its motion around the Sun. (In Sec. 6 below, we will discuss some very slow motions of this axis, due to gravity effects.)

Spherical tops are also used in the most accurate gyroscopes, usually with gas or magnetic suspension in vacuum. If done carefully, such systems may have spectacular stability. For example, the gyroscope system of the Gravity Probe B satellite experiment, flown in 2004-2005, was based on quartz spheres - round with precision of about 10 nm and covered by superconducting thin films (which have enabled their magnetic suspension and SQUID monitoring). The whole system was stable enough to measure that the so-called geodetic effect in general relativity (essentially, the space curving by Earth's mass), resulting in the axis precession by just 6.6 arcseconds per year, i.e. with a precession frequency of just $\sim 10^{-11} \mathrm{~s}^{-1}$, agrees with theory with a record $\sim 0.3 \%$ accuracy. ${ }^{5}$

The second simple case is that of the "symmetric top" $\left(I_{1}=I_{2} \neq I_{3}\right)$, with the initial vector $\mathbf{L}$ aligned with the main principal axis. In this case, $\omega=\mathbf{L} / I_{3}=$ const, so that the rotation axis is conserved. ${ }^{6}$ Such tops, typically in the shape of a flywheel (rotor) supported by a "gimbal" system (Fig. 8), are broadly used in more common gyroscopes, core parts of automatic guidance systems, for

[^81]example, in ships, airplanes, missiles, etc. Even if the ship's hull wobbles, the suspended gyroscope sustains its direction relative to Earth (which is sufficiently inertial for these applications). ${ }^{7}$


Fig. 6.8. Typical gyroscope. (Adapted from http://en.wikipedia.org/wiki/Gyroscope.)

However, in the general case with no such special initial alignment, the dynamics of symmetric tops is more complex. In this case, vector $\mathbf{L}$ is still conserved, including its direction, but vector $\omega$ is not. Indeed, let us direct axis $\mathbf{n}_{2}$ perpendicular to the common plane of vectors $\mathbf{L}$ and the instantaneous direction $\mathbf{n}_{3}$ of the main principal axis (in Fig. 9, the plane of drawing); then, in that particular instant, $L_{2}=0$. Now let us recall that in a symmetric top, axis $\mathbf{n}_{2}$ is a principal one. According to Eq. (26) with $j$ $=2$, the corresponding component $\omega_{2}$ has to be equal to $L_{2} / I_{2}$, so it vanishes. This means that vector $\omega$ lies in this plane (the common plane of vectors $\mathbf{L}$ and $\mathbf{n}_{3}$ ) as well - see Fig. 9a.

(b)

Fig. 6.9. Free rotation of a symmetric top: (a) the general configuration of vectors, and (b) calculating the free precession frequency.

Now consider any point of the body, located on axis $\mathbf{n}_{3}$, and hence within plane $\left[\mathbf{n}_{3}, \mathbf{L}\right]$. Since $\omega$ is the instantaneous axis of rotation, according to Eq. (9), the point has instantaneous velocity $\mathbf{v}=\boldsymbol{\omega} \times \mathbf{r}$ directed normally to that plane. Since this is true for each point of the main axis (besides only one, with $\mathbf{r}=0$, i.e. the center of mass, which does not move), this axis as a whole has to move perpendicular to the common plane of vectors $\mathbf{L}, \omega$, and $\mathbf{n}_{3}$. Since such conclusion is valid for any moment of time, it means that vectors $\omega$ and $\mathbf{n}_{3}$ rotate about the space-fixed vector $\mathbf{L}$ together, with some angular velocity $\omega_{\text {pre }}$, at each moment staying in one plane. This effect is usually called the free precession (or "torque-

[^82]free", or "regular") precession, and has to be clearly distinguished it from the completely different effect of the torque-induced precession which will be discussed in the next section.

In order to calculate $\omega_{\text {pre }}$, let us present the instant vector $\omega$ as a sum of not its Cartesian coordinates (as in Fig. 9a), but rather of two non-orthogonal vectors directed along $\mathbf{n}_{3}$ and $\mathbf{L}$ (Fig. 9b):

$$
\begin{equation*}
\boldsymbol{\omega}=\omega_{\mathrm{rot}} \mathbf{n}_{3}+\omega_{\mathrm{pre}} \mathbf{n}_{L}, \quad \mathbf{n}_{L} \equiv \frac{\mathbf{L}}{L} . \tag{6.57}
\end{equation*}
$$

It is clear from Fig. 9 b that $\omega_{\text {rot }}$ has the meaning of the angular velocity of body rotation of the body about its main principal axis, while $\omega_{\text {pre }}$ is the angular velocity of rotation of that axis about the constant direction of vector $\mathbf{L}$, i.e. the frequency of precession. Now the latter frequency may be readily calculated from the comparison of two panels of Fig. 9, by noticing that the same angle $\theta$ between vectors $\mathbf{L}$ and $\mathbf{n}_{3}$ participates in two relations:

$$
\begin{equation*}
\sin \theta=\frac{L_{1}}{L}=\frac{\omega_{1}}{\omega_{\mathrm{pre}}} \tag{6.58}
\end{equation*}
$$

Since axis $\mathbf{n}_{1}$ is principal, we may use Eq. (26) for $j=1$, i.e. $L_{1}=I_{1} \omega_{1}$, to eliminate $\omega_{1}$ from Eq. (58), and get a very simple formula

$$
\begin{equation*}
\omega_{\mathrm{pre}}=\frac{L}{I_{1}} . \tag{6.59}
\end{equation*}
$$

[^83]This result shows that the precession frequency is constant and independent of the alignment of vector $\mathbf{L}$ with the main principal axis $\mathbf{n}_{3}$, while the amplitude of this motion (characterized by angle $\theta$ ) does depend on the alignment, and vanishes if $\mathbf{L}$ is parallel to $\mathbf{n}_{3} .{ }^{8}$ Note also that if all principal moments of inertia are of the same order, $\omega_{\text {pre }}$ is of the same order as the total angular velocity $\omega=|\omega|$ of rotation.

Now, let us briefly discuss the free precession in the general case of an "asymmetric top", i.e. a body with $I_{1} \neq I_{2} \neq I_{3}$. In this case the effect is more complex because here not only the direction but also the magnitude of the instantaneous angular velocity $\omega$ may evolve in time. If we are only interested in the relation between the instantaneous values of $\omega_{j}$ and $L_{j}$, i.e. the "trajectories" of vectors $\omega$ and $\mathbf{L}$ as observed from the reference frame $\left\{\mathbf{n}_{1}, \mathbf{n}_{2}, \mathbf{n}_{3}\right\}$ of the principal axes of the body (rather than an explicit law of their time evolution), they may be found directly from the conservation laws. (Let me emphasize again that vector $\mathbf{L}$, being constant in an inertial frame, generally evolves in the frame rotating with the body.) Indeed, Eq. (55) may be understood as the equation of an ellipsoid in Cartesian coordinates $\left\{\omega_{1}\right.$, $\left.\omega_{2}, \omega_{3}\right\}$, so that for free body, vector $\omega$ has to stay on the surface of that ellipsoid. ${ }^{9}$ On the other hand, since the reference frame rotation preserves the length of any vector, the magnitude (but not direction!) of vector $\mathbf{L}$ is also an integral of motion in the moving frame, and we can write

$$
\begin{equation*}
L^{2} \equiv \sum_{j=1}^{3} L_{j}^{2}=\sum_{j=1}^{3} I_{j}^{2} \omega_{j}^{2}=\text { const } \tag{6.60}
\end{equation*}
$$

[^84]Hence the trajectory of vector $\omega$ follows the closed curve formed by the intersection of two ellipsoids, (55) and (60). It is evident that this trajectory is generally "taco-edge-shaped", i.e. more complex than a plane circle but never very complex either.

The same argument may be repeated for vector $\mathbf{L}$, for whom the first form of Eq. (60) descries a sphere, and Eq. (55), another ellipsoid:

$$
\begin{equation*}
T_{\mathrm{rot}}=\sum_{j=1}^{3} \frac{1}{2 I_{j}} L_{j}^{2}=\text { const } . \tag{6.61}
\end{equation*}
$$

On the other hand, if we are interested in the trajectory of vector $\omega$ in an inertial frame (in which vector $\mathbf{L}$ stays still), we may note that the general relation (15) for the same rotational energy $T_{\text {rot }}$ may also be rewritten as

$$
\begin{equation*}
T_{\mathrm{rot}}=\frac{1}{2} \sum_{j=1}^{3} \omega_{j} \sum_{j^{\prime}=1}^{3} I_{i j^{\prime}} \omega_{j^{\prime}} \tag{6.62}
\end{equation*}
$$

But according to the Eq. (22), the second sum in the right-hand part is nothing more than $L_{j}$, so that

$$
\begin{equation*}
T_{\mathrm{rot}}=\frac{1}{2} \sum_{j=1}^{3} \omega_{j} L_{j}=\frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{L} . \tag{6.63}
\end{equation*}
$$

This equation shows that for a free body ( $T_{\text {rot }}=$ const, $\mathbf{L}=$ const), even is vector $\omega$ changes in time, its end point should stay within a plane perpendicular to angular momentum $\mathbf{L}$. (Earlier, we have seen that for the particular case of the symmetric top - see Fig. 9b, but for an asymmetric top, the trajectory of the end point may not be circular.)

If we are interested not only in the trajectory of vector $\omega$, but also its explicit evolution in time, it may be calculated using the general Eq. (33) presented in principal components $\omega_{j}$. For that, we have to recall that Eq. (33) is only valid in an inertial reference frame, while the frame $\left\{\mathbf{n}_{1}, \mathbf{n}_{2}, \mathbf{n}_{3}\right\}$ may rotate with the body and hence is generally not inertial. We may handle this problem by applying to vector $\mathbf{L}$ the general relation (8):

$$
\begin{equation*}
\left.\frac{d \mathbf{L}}{d t}\right|_{\text {in lab }}=\left.\frac{d \mathbf{L}}{d t}\right|_{\text {in mov }}+\boldsymbol{\omega} \times \mathbf{L} . \tag{6.64}
\end{equation*}
$$

Combining it with Eq. (33), in the moving frame we get

$$
\begin{equation*}
\frac{d \mathbf{L}}{d t}+\boldsymbol{\omega} \times \mathbf{L}=\boldsymbol{\tau} \tag{6.65}
\end{equation*}
$$

where $\tau$ is the external torque. In particular, for the principal-axis components $L_{j}$, related to components $\omega_{j}$ by Eq. (26), Eq. (65) is reduced to a set of three scalar Euler equations

$$
\begin{equation*}
I_{j} \dot{\omega}_{j}+\left(I_{j^{\prime \prime}}-I_{j^{\prime}}\right) \omega_{j^{\prime}} \omega_{j^{\prime \prime}}=\tau_{j} \tag{6.66}
\end{equation*}
$$

where the set of indices $\left\{j, j^{\prime}, j^{\prime \prime}\right\}$ has to follow the usual "right" order-e.g., $\{1,2,3\}$, etc. ${ }^{10}$

[^85]In order to get a feeling how do the Euler equations work, let us return to the case of a free symmetric top ( $\tau_{1}=\tau_{2}=\tau_{3}=0, I_{1}=I_{2} \neq I_{3}$ ). In this case, $I_{1}-I_{2}=0$, so that Eq. (66) with $j=3$ yields $\omega_{3}$ $=$ const, while the equations for $j=1$ and $j=2$ take the simple form

$$
\begin{equation*}
\dot{\omega}_{1}=-\Omega_{\mathrm{pre}} \omega_{2}, \quad \dot{\omega}_{2}=\Omega_{\mathrm{pre}} \omega_{1}, \tag{6.67}
\end{equation*}
$$

where $\Omega_{\text {pre }}$ is a constant determined by the system parameters and initial conditions:

$$
\begin{equation*}
\Omega_{\mathrm{pre}} \equiv \omega_{3} \frac{I_{3}-I_{1}}{I_{1}} \tag{6.68}
\end{equation*}
$$

Obviously, Eqs. (67) have a sinusoidal solution with frequency $\Omega_{\text {pre }}$, and describe uniform rotation of vector $\omega$, with that frequency, about the main axis $\mathbf{n}_{3}$. This is just another presentation of the torque-free precession analyzed above, this time as observed from the rotating body. Evidently, $\Omega_{\text {pre }}$ is substantially different from the frequency $\omega_{\text {pre }}(59)$ of the precession as observed from the lab frame; for example, the former frequency vanishes for the spherical top (with $I_{1}=I_{2}=I_{3}$ ), while the latter frequency tends to the rotation frequency.

Unfortunately, for the rotation of an asymmetric top (i.e., an arbitrary rigid body), when no component $\omega_{j}$ is conserved, the Euler equations (66) are strongly nonlinear even in the absence of the external torque, and a discussion of their solutions would take more time than I can afford. ${ }^{11}$

### 6.5. Torque-induced precession

The dynamics of rotation becomes even more complex in the presence of external forces. Let us consider the most important and counter-intuitive effect of torque-induced precession, for the simplest case of an axially-symmetric body (which is a particular case of the symmetric top, $I_{1}=I_{2} \neq I_{3}$ ) rapidly spinning about his symmetry axis, and supported at some point $A$ of that axis, that does not coincide with the center of mass $O$ - see Fig. 10. Without external forces, such top would retain the direction of its rotation axis that would always coincide with the direction of the angular momentum:

$$
\begin{equation*}
\mathbf{L}=I_{3} \mathbf{\omega}=I_{3} \omega_{\mathrm{rot}} \mathbf{n}_{3} \tag{6.69}
\end{equation*}
$$


(a)

(b)

[^86]The uniform gravity field creates bulk-distributed forces that, as we know from the analysis of the physical pendulum in Sec. 3, are equivalent to a single force $M \mathbf{g}$ applied in the center of mass - in Fig. 10, point $O$. The torque of the force relative to the support point $A$ is

$$
\begin{equation*}
\boldsymbol{\tau}=\left.\mathbf{r}_{O}\right|_{\text {in } A} \times M \mathbf{g}=M / \mathbf{n}_{3} \times \mathbf{g} . \tag{6.70}
\end{equation*}
$$

Hence the general equation (33) of the angular momentum (valid in the inertial "lab" frame, in which point $A$ rests) becomes

Precession: equation

$$
\begin{equation*}
\dot{\mathbf{L}}=M l \mathbf{n}_{3} \times \mathbf{g} . \tag{6.71}
\end{equation*}
$$

Despite the apparent simplicity of this (exact!) equation, its analysis is straightforward only in the limit of relatively high rotation velocity $\omega_{\text {rot }}$ or, alternatively, very small torque. In this limit, we may, in the $0^{\text {th }}$ approximation, still use Eq. (69) for $\mathbf{L}$. Then Eq. (71) shows that vector $\dot{\mathbf{L}}$ is perpendicular to both $\mathbf{n}_{3}$ (and hence $\mathbf{L}$ ) and $\mathbf{g}$, i.e. lies within the horizontal plane, and is perpendicular to the horizontal component $\mathbf{L}_{x y}$ of vector $\mathbf{L}$ - see Fig. 10b. Since the magnitude of this vector is constant, $|\dot{\mathbf{L}}|=m g l \sin \theta$, vector $\mathbf{L}$ (and hence the body's main axis) rotates about the vertical axis with angular velocity

Precession: frequency

$$
\begin{equation*}
\omega_{\mathrm{pre}}=\frac{|\dot{\mathbf{L}}|}{L_{x y}}=\frac{M g l \sin \theta}{L \sin \theta}=\frac{M g l}{L}=\frac{M g l}{I_{3} \omega_{\mathrm{rot}}} . \tag{6.72}
\end{equation*}
$$

Thus, very counter-intuitively, the fast-rotating top "does not want to" follow the external, vertical force and, in addition to fast spinning about the symmetry axis $\mathbf{n}_{3}$, also performs a revolution, called the torque-induced precession, about the vertical axis. Note that, similarly to the free-precession frequency (59), the torque-induced precession frequency (72) does not depend on the initial (and sustained) angle $\theta$. However, the torque-induced precession frequency is inversely (rather than directly) proportional to $\omega$, and is typically much lower. This relative slowness is also required for the validity of our simple theory of this effect. Indeed, in our approximate treatment we have used Eq. (69), i.e. neglected precession's contribution to the angular momentum vector $\mathbf{L}$. This is only possible if the contribution is relatively small, $I \omega_{\text {pre }} \ll I_{3} \omega_{\text {rot }}$, where $I$ is a certain effective moment of inertia for the precession (to be worked out later). Using our result (72), this condition may be rewritten as

$$
\begin{equation*}
\omega_{\mathrm{rot}} \gg\left(\frac{M g l I}{I_{3}^{2}}\right)^{1 / 2} \tag{6.73}
\end{equation*}
$$

For a body of not too extreme proportions, i.e. with all linear dimensions of the order of certain length $l$, all inertia moments are of the order of $M l^{2}$, so that the right-hand part of Eq. (73) is of the order of $(g / l)^{1 / 2}$, i.e. comparable with the eigenfrequency of the same body as the physical pendulum, i.e. at the absence of fast rotation.

In order to develop a qualitative theory that could take us beyond such approximate treatment, the Euler equations (66) may be used, but are not very convenient. A better approach, suggested by the same L. Euler, is to introduce a set of three independent angles between the principal axes $\left\{\mathbf{n}_{1}, \mathbf{n}_{2}, \mathbf{n}_{3}\right\}$ bound to the rigid body, and axes $\left\{\mathbf{n}_{x}, \mathbf{n}_{y}, \mathbf{n}_{z}\right\}$ of an inertial reference frame (Fig. 11), and then express the basic equation (33) of rotation, via these angles. There are several possible options for the definition of
such angles, ${ }^{12}$ Fig. 11 shows the set of Euler angels, most convenient for discussion of fast rotation. As one can see at the figure, the first Euler angle, $\theta$, is the usual polar angle measured from axis $\mathbf{n}_{z}$ to axis $\mathbf{n}_{3}$. The second one is the azimuthal angle $\varphi$, measured from axis $\mathbf{n}_{x}$ to the so-called line of nodes formed by the intersection of planes $\left[\mathbf{n}_{x}, \mathbf{n}_{y}\right]$ and $\left[\mathbf{n}_{1}, \mathbf{n}_{2}\right]$. The last Euler angle, $\psi$, is measured within plane [ $\mathbf{n}_{1}, \mathbf{n}_{2}$ ], from the line of nodes to axis $\mathbf{n}_{1}$. In the simple picture of the force-induced precession of a symmetric top, which was derived above, angle $\theta$ is constant, angle $\psi$ changes very rapidly, with the rotation velocity $\omega_{\text {rot }}$, while angle $\varphi$ grows with the precession frequency $\omega_{\text {pre }}(72)$.
 the Euler angles.

Now we can express the principal-axes components of the instantaneous angular velocity vector, $\omega_{1}, \omega_{2}$, and $\omega_{3}$, as measured in the lab reference frame, in terms of the Euler angles. It may be easily done calculating, from Fig. 11, the contributions to the change of Euler angles to each principal axis, and then adding them up. The result is

$$
\begin{aligned}
& \omega_{1}=\dot{\varphi} \sin \theta \sin \psi+\dot{\theta} \cos \psi, \\
& \omega_{2}=\dot{\varphi} \sin \theta \cos \psi-\dot{\theta} \sin \psi, \\
& \omega_{3}=\dot{\varphi} \cos \theta+\dot{\psi}
\end{aligned}
$$

These formulas allow the expression of the kinetic energy of rotation (25) and the angular momentum components (26) in terms of the generalized coordinates $\theta, \varphi$, and $\psi$, and use then powerful Lagrangian formalism to derive their equations of motion. This is especially simple to do in the case of symmetric tops (with $I_{1}=I_{2}$ ), because plugging Eqs. (74) into Eq. (25) we get an expression,

$$
\begin{equation*}
T_{\mathrm{rot}}=\frac{I_{1}}{2}\left(\dot{\theta}^{2}+\dot{\varphi}^{2} \sin ^{2} \theta\right)+\frac{I_{3}}{2}(\dot{\varphi} \cos \theta+\dot{\psi})^{2}, \tag{6.75}
\end{equation*}
$$

which does not include explicitly either $\varphi$ or $\psi$. (This reflects the fact that for a symmetric top we can always select axis $\mathbf{n}_{1}$ to coincide with the line of nodes, and hence take $\psi=0$ at the considered moment of time. Note that this trick does not mean we can take $\dot{\psi}=0$, because axis $\mathbf{n}_{1}$, as observed from the inertial reference frame, moves!) Now we should not forget that at the torque-induced precession, the center of mass moves as well (see Fig. 10), so that according to Eq. (14), the total kinetic energy of the body is the sum of two terms,

[^87]\[

$$
\begin{equation*}
T=T_{\mathrm{rot}}+T_{\mathrm{tran}}, \quad T_{\mathrm{tran}}=\frac{M}{2} V^{2}=\frac{M}{2} l^{2}\left(\dot{\theta}^{2}+\dot{\varphi}^{2} \sin ^{2} \theta\right), \tag{6.76}
\end{equation*}
$$

\]

while the potential energy is just

$$
\begin{equation*}
U=\text { Mgl } \cos \theta+\text { const } \tag{6.77}
\end{equation*}
$$

Now we could readily write the Lagrangian equations of motion for the Euler angles, but it is better to immediately notice that according to Eqs. (75)-(77), the Lagrangian function, $T-U$, does not depend explicitly on "cyclic" coordinates $\varphi$ and $\psi$, so that the corresponding generalized momenta are conserved:

$$
\begin{gather*}
p_{\varphi} \equiv \frac{\partial T}{\partial \dot{\varphi}}=I_{A} \dot{\varphi} \sin ^{2} \theta+I_{3}(\dot{\varphi} \cos \theta+\dot{\psi}) \cos \theta=\text { const },  \tag{6.78}\\
p_{\psi} \equiv \frac{\partial T}{\partial \dot{\psi}}=I_{3}(\dot{\varphi} \cos \theta+\dot{\psi})=\text { const }, \tag{6.79}
\end{gather*}
$$

where, according to Eq. (29), $I_{A} \equiv I_{1}+M l^{2}$ is just the body's moment of inertia for rotation about a horizontal axis passing through the support point $A$. According to the last of Eqs. (74), $p_{\psi}$ is just $L_{3}$, the angular momentum's component along the rotating axis $\mathbf{n}_{3}$. On the other hand, by its definition $p_{\varphi}$ is $L_{z}$, the same vector L's component along the static axis z. (Actually, we could foresee in advance the conservation of both these components of $\mathbf{L}$, because vector (70) of the external torque is perpendicular to both $\mathbf{n}_{3}$ and $\mathbf{n}_{\mathrm{z}}$.) Using these notions, and solving the simple system of linear equations (78)-(79) for the angle derivatives, we get

$$
\begin{equation*}
\dot{\varphi}=\frac{L_{z}-L_{3} \cos \theta}{I_{A} \sin ^{2} \theta}, \quad \dot{\psi}=\frac{L_{3}}{I_{3}}-\frac{L_{z}-L_{3} \cos \theta}{I_{A} \sin ^{2} \theta} \cos \theta \tag{6.80}
\end{equation*}
$$

One more conserved quantity in this problem is the full mechanical energy ${ }^{13}$

$$
\begin{equation*}
E \equiv T+U=\frac{I_{A}}{2}\left(\dot{\theta}^{2}+\dot{\varphi}^{2} \sin ^{2} \theta\right)+\frac{I_{3}}{2}(\dot{\varphi} \cos \theta+\dot{\psi})^{2}+M g l \cos \theta . \tag{6.81}
\end{equation*}
$$

Plugging Eqs. (80) into Eq. (81), we get a first-order differential equation for angle $\theta$, which may be presented in the following physically transparent form:

$$
\begin{equation*}
\frac{I_{A}}{2} \dot{\theta}^{2}+U_{\mathrm{ef}}(\theta)=E, \quad U_{\mathrm{ef}}(\theta) \equiv \frac{\left(L_{z}-L_{3} \cos \theta\right)^{2}}{2 I_{A} \sin ^{2} \theta}+\frac{L_{3}^{2}}{2 I_{3}}+M g l \cos \theta+\text { const } . \tag{6.82}
\end{equation*}
$$

Thus, similarly to the planetary problems considered in Sec. 3.5 , the symmetric top precession has been reduced (without any approximations!) to a 1 D problem of motion of one of its degrees of freedom, the polar angle $\theta$, in an effective potential $U_{\text {ef }}(\theta)$, which is the sum of the real potential energy $U(77)$ and a contribution from the kinetic energy of motion along two other angles. In the absence of rotation about axes $\mathbf{n}_{z}$ and $\mathbf{n}_{3}$ (i.e., $L_{z}=L_{3}=0$ ), Eq. (82) is reduced to the first integral of the equation (40) of motion of a physical pendulum. If the rotation is present, then (besides the case of special initial

[^88]conditions when $\theta(0)=0$ and $\left.L_{z}=L_{3}\right),{ }^{14}$ the first contribution to $U_{\text {ef }}(\theta)$ diverges at $\theta \rightarrow 0$ and $\pi$, so that the effective potential energy has a minimum at some finite value $\theta_{0}$ of the polar angle $\theta$.

If the initial angle $\theta(0)$ equals this $\theta_{0}$, i.e. if the initial effective energy is equal to its minimum value $U_{\text {eff }}\left(\theta_{0}\right)$, the polar angle remains constant through the motion: $\theta(t)=\theta_{0}$. This corresponds to the pure torque-induced precession whose angular velocity is given by the first of Eqs. (80):

$$
\begin{equation*}
\omega_{\mathrm{pre}} \equiv \dot{\varphi}=\frac{L_{z}-L_{3} \cos \theta_{0}}{I_{A} \sin ^{2} \theta_{0}} . \tag{6.83}
\end{equation*}
$$

The condition for finding $\theta_{0}, d U_{\mathrm{ef}} / d \theta=0$, is a transcendent algebraic equation that cannot be solved analytically for arbitrary parameters. However, in the high spinning speed limit (73), this is possible. Indeed, in this limit the potential energy contribution to $U_{\text {ef }}$ is small, and we may analyze its effect by successive approximations. In the $0^{\text {th }}$ approximation, i.e. at $\mathrm{Mgl}=0$, the minimum of $U_{\text {ef }}$ is evidently achieved at $\cos \theta_{0}=L_{z} / L_{3}$, giving zero precession frequency (83). In the next, $1^{\text {st }}$ approximation, we may require that at $\theta=\theta_{0}$, the derivative of first term in the right-hand part of Eq. (82) for $U_{\text {ef }}$ over $\cos \theta$, equal to $-L_{z}\left(L_{z}-L_{3} \cos \theta\right) / I_{A} \sin ^{2} \theta,{ }^{15}$ is cancelled with that of the gravity-induced term, equal to Mgl . This immediately yields $\omega_{\text {pre }}=\left(L_{z}-L_{3} \cos \theta_{0}\right) / I_{A} \sin ^{2} \theta_{0}=\mathrm{Mgl} / L_{3}$, so that taking $L_{3}=I_{3} \omega_{\text {rot }}$ (as we may in the high spinning speed limit), we recover the simple expression (72).

The second important result that readily follows from Eq. (82) is the exact expression the threshold value of the spinning speed for a vertically rotating top $\left(\theta=0, L_{z}=L_{3}\right)$. Indeed, in the limit $\theta$ $\rightarrow 0$ this expression may be readily simplified:

$$
\begin{equation*}
U_{\mathrm{ef}}(\theta) \approx \mathrm{const}+\left(\frac{L_{3}^{2}}{8 I_{A}}-\frac{M g l}{2}\right) \theta^{2} . \tag{6.84}
\end{equation*}
$$

This formula shows that if $\omega_{3}=L_{3} / I_{3}$ (i.e. the angular velocity that was called $\omega_{\text {rot }}$ in the approximate theory) is higher than the following threshold value,

$$
\begin{equation*}
\omega_{\mathrm{th}} \equiv 2\left(\frac{M g l I_{A}}{I_{3}^{2}}\right)^{1 / 2} \tag{6.85}
\end{equation*}
$$

then the coefficient at $\theta^{2}$ in Eq. (84) is positive, so that $U_{\text {ef }}$ has a stable minimum at $\theta_{0}=0$. On the other hand, if $\omega_{3}$ is decreased below $\omega_{\mathrm{th}}$, the fixed point becomes unstable, so that the top falls down. Note that if we take $I=I_{A}$ in condition (73) of the approximate treatment, it acquires a very simple sense: $\omega_{\text {rot }}$ $\gg \omega_{\mathrm{th}}$.

Finally, Eqs. (82) give a natural description of one more phenomenon. If the initial energy is larger than $U_{\text {ef }}\left(\theta_{0}\right)$, angle $\theta$ oscillates between two classical turning points on both sides of the fixed point $\theta_{0}$. The law and frequency of these oscillations may be found exactly as in Sec. 3.3 - see Eqs. (3.27) and (3.28). At $\omega_{3} \gg \omega_{\mathrm{th}}$, this motion is a fast rotation of the symmetry axis $\mathbf{n}_{3}$ of the body about its average position performing the slow precession. These oscillations are called nutations, but

[^89]physically they are absolutely similar to the free precession that was analyzed in the previous section, and the order of magnitude of their frequency is still given by Eq. (59).

It may be proved that small energy dissipation (not taken into account in our analysis) leads first to a decay of nutations, then to a slower drift of the precession angle $\theta_{0}$ to zero and, finally, to a gradual decay of the spinning speed $\omega_{3}$ until it reaches the threshold (85) and the top falls down.

### 6.6. Non-inertial reference frames

Before moving on to the next chapter, let us use the results of our discussion of rotation kinematics in Sec. 1 to complete the analysis of transfer between two reference frames, started in the introductory Chapter 1 - see Fig. 1.2. Indeed, the differentiation rule described by Eq. (8) and derived for an arbitrary vector $\mathbf{A}$ enables us to relate not only radius-vectors, but also the velocities and accelerations of a particle as measured in two reference frames: the "lab" frame $O$ ' (which will be later assumed inertial) and the "moving" (possibly rotating) frame $O-$ see Fig. 12.


Fig. 6.12. General case of transfer between two reference frames.

As this picture shows, even if frame $O$ rotates relative to the lab frame, the radius-vectors are still related, at any moment of time, by the simple Eq. (1.7). In the notation of Fig. 12 it reads

$$
\begin{equation*}
\left.\mathbf{r}^{\prime}\right|_{\text {in lab }}=\left.\mathbf{r}_{O}\right|_{\text {in lab }}+\left.\mathbf{r}\right|_{\text {in lab }} . \tag{6.86}
\end{equation*}
$$

However, as was discussed in Sec. 1, for velocities the general addition rule is already more complex. In order to find it, let us differentiate Eq. (86) over time:

$$
\begin{equation*}
\left.\frac{d}{d t} \mathbf{r}^{\prime}\right|_{\text {in lab }}=\left.\frac{d}{d t} \mathbf{r}_{O}\right|_{\text {in lab }}+\left.\frac{d}{d t} \mathbf{r}\right|_{\text {in lab }} . \tag{6.87}
\end{equation*}
$$

The left-hand part of this relation is evidently particle's velocity as measured in the lab frame, and the first term in the right-hand part of Eq. (87) is the velocity of point $O$, as measured in the same frame. The last term is more complex: we need to differentiate vector $\mathbf{r}$ that connects point $O$ with the particle (Fig. 12), considering how its evolution looks from the lab frame. Due to the possible mutual rotation of frames $O$ and $O$ ', that term may not be zero even if the particle does not move relative to frame $O$.

Fortunately, we have already derived the general Eq. (8) to analyze situations exactly like this one. Taking $\mathbf{A}=\mathbf{r}$, we may apply it to the last term of Eq. (87), to get

$$
\begin{equation*}
\left.\mathbf{v}\right|_{\text {in lab }}=\left.\mathbf{v}_{O}\right|_{\text {in lab }}+(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r}) \tag{6.88}
\end{equation*}
$$

where $\omega$ is the instantaneous angular velocity of an imaginary rigid body connected to the moving reference frame (or we may say, of the frame as such), an $\mathbf{v}$ is $d \mathbf{r} / d t$, as measured in the moving frame $O$, (Here and later in this section, all vectors without indices imply their observation from the moving frame.) Relation (88), on one hand, is a natural generalization of Eq. (10) for $\mathbf{v} \neq 0$; on the other hand, if $\omega=0$, it is reduced to simple Eq. (1.8) for the translational motion of frame $O$.

Now, in order to calculate acceleration, me may just repeat the trick: differentiate Eq. (88) over time, and then use Eq. (8) again, now for vector $\mathbf{A}=\mathbf{v}+\omega \times \mathbf{r}$. The result is

$$
\begin{equation*}
\left.\left.\mathbf{a}\right|_{\text {in lab }} \equiv \mathbf{a}_{o}\right|_{\text {in lab }}+\frac{d}{d t}(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r})+\boldsymbol{\omega} \times(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r}) . \tag{6.89}
\end{equation*}
$$

Carrying out the differentiation in the second term, we finally get the goal equation,

$$
\begin{equation*}
\left.\left.\mathbf{a}\right|_{\text {in lab }} \equiv \mathbf{a}_{o}\right|_{\text {in lab }}+\mathbf{a}+\dot{\boldsymbol{\omega}} \times \mathbf{r}+2 \boldsymbol{\omega} \times \mathbf{v}+\boldsymbol{\omega} \times(\boldsymbol{\omega} \times \mathbf{r}), \tag{6.90}
\end{equation*}
$$

where a is particle's acceleration, as measured in the moving frame. Evidently, Eq. (90) is a natural generalization of the simple Eq. (1.9) to the rotating frame case.

Now let the lab frame $O$ ' be inertial; then the $2^{\text {nd }}$ Newton law for a particle of mass $m$ is

$$
\begin{equation*}
\left.m \mathbf{a}\right|_{\text {in lab }}=\mathbf{F}, \tag{6.91}
\end{equation*}
$$

where $\mathbf{F}$ is the vector sum of all forces action on the particle. This is simple and clear; however, in many cases it is much more convenient to work in a non-inertial reference frames. For example, describing most phenomena on Earth's surface, in is rather inconvenient to use a reference frame resting on the Sun (or in the galactic center, etc.). In order to understand what we should pay for the convenience of using the moving frame, we may combine Eqs. (90) and (91) to write

$$
\begin{equation*}
m \mathbf{a}=\mathbf{F}-\left.m \mathbf{a}_{o}\right|_{\text {in lab }}-m \boldsymbol{\omega} \times(\boldsymbol{\omega} \times \mathbf{r})-2 m \boldsymbol{\omega} \times \mathbf{v}-m \dot{\boldsymbol{\omega}} \times \mathbf{r} . \tag{6.92}
\end{equation*}
$$

This result may be interpreted in the following way: if we want to use the $2^{\text {nd }}$ Newton law's analog in a non-inertial reference frame, we have to add, to the real net force $\mathbf{F}$ acting on a particle, four pseudoforce terms, called inertial forces, all proportional to particle's mass. Let us analyze them, while always remembering that these are just mathematical terms, not real forces. (In particular, it would be futile to seek for the $3^{\text {rd }}$ Newton law's counterpart for an inertial force.)

The first term, $-\left.m \mathbf{a}_{0}\right|_{\text {in }}$ lab, is the only one not related to rotation, and is well known from the undergraduate mechanics. (Let me hope the reader remembers all these weight-in-the-moving-elevator problems.) Despite its simplicity, this term has subtle and interesting consequences. As an example, let us consider a planet, such as our Earth, orbiting a star and also rotating about its own axis - see Fig. 13. The bulk-distributed gravity forces, acting on a planet from its star, are not quite uniform, because they obey the $1 / r^{2}$ gravity law (1.16a), and hence are equivalent to a single force applied to a point $A$ slightly offset from the planet's center of mass $O$ toward the star. For a spherically-symmetric planet, points $O$ and $A$ would be exactly aligned with the direction toward the star. However, real planets are not absolutely rigid, so that, due to the centrifugal "force" (to be discussed shortly), their rotation about their own axis makes them slightly elliptic - see Fig. 13. (For our Earth, this equatorial bulge is about 10 km in each direction.) As a result, the net gravity force does create a small torque relative to the center of mass $O$. On the other hand, repeating all the arguments of this section for a body (rather than a point), we may see that, in the reference frame moving with the planet, the inertial "force" $-\mathrm{Ma}_{O}$ (which is of
course equal to the total gravity force and directed from the star) is applied exactly to the center of mass and does not create a torque. As a result, this pair of forces creates a torque $\tau$ perpendicular to both the direction toward the star and the vector connecting points $O$ and $A$. (In Fig. 13, the torque vector is perpendicular to the plane of drawing). If angle $\delta$ between the planet's "polar" axis of rotation and the direction towards the star was fixed, then, as we have seen in the previous section, this torque would induce a slow axis precession about that direction. However, as a result of orbital motion, angle $\delta$ oscillates in time much faster (once a year) between values $(\pi / 2+\varepsilon)$ and $(\pi / 2-\varepsilon)$, where $\varepsilon$ is the axis tilt, i.e. angle between the polar axis (direction of vectors $\mathbf{L}$ and $\omega_{\text {rot }}$ ) and the normal to the ecliptic plane of the planet's orbit. (For the Earth, $\varepsilon \approx 23.4^{\circ}$.) A straightforward averaging over these fast oscillations ${ }^{16}$ shows that the torque leads to the polar axis precession about the axis perpendicular to the ecliptic plane, keeping angle $\varepsilon$ constant. For the Earth, the period, $T_{\text {pre }}=2 \pi / \omega_{\text {pre }}$, of this precession of the equinoxes (or "precession of the equator"), corrected to the substantial effect of Moon's gravity, is close to 26,000 years.


Fig. 6.13. Axial precession of a planet (with the equatorial bulge and the force line offset strongly exaggerated).

Returning to Eq. (92), the direction of the second term of its right-hand part, $\mathbf{F}_{c}=-m \omega \times(\omega \times \mathbf{r})$, called the centrifugal force, is always perpendicular to, and directed out of the instantaneous rotation axis - see Fig. 14.


Indeed, vector $\omega \times \mathbf{r}$ is perpendicular to both $\omega$ and $\mathbf{r}$ (in Fig. 14, normal to the picture plane and directed from the reader) and has magnitude $\omega r \sin \theta=\omega \rho$, where $\rho$ is the distance of the particle from the rotation axis. Hence the outer vector product, with the account of the minus sign, is normal to the rotation axis $\omega$, directed out from the axis, and equal to $\omega^{2} r \sin \theta=\omega^{2} \rho$. The "centrifugal force" is of

[^90]course just the result of the fact that the centripetal acceleration $\omega^{2} \rho$, explicit in the inertial reference frame, disappears in the rotating frame. For a typical location of the Earth ( $\rho \sim R_{\mathrm{E}} \approx 6 \times 10^{6} \mathrm{~m}$ ), with its angular velocity $\omega_{\mathrm{E}} \approx 10^{-4} \mathrm{~s}^{-1}$, the acceleration is rather considerable, of the order of $3 \mathrm{~cm} / \mathrm{s}^{2}$, i.e. $\sim 0.003$ $g$, and is responsible, in particular, for the largest part of the equatorial bulge mentioned above.

As an example of using the centrifugal "force" concept, let us return again to our "testbed" problem on the bead sliding along a rotating ring - see Figs. 1.5 and 2.1. In the non-inertial reference frame attached to the ring, we have to add, to real forces $m \mathbf{g}$ and $\mathbf{N}$ acting on the bead, the horizontal centrifugal "force" ${ }^{17}$ directed out of the rotation axis, with magnitude $m \omega^{2} \rho$. In the notations of Fig. 2.1, its component tangential to the ring equals $m \omega^{2} \rho \cos \theta=m \omega^{2} R \sin \theta \cos \theta$, and hence the Cartesian component of Eq. (92) along this direction is

$$
\begin{equation*}
m a=-m g \sin \theta+m \omega^{2} R \sin \theta \cos \theta . \tag{6.93}
\end{equation*}
$$

With $a=R \ddot{\theta}$, this gives us the equation of motion equivalent to Eq. (2.25), which had been derived in Sec. 2.2 (in the inertial frame) using the Lagrangian formalism.

The third term in the right-hand part of Eq. (92) is the so-called Coriolis force, ${ }^{18}$ which exists only if the particle moves in the rotating reference frame. Its physical sense may be understood by considering a projectile fired horizontally, say from the North Pole. From the point of view of the Earthbased observer, it will a subject of an additional Coriolis force $\mathbf{F}_{\mathrm{C}}=-2 m \omega \times \mathbf{v}$, directed westward, with magnitude $2 m \omega_{E} v$, where $\mathbf{v}$ is the main, southward component of the velocity. This force would cause the westward acceleration $a=2 \omega_{\mathrm{E}} \mathrm{V}$, and the resulting eastward deviation growing with time as $d=a t^{2} / 2$ $=\omega_{\mathrm{E}} v t^{2}-$ see Fig. 15. (This formula is exact only if $d$ is much smaller than the distance $r=v t$ passed by the projectile.) On the other hand, from the point of view of the inertial-frame observer, the projectile trajectory in the horizontal plane is a straight line, but during the flight time $t$, the Earth surface slips eastward from under the trajectory by distance $d=r \varphi=(v t)\left(\omega_{E} t\right)=\omega_{E} v t^{2}$ where $\varphi=\omega_{E} t$ is the azimuthal angle of the Earth rotation during the flight). Thus, both approaches give the same result.


Fig. 6.15. Trajectory of a projectile fired horizontally from the North Pole, from the point of view of an Earth-bound observer looking down. Circles show parallels, straight lines mark meridians.

Hence, the Coriolis "force" is just a fancy (but frequently very convenient) way of description of a purely geometric effect pertinent to rotation, from the point of view of the observer participating in it. This force is responsible, in particular, for the higher right banks of rivers in the Northern hemisphere, regardless of the direction of their flow - see Fig. 16. Despite the smallness of the Coriolis force (for a

[^91]typical velocity of the water in a river, $v \sim 1 \mathrm{~m} / \mathrm{s}$, it is equivalent to acceleration $a_{\mathrm{C}} \sim 10^{-2} \mathrm{~cm} / \mathrm{s}^{2} \sim 10^{-5}$ $g$ ), its multi-century effects may be rather prominent. ${ }^{19}$


Fig. 6.16. Coriolis "forces" due to Earth's rotation, in the Northern hemisphere.

The last, fourth term of Eq. (92), $-m \dot{\boldsymbol{\omega}} \times \mathbf{r}$, exists only when the rotation frequency changes in time, and may be interpreted as a local-position-specific addition to the first term.

Equation (92), derived above from the Newton equation (91), may be alternatively obtained from the Lagrangian approach, which also gives some important insights on energy at rotation. Let us use Eq. (88) to present the kinetic energy of the particle in an inertial frame in terms of $\mathbf{v}$ and $\mathbf{r}$ measured in a rotating frame:

$$
\begin{equation*}
T=\frac{m}{2}\left[\left.\mathbf{v}_{O}\right|_{\text {in lab }}+(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r})\right]^{2}, \tag{6.94}
\end{equation*}
$$

and use this expression to calculate the Lagrangian function. For the relatively simple case of particle motion in the field of potential forces, measured from a reference frame that performs pure rotation (so that $\mathbf{v}_{\text {O }}^{\text {in lab }}=0$ ) with a constant angular velocity $\omega$, the result is

$$
\begin{equation*}
L \equiv T-U=\frac{m}{2} v^{2}+m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})+\frac{m}{2}(\boldsymbol{\omega} \times \mathbf{r})^{2}-U=\frac{m}{2} v^{2}+m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})-U_{\mathrm{ef}}, \tag{6.95}
\end{equation*}
$$

where the effective potential energy, ${ }^{20}$

$$
\begin{equation*}
U_{\mathrm{ef}} \equiv U-\frac{m}{2}(\boldsymbol{\omega} \times \mathbf{r})^{2}, \tag{6.96}
\end{equation*}
$$

is just the sum of the real potential energy $U$ of the particle and the so-called centrifugal potential energy associated with the centrifugal "inertial force":

[^92]\[

$$
\begin{equation*}
\mathbf{F}_{c} \equiv-m \boldsymbol{\omega} \times(\boldsymbol{\omega} \times \mathbf{r})=-\nabla\left[-\frac{m}{2}(\boldsymbol{\omega} \times \mathbf{r})^{2}\right] . \tag{6.97}
\end{equation*}
$$

\]

Of course, the Lagrangian equations of motion derived from Eq. (95), considering the Cartesian components of $\mathbf{r}$ and $\mathbf{v}$ as generalized coordinates and velocities, coincide with Eq. (92) (with $\mathbf{a}_{\circ} \mathrm{lin}_{\mathrm{in}}=$ $\dot{\boldsymbol{\omega}}=0$, and $\mathbf{F}=-\nabla U$ ), but it is very informative to have a look at a by-product of this derivation, the generalized momentum corresponding to particle's coordinate $\mathbf{r}$ as measured in the rotating reference frame, ${ }^{21}$

$$
\begin{equation*}
\boldsymbol{p} \equiv \frac{\partial L}{\partial \mathbf{v}}=m(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r}) . \tag{6.98}
\end{equation*}
$$

According to Eq. (88), with $\left.\mathbf{v}_{O}\right|_{\text {in lab }}=0$, the expression in parentheses is just $\left.m \mathbf{v}\right|_{\text {in lab. }}$. However, from the point of view of the moving frame, i.e. not knowing about the physical sense of vector $\boldsymbol{p}=\left.m \mathbf{v}\right|_{\text {in lab }}$, we would have a reason to speak about two different momenta of the same particle, the so-called kinetic momentum $\mathbf{p}=m \mathbf{v}$ and the canonical momentum $\boldsymbol{p}=\mathbf{p}+m \omega \times \mathbf{r} .{ }^{22}$

Now let us calculate the Hamiltonian function $H$ and energy $E$ as functions of the same movingframe variables:

$$
\begin{align*}
H & \equiv \sum_{j=1}^{3} \frac{\partial L}{\partial v_{j}} v_{j}-L=\boldsymbol{p} \cdot \mathbf{v}-L=m \mathbf{v} \cdot(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r})-\left[\frac{m}{2} v^{2}+m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})-U_{\mathrm{ef}}\right]=\frac{m v^{2}}{2}+U_{\mathrm{ef}},  \tag{6.99}\\
E & \equiv T+U=\frac{m}{2} v^{2}+m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})+\frac{m}{2}(\boldsymbol{\omega} \times \mathbf{r})^{2}+U=\frac{m}{2} v^{2}+U_{\mathrm{ef}}+m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})+m(\boldsymbol{\omega} \times \mathbf{r})^{2} . \tag{6.100}
\end{align*}
$$

These expressions clearly show that $E$ and $H$ are not equal. In hindsight, this is not surprising, because the kinetic energy (94), expressed in the moving-frame variables, includes a term linear in $\mathbf{v}$, and hence is not a quadratic-homogeneous function of this generalized velocity. The difference of these functions may be presented as

$$
\begin{equation*}
E-H=m \mathbf{v} \cdot(\boldsymbol{\omega} \times \mathbf{r})+m(\boldsymbol{\omega} \times \mathbf{r})^{2}=m(\mathbf{v}+\boldsymbol{\omega} \times \mathbf{r}) \cdot(\boldsymbol{\omega} \times \mathbf{r})=\left.m \mathbf{v}\right|_{\text {in lab }} \cdot(\boldsymbol{\omega} \times \mathbf{r}) . \tag{6.101}
\end{equation*}
$$

Now using the operand rotation rule again, we may transform this expression into a even simpler form: ${ }^{23}$

$$
\begin{equation*}
E-H=\boldsymbol{\omega} \cdot\left(\mathbf{r} \times\left. m \mathbf{v}\right|_{\text {in lab }}\right)=\boldsymbol{\omega} \cdot(\mathbf{r} \times \boldsymbol{p})=\left.\boldsymbol{\omega} \cdot \mathbf{L}\right|_{\text {in lab }} \tag{6.102}
\end{equation*}
$$

$E$ and $H$ at rotation

Let us evaluate this difference for our testbed problem - see Fig. 2.1. In this case, vector $\omega$ is aligned with axis $z$, so that of all Cartesian components of vector $\mathbf{L}$, only component $L_{z}$ is important for the scalar product (102). This component evidently equals $I_{z} \omega=m \rho^{2} \omega=m \omega R^{2} \sin ^{2} \theta$, so that

$$
\begin{equation*}
E-H=m \omega^{2} R^{2} \sin ^{2} \theta, \tag{6.103}
\end{equation*}
$$

[^93]i.e. the same result that follows from the direct subtraction of Eqs. (2.40) and (2.41).

The last form of Eq. (99) shows that in the rotating frame, the Hamiltonian function of a particle has a very simple physical sense. It is conserved, and hence may serve as an integral of motion, in many important situations when $\mathbf{L}$, and hence $E$, are not - our testbed problem is again a very good example.

### 6.7. Exercise problems

6.1. Calculate the principal moments of inertia for the following rigid bodies:
(i)

(ii)

(iii)

(iv)

(i) a thin, plane round hoop,
(ii) a flat uniform round disk,
(iii) a thin spherical shell, and
(iv) a uniform solid sphere.

Compare the results assuming that all the bodies have the same radius $R$ and mass $M$.
6.2. Calculate the principal moments of inertia for the following rigid bodies (see Fig. below):

(i) an equilateral triangle made of thin rods with a uniform linear mass density $\mu$,
(ii) a thin plate in the shape of an equilateral triangle, with a uniform areal mass density $\sigma$, and
(iii) a tetrahedral pyramid made of a heavy material with a uniform bulk mass density $\rho$.

Assuming that the total mass of the three bodies is the same, compare the results and give an interpretation of their difference.
6.3. Prove that Eqs. (34)-(36) are valid for rotation about a fixed axis, even if it does not pass through the center of mass, if all distances $\rho_{z}$ are measured from that axis.
6.4. The end of a uniform, thin, heavy rod of length $2 l$ and mass $m$, initially at rest, is hit by a bullet of mass $m^{\prime}$, flying with velocity $v_{0}$, which gets stuck in the stick - see Fig. on the right. Use two different approaches to calculate the velocity of the opposite end of the rod right after the collision.

6.5. A uniform ball is placed on a horizontal plane, while rotating with an angular velocity $\omega_{0}$, but having no initial linear velocity. Calculate the angular velocity after ball's slippage stops, assuming the usual simple approximation of the kinetic friction force: $F_{f}=\mu N$, where $N$ is a pressure between the surfaces, and $\mu$ is a velocity-independent coefficient.
6.6. A body may rotate about fixed horizontal axis $A$ - see Fig. 5. Find the frequency of its small oscillations, in a uniform gravity field, as a function of distance $l$ of the axis from body's center of mass $O$, and analyze the result.
6.7. A thin uniform bar of mass $M$ and length $l$ is hung on a light thread of length $l$ ' (like a "chime" bell - see Fig. on the right). Find:
(i) the equations of motion of the system (within the plane of drawing);
(ii) the eigenfrequencies of small oscillations near the equilibrium;
(iii) the distribution coefficients for each oscillation mode.

Sketch the oscillation modes for the particular case $l=l$ '.

6.8. A solid, uniform, round cylinder of mass $M$ can roll, without slipping, over a concave, round cylindrical surface of a block of mass $M^{\prime}$, in a uniform gravity field - see Fig. on the right. The block can slide without friction on a horizontal surface. Using the Lagrangian formalism,

(i) find the frequency of small oscillations of the system near the equilibrium, and
(ii) sketch the oscillation mode for the particular case $M^{\prime}=M, R^{\prime}=2 R$.
6.9. A uniform solid hemisphere of radius $R$ is placed on a horizontal plane - see Fig. on the right. Find the frequency of its small oscillations within a vertical plane, for two ultimate cases:
(i) there is no friction between the hemisphere and plane surfaces, and
(ii) the static friction is so strong that there is no slippage between
 these surfaces.
6.10. For the "sliding ladder" problem started in Sec. 3 (see Fig. 7), find the critical value $\alpha_{\mathrm{c}}$ of angle $\alpha$ at which the ladder loses contact with the vertical wall, assuming that it starts sliding from the vertical position with a negligible initial velocity.
6.11.* A rigid, straight, uniform rod of length $l$, with the lower end on a pivot, falls in a uniform gravity field - see Fig. on the right. Neglecting friction, calculate the distribution of the bending torque $\tau$ along its length, and analyze the result.

6.12. Six similar, uniform rods of length $l$ and mass $m$ are connected by light joints so that they may rotate, without friction, versus each other, forming a planar polygon. Initially, the polygon was at rest, and had the correct hexagon shape - see Fig. on the right. Suddenly, an external force $\mathbf{F}$ is applied to the middle of one rod, in the direction of hexagon's symmetry center. Calculate the accelerations: of the rod to which the force is applied (a), and of the opposite $\operatorname{rod}\left(a^{\prime}\right)$, immediately after the application of the force.

6.13. A rectangular cuboid (parallelepiped) with sides $a_{1}, a_{2}$, and $a_{3}$, made of a material with constant density $\rho$, is rotated, with a constant angular velocity $\omega$, about one of its space diagonals - see Fig. on the right. Calculate the torque $\tau$ necessary to sustain such rotation.

6.14. One end of a light shaft of length $l$ is firmly attached to the center of a uniform solid disk of radius $R \ll l$ and mass $M$, whole plane is perpendicular to the shaft. Another end of the shaft is attached to a vertical axis (see Fig. on the right) so that the shaft may rotate about the axis without friction. The disk rolls, without slippage, over a horizontal surface, so
 that the whole system rotates about the vertical axis with a constant angular velocity $\omega$. Calculate the (vertical) supporting force exerted on the disk by the surface.
6.15. An air-filled balloon is placed inside a container filled with water that moves in space, in a negligible gravity field. Suddenly, force $\mathbf{F}$ is applied to the container, pointing in a certain direction. What direction would the balloon move relative to the container?
6.16. Calculate the height of solar tides on a large ocean, using the following simplifying assumptions: the tide period ( $1 / 2$ of Earth's day) is much longer than the period of all ocean waves, the Earth (of mass $M_{\mathrm{E}}$ ) is a sphere of radius $R_{\mathrm{E}}$, and its distance $r_{\mathrm{S}}$ from the Sun (of mass $M_{\mathrm{S}}$ ) is constant and much larger than $R_{\mathrm{E}}$.
6.17.* A satellite is on a circular orbit, of radius $R$, around the Earth.
(i) Write the equations of motion of a small body as observed from the satellite, and simplify them for the case when body's motion is limited to a close vicinity of the satellite.
(ii) Use the equations to prove that at negligible external forces (in particular, negligible gravitational attraction to the satellite) the body may be placed on an elliptical trajectory around satellite's center of mass, within its plane of rotation about Earth. Calculate the ellipse's orientation and eccentricity.
6.18.* A non-spherical shape of an artificial satellite may ensure its stable angular orientation relative to Earth's surface, advantageous for many practical goals. Modeling the satellite as a strongly elongated, axially-symmetric body, moving around the Earth on a circular orbit of radius $R$, find its
stable orientation, and analyze possible small oscillations of the satellite's symmetry axis around this equilibrium position.
6.19. A thin coin of radius $r$ is rolled, with velocity $V$, on a horizontal surface without slippage. What should be coin's tilt angle $\theta$ (see Fig. on the right) for it to roll on a circle of radius $R \gg r$ ? Modeling the coin as a very thin, uniform disk, and assuming that angle $\theta$ is small, solve this problem in:

(i) an inertial ("lab") reference frame, and
(ii) the non-inertial reference frame moving with coin's center of mass (but not rotating with it).
6.20. Two planets are on the circular orbit around their common center of mass. Calculate the effective potential energy of a much lighter mass (say, a spaceship) rotating with the same angular velocity, on the line connecting the planets. Sketch the plot of function the radial dependence of $U_{\text {ef }}$ and find out the number of so-called Lagrange points is which the potential energy has local maxima. Calculate their position approximately in the limit when one of the planets is much more massive than the other one.
6.21. A small body is dropped down to the surface of Earth from height $h \ll R_{\mathrm{E}}$, without initial velocity. Calculate the magnitude and direction of its deviation from the vertical, due to the Earth rotation. Estimate the effect's magnitude for a body dropped from the Empire State Building.
6.22. Use Eq. (94) to calculate the generalized momentum and derive the Lagrange equation of motion of a particle, considering $L$ a function of $\mathbf{r}$ and $\mathbf{v}$ as measured in a non-inertial but non-rotating reference frame.

## Chapter 7. Deformations and Elasticity

The objective of this chapter is a brief discussion of small deformations of $3 D$ continuous media, with a focus on elastic properties of solids. The reader will see that deformation of solids is nontrivial even in the absence of motion, so that several key problems of statics will need to be discussed before proceeding to such dynamic phenomena as elastic waves in infinite media and thin rods.

### 7.1. Strain

Rigid bodies discussed in the previous chapter are just a particular case of continuous media. As has already been mentioned, these are systems of particles so close to each other that the system discreteness may be neglected, so that the particle displacement $\mathbf{q}$ may be considered as a continuous function of space and time. The subject of this chapter is small deviations from the rigid-body approximation discussed in Chapter 6, i.e. small deformations. The deformation smallness allows one to consider the displacement vector $\mathbf{q}$ as a function of the initial (pre-deformation) position of the particle $\mathbf{r}$, and time $t$ - just as was done in the Secs. 5.3-5.5 for 1D waves.

The first task of the deformation theory is to exclude from consideration the types of motion considered in Chapter 6, namely the translation and rotation unrelated to deformations. This means, first of all, the variables describing deformations should not depend on the part of displacement $\mathbf{q}$ that does not depend on position $\mathbf{r}$ (i.e. is common for the whole media), because that part corresponds to a translational shift rather than to a deformation (Fig. 1a). Moreover, even certain non-uniform displacements do not contribute to deformation. For example, Eq. (6.7) (with $d \mathbf{r}$ replaced with $d \mathbf{q}$ to comply with our current notation) shows that a small displacement of the type

$$
\begin{equation*}
\left.d \mathbf{q}\right|_{\text {rotation }}=d \varphi \times \mathbf{r} \tag{7.1}
\end{equation*}
$$

where $d \varphi=\omega d t$ is an infinitesimal vector common for the whole continuum, corresponds to its rotation about the direction of that vector, and has nothing to do with the body deformation (Fig. 1b).


Fig. 7.1. Two types of displacement vector distributions that are unrelated to deformation:
(a) translation and (b) rotation.

This is why in order to develop an adequate quantitative characterization of deformation, we should start with finding suitable appropriate functions of the spatial distribution of displacements, $\mathbf{q}(\mathbf{r})$, that exist only due to deformations. One of such measures is the change of distance $d l=|d \mathbf{r}|$ between two close points:

$$
\begin{equation*}
\left.(d l)^{2}\right|_{\text {after deformation }}-\left.(d l)^{2}\right|_{\text {before deformation }}=\sum_{j=1}^{3}\left(d r_{j}+d q_{j}\right)^{2}-\sum_{j=1}^{3}\left(d r_{j}\right)^{2}, \tag{7.2}
\end{equation*}
$$

where $d q_{j}$ is the $j^{\text {th }}$ Cartesian component of the difference $d \mathbf{q}$ between the displacements $\mathbf{q}$ of the two points. If the deformation is small in the sense $|d \mathbf{q}| \ll|d \mathbf{r}|=d l$, we may keep in Eq. (2) only the terms proportional to the first power of the infinitesimal vector $d \mathbf{q}$ :

$$
\begin{equation*}
\left.(d l)^{2}\right|_{\text {after deformation }}-\left.(d l)^{2}\right|_{\text {before deformation }}=\sum_{j=1}^{3}\left[2 d r_{j} d q_{j}+\left(d q_{j}\right)^{2}\right] \approx 2 \sum_{j=1}^{3} d r_{j} d q_{j} \tag{7.3}
\end{equation*}
$$

Since $q_{j}$ is a function of 3 independent scalar arguments $r_{j}$, its differential may be presented as

$$
\begin{equation*}
d q_{j}=\sum_{j^{\prime}=1}^{3} \frac{\partial q_{j}}{\partial r_{j^{\prime}}} d r_{j^{\prime}} \tag{7.4}
\end{equation*}
$$

Coefficients $\partial q_{j} / \partial r_{j}$, may be considered as elements of a tensor ${ }^{1}$ providing a linear relation between vectors dr and dq. Plugging Eq. (4) into Eq. (2), we get

$$
\begin{equation*}
\left.(d l)^{2}\right|_{\text {after deformation }}-(d l)_{\mid \text {before deformation }}^{2}=2 \sum_{j, j^{\prime}=1}^{3} \frac{\partial q_{j}}{\partial r_{j^{\prime}}} d r_{j} d r_{j^{\prime}} . \tag{7.5}
\end{equation*}
$$

A convenience of tensor $\partial q_{j} / \partial r_{j}$, for characterizing deformations is that it automatically excludes the translation displacement (Fig. 1a) that is independent of $r_{j}$. Its drawback is that its particular components are still affected by the rotation of the body (though the sum (5) is not). Indeed, according to the vector product definition, Eq. (1) may be presented in Cartesian coordinates as

$$
\begin{equation*}
\left.d q_{j}\right|_{\text {rotation }}=\left(d \varphi_{j^{\prime}} r_{j^{\prime \prime}}-d \varphi_{j^{\prime \prime}} r_{j^{\prime}}\right) \varepsilon_{i j j^{\prime \prime}} \tag{7.6}
\end{equation*}
$$

where $\varepsilon_{i j j^{\prime} "}$ is the Levi-Civita symbol ${ }^{2}$ equal to (+1) if all indices $j, j^{\prime}$, and $j^{\prime \prime}$ are different and run in a "right" order - $\{1,2,3\}$, etc., and ( -1 ) otherwise, so that for any order of non-equal indices, $\varepsilon_{i j j} j^{\prime \prime}=-\varepsilon_{j i j j}$ ". Differentiating Eq. (6) over a particular Cartesian coordinate of vector $\mathbf{r}$, and taking into account that this partial differentiation $(\partial)$ is independent of (and hence may be swapped with) the differentiation (d) over the rotation angle $\varphi$, we get the amounts,

$$
\begin{equation*}
d\left(\frac{\partial q_{j}}{\partial r_{j^{\prime}}}\right)_{\text {rotation }}=-\varepsilon_{i j j^{\prime \prime}} d \varphi_{j^{\prime \prime}}, d\left(\frac{\partial q_{j^{\prime}}}{\partial r_{j}}\right)_{\text {rotation }}=-\varepsilon_{j j j^{\prime \prime}} d \varphi_{j^{\prime \prime}}=\varepsilon_{j j j^{\prime \prime}} d \varphi_{j "}, \tag{7.7}
\end{equation*}
$$

which may differ from 0 . However, notice that the sum of these two differentials equals zero for any $d \varphi$, which is possible only if

$$
\begin{equation*}
\left(\frac{\partial q_{j^{\prime}}}{\partial r_{j}}+\frac{\partial q_{j}}{\partial r_{j^{\prime}}}\right)_{\text {rotation }}=0, \text { for } j \neq j^{\prime} \tag{7.8}
\end{equation*}
$$

[^94]so that the full sum (5), that includes 3 such partial sums, is not affected by rotation - as we already know. This is why it is convenient to rewrite Eq. (5) in a mathematically equivalent form
\[

$$
\begin{equation*}
\left.(d l)^{2}\right|_{\text {after deformation }}-(d l)_{\mid \text {before deformation }}^{2}=2 \sum_{j, j^{\prime}=1}^{3} s_{j j^{\prime}} d r_{j} d r_{j^{\prime}}, \tag{7.9a}
\end{equation*}
$$

\]

where $s_{j j}$ are the elements of the so-called symmetrized strain tensor defined as

Strain tensor

$$
\begin{equation*}
s_{i j^{\prime}} \equiv \frac{1}{2}\left(\frac{\partial q_{j}}{\partial r_{j^{\prime}}}+\frac{\partial q_{j^{\prime}}}{\partial r_{j}}\right) \tag{7.9b}
\end{equation*}
$$

(Note that this modification does not affect the diagonal elements: $s_{j j}=\partial q_{j} / \partial r_{j}$.). The advantage of symmetrized tensor ( 9 b ) over the initial tensor $\partial q_{j} / \partial r_{j}$, is that according to Eq. (8), at pure rotation all elements of the symmetrized strain tensor vanish.

Now let us discuss the physical meaning of this tensor. At was already mentioned in Sec. 6.2, any symmetric tensor may be diagonalized by an appropriate selection of the reference frame axes. In such principal axes, $s_{j j^{\prime}}=s_{j j} \delta_{j j^{\prime}}$, so that Eq. (4) takes the simple form

$$
\begin{equation*}
d q_{j}=\frac{\partial q_{j}}{\partial r_{j}} d r_{j}=s_{i j} d r_{j} \tag{7.10}
\end{equation*}
$$

We may use this expression to calculate the change of each side of an infinitesimal cuboid (parallelepiped) with sides $d q_{j}$ parallel to the principal axes:

$$
\begin{equation*}
\left.d r_{j}\right|_{\text {after deformation }}-\left.d r_{j}\right|_{\text {before deformation }} \equiv d q_{j}=s_{j j} d r_{j}, \tag{7.11}
\end{equation*}
$$

and of cuboid's volume $d V=d r_{1} d r_{2} d r_{3}$ :

$$
\begin{equation*}
\left.d V\right|_{\text {after deformation }}-\left.d V\right|_{\text {before deformation }}=\prod_{j=1}^{3}\left(d r_{j}+s_{j j} d r_{j}\right)-\prod_{j=1}^{3} d r_{j}=d V\left[\prod_{j=1}^{3}\left(1+s_{j j}\right)-1\right], \tag{7.12}
\end{equation*}
$$

Since all our analysis is only valid in the linear approximation in small $s_{j j}$, Eq. (12) is reduced to

$$
\begin{equation*}
\left.d V\right|_{\text {after deformation }}-\left.d V\right|_{\text {before deformation }} \approx d V \sum_{j=1}^{3} s_{j j} \equiv d V \operatorname{Tr}(\mathrm{~s}), \tag{7.13}
\end{equation*}
$$

where $\operatorname{Tr}(\text { trace })^{3}$ of any matrix (in particular, tensor) is the sum of its diagonal elements; in our case ${ }^{4}$

$$
\begin{equation*}
\operatorname{Tr}(\mathrm{s}) \equiv \sum_{j=1}^{3} s_{j j} \tag{7.14}
\end{equation*}
$$

So, the diagonal components of the tensor characterize medium's compression/extension; then what is the meaning of the off-diagonal components of the tensor? It may be illustrated on the simplest example of a purely shear deformation, shown in Fig. 2 (the geometry is assumed to be uniform along axis $z$ ). In this case, all displacements (assumed small) have just one Cartesian component, in Fig. 2

[^95]along axis $x$ : $\mathbf{q}=\mathbf{n}_{x} \alpha y$ (with $\alpha \ll 1$ ), so that the only nonvanishing component of the initial strain tensor $\partial q_{j} / \partial r_{j}$, is $\partial q_{x} / \partial y=\alpha$, and the symmetrized tensor (9b) is
\[

\mathrm{s}=\left($$
\begin{array}{ccc}
0 & \alpha / 2 & 0  \tag{7.15}\\
\alpha / 2 & 0 & 0 \\
0 & 0 & 0
\end{array}
$$\right)
\]

Evidently, the change (13) of volume vanishes in this case. Thus, off-diagonal elements of tensor s characterize shear deformations.


Fig. 7.2. Example of a pure shear.

To conclude this section, let me note that Eq. (9) is only valid in Cartesian coordinates. For the solution of some important problems, especially those with a spherical or axial symmetry, it is frequently convenient to express six different components of the symmetric strain tensor via three components of the displacement vector $\mathbf{q}$ in either spherical or cylindrical coordinates. A straightforward differentiation, using the definition of such coordinates, ${ }^{5}$ yields, in particular, the following formulas for the diagonal elements of the tensor in the local mutually orthogonal coordinates that are directed along unit vectors - either $\left\{\mathbf{n}_{r}, \mathbf{n}_{\theta}, \mathbf{n}_{\varphi}\right\}$ or $\left\{\mathbf{n}_{\rho}, \mathbf{n}_{\varphi,}, \mathbf{n}_{z}\right\}$ - at the given point:
(i) in the spherical coordinates:

$$
\begin{equation*}
s_{r r}=\frac{\partial q_{r}}{\partial r}, \quad s_{\theta \theta}=\frac{q_{r}}{r}+\frac{1}{r} \frac{\partial q_{\theta}}{\partial \theta}, \quad s_{\varphi \varphi}=\frac{q_{r}}{r}+\frac{q_{\theta}}{r} \frac{\cos \theta}{\sin \theta}+\frac{1}{r \sin \theta} \frac{\partial q_{\varphi}}{\partial \varphi} ; \tag{7.16}
\end{equation*}
$$

(ii) in the cylindrical coordinates:

$$
\begin{equation*}
s_{\rho \rho}=\frac{\partial q_{\rho}}{\partial \rho}, \quad s_{\varphi \varphi}=\frac{q_{\rho}}{\rho}+\frac{1}{\rho} \frac{\partial q_{\varphi}}{\partial \varphi}, \quad s_{z z}=\frac{\partial q_{z}}{\partial z} . \tag{7.17}
\end{equation*}
$$

These expressions, that will be used below for solution of some problems for symmetrical geometries, may be a bit counter-intuitive. Indeed, Eq. (16) shows that even for a purely radial, axiallysymmetric deformation, $\mathbf{q}=\mathbf{n}_{r} q(r)$, diagonal angular components of strain do not vanish: $s_{\theta \theta}=s_{\varphi \varphi}=q / r$. (According to Eq. (17), in cylindrical coordinates, the same effect is exhibited by the only angular component of the tensor.) Note, however, that these relations describe a very simple geometric effect: the change of the lateral distance $r d \gamma \ll r$ between two close points with the same distance $r$ from a central point, at a small change of $r$ that keeps the angle $d \gamma$ between their radius-vectors $\mathbf{r}$ constant.

[^96]
### 7.2. Stress

Now let us discuss the forces that cause deformations. Internal forces acting inside (i.e. between arbitrarily defined parts of) a continuous media may be also characterized by a tensor. This stress tensor, ${ }^{6}$ with elements $\sigma_{j j}$, relates components of the elementary vector $d \mathbf{F}$ of the force acting on an elementary area $d A$ of an (possibly, imaginary) interface between two parts of a continuous media with elementary vector $d \mathbf{A}=\mathbf{n} d A$ normal to the area (Fig. 3):

Stress tensor

$$
\begin{equation*}
d F_{j}=\sum_{j^{\prime}=1}^{3} \sigma_{i j^{\prime}} d A_{j^{\prime}} \tag{7.18}
\end{equation*}
$$

The usual sign convention here is to take the outer normal $d \mathbf{n}$, i.e. to direct $d \mathbf{A}$ out of "our" part of the continuum, i.e. the part on which the calculated force $d \mathbf{F}$ is exerted.


Fig. 7.3. Definition of vectors $d \mathbf{A}$ and $d \mathbf{F}$.

In some cases the stress tensor's structure is very simple. For example, as will be discussed in detail in the next chapter, static or frictionless fluids may only provide a force normal to any surface and usually directed toward "our" part of the body, so that

$$
\begin{equation*}
d \mathbf{F}=-P d \mathbf{A}, \quad \text { i.e. } \sigma_{i j^{\prime}}=-P \delta_{i j^{\prime}}, \tag{7.19}
\end{equation*}
$$

where scalar $P$ (in most cases positive) is called pressure, and generally depends on both the spatial position and time. This type of stress, with $P>0$, is frequently called the hydrostatic compression - even if it takes place in solids.

However, in the general case the stress tensor also has off-diagonal terms, which characterize shear stress. For example, if the shear strain shown in Fig. 2 is caused by a pair of forces $\pm \mathbf{F}$, they create internal forces $F_{x} \mathbf{n}_{x}$, with $F_{x}>0$ if we speak about the force acting upon a part of the sample below the imaginary horizontal interface we are discussing. In order to avoid horizontal acceleration of each horizontal slice of the sample, the forces should not depend on $y$, i.e. $F_{x}=$ const $=F$. Superficially, it may look that this is the only nonvanishing component of the stress tensor is $d F_{x} / d A_{y}=F / A=$ const, so that tensor is asymmetric, in contrast to the strain tensor (15) of the same system. Note, however, that the pair of forces $\pm \mathbf{F}$ creates not only the shear stress, but also a nonvanishing rotating torque $\tau=-F h \mathbf{n}_{z}$ $=-\left(d F_{x} / d A_{y}\right) A h \mathbf{n}_{z}=-\left(d F_{x} / d A_{y}\right) V \mathbf{n}_{z}$, where $V=A h$ is sample's volume. So, if we want to perform a static stress experiment, i.e. avoid sample's rotation, we need to apply some other forces, e.g., a pair of vertical forces creating an equal and opposite torque $\tau^{\prime}=\left(d F_{y} / d A_{x}\right) V \mathbf{n}_{z}$, implying that $d F_{y} / d A_{x}=d F_{x} / d A_{y}$ $=F / A$. As a result, the stress tensor becomes symmetric, and similar in structure to the symmetrized strain tensor (15):

[^97]\[

\sigma=\left($$
\begin{array}{ccc}
0 & F_{0} / A & 0  \tag{7.20}\\
F_{0} / A & 0 & 0 \\
0 & 0 & 0
\end{array}
$$\right)
\]

In many situations, the body may be stressed not only by forces applied to their surfaces, but also by some volume-distributed (bulk) forces $d \mathbf{F}=\mathbf{f} d V$, whose certain effective bulk density $\mathbf{f}$. (The most evident example of such forces is gravity. If its field is uniform as described by Eq. (1.16b), then $\mathbf{f}=\rho \mathbf{g}$, where $\rho$ is the mass density.) Let us derive the key formula describing the correct summation of the surface and bulk forces. For that, consider again an infinitesimal cuboid with sides $d r_{j}$ parallel to the corresponding coordinates axes (Fig. 4) - now not necessarily the principal axes of the stress tensor.


Fig. 7.4. Deriving Eq. (23).

If elements $\sigma_{j j}$, of the tensor do not depend on position, the force $d \mathbf{F}^{\left(j^{\prime}\right)}$ acting on $j$ '-th face of the cuboid is exactly balanced by the equal and opposite force acting on the opposite face, because vectors $d \mathbf{A}^{\left(j^{\prime}\right)}$ of these faces are equal and opposite. However, if $\sigma_{j j}$, is a function of $\mathbf{r}$, then the net force $d\left(d \mathbf{F}^{\left(j^{\prime}\right)}\right)$ does not vanish. Using the expression for to the $j$, th contribution to sum (18), in the first order in $d \mathbf{r}$, the $j^{\text {th }}$ components of this vector is

$$
\begin{equation*}
d\left(d F_{j}^{\left(j^{\prime}\right)}\right)=d\left(\sigma_{i j^{\prime}} d A_{j^{\prime}}\right)=\frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}} d r_{j^{\prime}} d A_{j^{\prime}}=\frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}} d V \tag{7.21}
\end{equation*}
$$

where cuboid's volume $d V=d r_{j} \cdot d A_{j^{\prime}}$ does not depend on $j^{\prime}$. The addition these force components for all three pairs of cuboid faces, i.e. the summation of Eqs. (21) for all 3 values of the upper index $j$ ', yields the following relation for the $j^{\text {th }}$ component of the net force exerted on the cuboid:

$$
\begin{equation*}
d\left(d F_{j}\right)=\sum_{j^{\prime}=1}^{3} d\left(d F_{j}^{\left(j^{\prime}\right)}\right)=\sum_{j^{\prime}=1}^{3} \frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}} d V . \tag{7.22}
\end{equation*}
$$

Since any volume may be broken into such infinitesimal cuboids, Eq. (22) shows that the space-varying stress is equivalent to a volume-distributed force $d \mathbf{F}_{\mathrm{ef}}=\mathbf{f}_{\mathrm{ef}} d V$, whose effective (not real!) bulk density $\mathbf{f}_{\mathrm{ef}}$ has the following Cartesian components

$$
\begin{equation*}
\left(f_{\mathrm{ef}}\right)_{j}=\sum_{j^{\prime}=1}^{3} \frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}} \tag{7.23}
\end{equation*}
$$

so that in the presence of genuinely bulk forces $d \mathbf{F}=\mathbf{f} d V$, densities $\mathbf{f}_{\text {ef }}$ and $\mathbf{f}$ just add up.
Let us use this addition rule to spell out the $2^{\text {nd }}$ Newton law for a unit volume of a continuous medium:

$$
\begin{equation*}
\rho \frac{\partial^{2} \mathbf{q}}{\partial t^{2}}=\mathbf{f}_{\mathrm{ef}}+\mathbf{f} . \tag{7.24}
\end{equation*}
$$

Using Eq. (23), the $j^{\text {th }}$ Cartesian component of Eq. (24) may be presented as

Medium dynamics equation

$$
\begin{equation*}
\rho \frac{\partial^{2} q_{j}}{\partial t^{2}}=\sum_{j^{\prime}=1}^{3} \frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}}+f_{j} \tag{7.25}
\end{equation*}
$$

This is the key equation of medium's dynamics, which will be repeatedly used below.
For solution of some problems, it is also convenient to have a general expression for work $\delta W$ of the stress forces at a virtual deformation $\delta \mathbf{q}$ - understood in the same variational sense as the virtual displacement $\delta \mathbf{r}$ in Sec. 2.1. Using the equivalence between the stress forces and the effective bulk forces with density $\mathbf{f}_{\mathrm{ef}}$, for any volume $V$ of the media we may write

$$
\begin{equation*}
\delta W=\int_{V} \mathbf{f}_{\mathrm{ef}} \cdot \delta \mathbf{q} d V=\sum_{j=1}^{3} \int_{V}\left(f_{\mathrm{ef}}\right)_{j} \delta q_{j} d V=\sum_{j, j^{\prime}=1}^{3} \int_{V} \frac{\partial \sigma_{i j^{\prime}}}{\partial r_{j^{\prime}}} \delta q_{j} d^{3} r . \tag{7.28}
\end{equation*}
$$

Let us take this integral by parts for a volume so large that deformations $\delta q_{j}$ on its surface are negligible. Then, swapping the operations of variations and spatial differentiation (just like it was done with the time derivative in Sec. 2.1), we get

$$
\begin{equation*}
\delta W=-\sum_{j, j^{\prime}=1}^{3} \int_{V} \sigma_{i j^{\prime}} \delta \frac{\partial q_{j}}{\partial r_{j^{\prime}}} d^{3} r . \tag{7.29}
\end{equation*}
$$

Assuming that tensor $\sigma_{j j}$, is symmetric, we may rewrite this expression as

$$
\begin{equation*}
\delta W=-\frac{1}{2} \sum_{j, j^{\prime}=1}^{3} \int_{V}\left(\sigma_{i j j^{\prime}} \delta \frac{\partial q_{j}}{\partial r_{j^{\prime}}}+\sigma_{j j^{\prime} j} \delta \frac{\partial q_{j}}{\partial r_{j^{\prime}}}\right) d^{3} r . \tag{7.30}
\end{equation*}
$$

Now, swapping indices $j$ and $j$ ' in the second expression, we finally get

$$
\begin{equation*}
\delta W=-\frac{1}{2} \sum_{j, j^{\prime}=1}^{3} \int_{V} \delta\left(\frac{\partial q_{j}}{\partial r_{j^{\prime}}} \sigma_{j j^{\prime}}+\frac{\partial q_{j^{\prime}}}{\partial r_{j}} \sigma_{j j^{\prime}}\right) d^{3} r=-\sum_{j, j^{\prime}=1}^{3} \int_{V} \sigma_{i j^{\prime}} \delta s_{j j^{\prime}} d^{3} r, \tag{7.31}
\end{equation*}
$$

where $s_{j j}$ are the components of strain tensor ( 9 b ). It is natural to rewrite this important formula as

Work of
stress forces

$$
\begin{equation*}
\delta W=\int_{V} \delta w(\mathbf{r}) d^{3} r, \quad \text { where } \delta w(\mathbf{r}) \equiv-\sum_{j, j^{\prime}=1}^{3} \sigma_{j j^{\prime}} \delta s_{j j^{\prime}} \tag{7.32}
\end{equation*}
$$

and interpret the locally-defined scalar function $\delta w(\mathbf{r})$ as the work of stress forces per unit volume, due to the small variation of the deformation.

### 7.3. Hooke's law

In order to form a complete system of equations describing media dynamics, one needs to complement Eq. (25) with an appropriate material equation describing the relation between the stress tensor $\sigma_{j j}$, and the deformation $\mathbf{q}$ described (in the small deformation limit) by the strain tensor $s_{j j}$. This
relation depends on the medium, and generally may be rather complex. Even leaving alone various anisotropic solids (e.g., crystals) and macroscopically-inhomogeneous materials (like ceramics or sand), strain typically depends not only on the current value of stress (possibly in a nonlinear way), but also on the previous history of stress application. Indeed, if strain exceeds a certain plasticity threshold, atoms (or nanocrystals) may slip to their new positions and never come back even if the strain is reduced. As a result, deformations become irreversible - see Fig. 5.


Fig. 7.5. Typical relation between stress and strain in solids (schematically).

Only below the thresholds of nonlinearity and plasticity (which are typically close to each other), strain is nearly proportional to stress, i.e. obeys the famous Hooke's law. ${ }^{7}$ However, even in this elastic range the law is not quite simple, and even for an isotropic medium is described not by one but by two constants, called elastic moduli. The reason for that is that most elastic materials resist the strain accompanied by the volume change (say, the hydrostatic compression) differently from how they resist the shear deformation. In order to describe this difference, let us first present the symmetrized strain tensor ( 9 b ) in the mathematically equivalent form

$$
\begin{equation*}
s_{i j j^{\prime}}=\left(s_{j j^{\prime}}-\frac{1}{3} \delta_{i j j^{\prime}} \operatorname{Tr}(\mathrm{s})\right)+\left(\frac{1}{3} \delta_{i j^{\prime}} \operatorname{Tr}(\mathrm{s})\right) . \tag{7.33}
\end{equation*}
$$

According to Eq. (13), the traceless tensor in the first parentheses of Eq. (33) does not give any contribution to the volume change, e.g., may be used to characterize purely shear deformation, while the second one describes the hydrostatic compression alone. Hence we may expect that the stress tensor may be presented (again, in the elastic deformation range only!) as

$$
\begin{equation*}
\sigma_{i j^{\prime}}=2 \mu\left(s_{j j^{\prime}}-\frac{1}{3} \operatorname{Tr}(\mathrm{~s}) \delta_{i j^{\prime}}\right)+3 K\left(\frac{1}{3} \operatorname{Tr}(\mathrm{~s}) \delta_{i j j^{\prime}}\right), \tag{7.34}
\end{equation*}
$$

## Hooke's law

where $K$ and $\mu$ are some constants. ${ }^{8}$ Indeed, experiments show that Hooke's law in this form is followed, at small strain, by all isotropic elastic materials. In accordance with the above discussion, constant $\mu$ (in some texts, denoted as $G$ ) is called the shear modulus, while constant $K$ (sometimes called $B$ ), the bulk modulus. Two columns of Table 1 below show the approximate values of these moduli for typical representatives of several major classes of materials. ${ }^{9}$

[^98]To better appreciate these values, let us first discuss the physical meaning of $K$ and $\mu$, using two simple examples of elastic deformation. For that it is convenient first to solve the set of 9 (or rather 6 different) linear equations (34) for $s_{j j}$. This is easy to do, due to the simple structure of these equations: they relate components $\sigma_{j j^{\prime}}$ and $s_{j j^{\prime}}$ with the same indices, besides the involvement of the tensor trace. This slight complication may be readily overcome by noticing that according to Eq. (34),

$$
\begin{equation*}
\operatorname{Tr}(\sigma) \equiv \sum_{j=1}^{3} \sigma_{j j}=3 K \operatorname{Tr}(\mathrm{~s}), \text { i.e. } \operatorname{Tr}(\mathrm{s})=\frac{1}{3 K} \operatorname{Tr}(\sigma) \tag{7.35}
\end{equation*}
$$

Plugging this result into Eq. (34) and solving it for $s_{i j}$, we readily get the reciprocal relation, which may be presented in a similar form:

$$
\begin{equation*}
s_{i j^{\prime}}=\frac{1}{2 \mu}\left(\sigma_{j j^{\prime}}-\frac{1}{3} \operatorname{Tr}(\sigma) \delta_{j j^{\prime}}\right)+\frac{1}{3 K}\left(\frac{1}{3} \operatorname{Tr}(\sigma) \delta_{i j j^{\prime}}\right) . \tag{7.36}
\end{equation*}
$$

Table 7.1. Elastic moduli, density, and sound velocities of a few representative materials (approximate values)

| Material | $K(\mathrm{GPa})$ | $\mu(\mathrm{GPa})$ | $E(\mathrm{GPa})$ | $v$ | $\rho\left(\mathrm{~kg} / \mathrm{m}^{3}\right)$ | $v_{l}(\mathrm{~m} / \mathrm{s})$ | $v_{t}(\mathrm{~m} / \mathrm{s})$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Diamond $^{(\mathrm{a})}$ | 600 | 450 | 1,100 | 0.20 | 3,500 | 1,830 | 1,200 |
| Hardened steel $^{\text {L }}$ | 170 | 75 | 200 | 0.30 | 7,800 | 5,870 | 3,180 |
| Water $^{(\mathrm{b})}$ | 2.1 | 0 | 0 | 0.5 | 1,000 | 1,480 | 0 |
| Air $^{(\mathrm{b})}$ | 0.00010 | 0 | 0 | 0.5 | 1.2 | 332 | 0 |

${ }^{(a)}$ Averages over crystallographic directions ( $\sim 10 \%$ anisotropy).
${ }^{(b)}$ At the so-called ambient conditions $\left(T=20^{\circ} \mathrm{C}, P=1 \mathrm{bar} \equiv 10^{5} \mathrm{~Pa}\right)$.

Now let us apply Hooke's law, in the form of Eqs. (34) or (36), to two simple situations in which the strain and stress tensors may be found without formulating the exact differential equations of the elasticity theory and boundary conditions for them. (That will be the subject of the next section.) The first experiment is the hydrostatic compression when the stress tensor is diagonal, and all its diagonal components are equal - see Eq. (19). ${ }^{10}$ For this case Eq. (36) yields

$$
\begin{equation*}
s_{i j^{\prime}}=-\frac{P}{3 K} \delta_{i j j^{\prime}}, \tag{7.37}
\end{equation*}
$$

which means that regardless of the shear modulus, the strain tensor is also diagonal, with all diagonal components equal. According to Eqs. (11) and (13), this means that all linear dimensions of the body are reduced by a similar fraction, so that its shape is preserved, while the volume is reduced by

[^99]\[

$$
\begin{equation*}
\frac{\Delta V}{V}=\sum_{j=1}^{3} s_{j j}=-\frac{P}{K} \tag{7.38}
\end{equation*}
$$

\]

This equation clearly shows the physical sense of the bulk modulus $K$ as the reciprocal compressibility.
As Table 1 shows, the values of $K$ may be dramatically different for various materials, and that even for such "soft stuff" as water this modulus in actually rather high. For example, even at the bottom of the deepest, $10-\mathrm{km}$ ocean well ( $P \approx 10^{3} \mathrm{bar} \approx 0.1 \mathrm{GPa}$ ), water density increases by just about $5 \%$. As a result, in most human-scale experiments, water may be treated as incompressible - a condition that will be widely used in the next chapter. Many solids are even much less compressible - see the first two rows of Table 1.

The most compressible media are gases. For a gas, certain background pressure $P$ is necessary just for containing it within certain volume $V$, so that Eq. (38) is only valid for small increments of pressure, $\Delta P$ :

$$
\begin{equation*}
\frac{\Delta V}{V}=-\frac{\Delta P}{K} \tag{7.39}
\end{equation*}
$$

Moreover, gas compression also depends on thermodynamic conditions. (For most condensed media, the temperature effects are very small.) For example, at ambient conditions most gases are reasonably well described by the equation of state for the model called the ideal classical gas:

$$
\begin{equation*}
P V=N k_{\mathrm{B}} T, \quad \text { i.e. } P=\frac{N k_{\mathrm{B}} T}{V} . \tag{7.40}
\end{equation*}
$$

where $N$ is the number of molecules in volume $V$, and $k_{\mathrm{B}} \approx 1.38 \times 10^{-23} \mathrm{~J} / \mathrm{K}$ is the Boltzmann constant. ${ }^{11}$ For a small volume change $\Delta V$ at constant temperature, this equation gives

$$
\begin{equation*}
\left.\Delta P\right|_{T=\text { const }}=-\frac{N k_{B} T}{V^{2}} \Delta V=-\frac{P}{V} \Delta V, \quad \text { i.e. }\left.\frac{\Delta V}{V}\right|_{T=\text { const }}=-\frac{\Delta P}{P} . \tag{7.41}
\end{equation*}
$$

Comparing this expression with Eq. (37), we get a remarkably simple result for the isothermal compression of gases,

$$
\begin{equation*}
\left.K\right|_{T=\mathrm{const}}=P, \tag{7.42}
\end{equation*}
$$

which means in particular that the bulk modulus listed in Table 1 is actually valid, at the ambient conditions, for almost any gas. Note, however, that the change of thermodynamic conditions (say, from isothermal to adiabatic ${ }^{12}$ ) may affect gas' compressibility.

Now let us consider the second, rather different, fundamental experiment: a pure shear deformation shown in Fig. 2. Since the traces of matrices (15) and (20), which describe this experiment, are equal to 0 , for their off-diagonal elements Eq. (34) gives simply $\sigma_{j j^{\prime}}=2 \mu s_{j j^{\prime}}$, so that the deformation angle $\alpha$ (see Fig. 2) is just

$$
\begin{equation*}
\alpha=\frac{1}{\mu} \frac{F}{A} . \tag{7.43}
\end{equation*}
$$

[^100]Notice that the angle does not depend on thickness $h$ of the sample, though of course the maximal linear deformation $q_{x}=\alpha h$ is proportional to the thickness. Naturally, as Table 1 shows, for all fluids (liquids and gases) $\mu=0$, because they cannot resist static shear stress.

However, not all experiments, even the apparently simple ones, involve just either $K$ or $\mu$. Let us consider stretching a long elastic rod of a small and uniform cross-section of area $A$ - the so-called tensile stress experiment shown in Fig. 6. ${ }^{13}$


Fig. 7.6. Tensile stress experiment.

Though the deformation of the rod near its clamped ends depends on the exact way forces $\mathbf{F}$ are applied (we will discuss this issue later on), we may expect that over most of its length the tension forces are directed virtually along the rod, $d \mathbf{F}=F_{z} \mathbf{n}_{z}$, and hence, with the coordinate choice shown in Fig. 6, $\sigma_{x j}=$ $\sigma_{y j}=0$ for all $j$, including the diagonal elements $\sigma_{x x}$ and $\sigma_{y y}$. Moreover, due to the open lateral surfaces, on which, evidently, $d F_{x}=d F_{y}=0$, there cannot be an internal stress force of any direction, acting on any elementary internal boundary parallel to these surfaces. This means that $\sigma_{z x}=\sigma_{z y}=0$. So, of all components of the stress tensor only one, $\sigma_{z z}$, is not equal to zero, and for a uniform sample, $\sigma_{z z}=$ const $=F / A$. For this case, Eq. (36) shows that the strain tensor is also diagonal, but with different diagonal elements:

$$
\begin{gather*}
s_{z z}=\left(\frac{1}{9 K}+\frac{1}{3 \mu}\right) \sigma_{z z},  \tag{7.44}\\
s_{x x}=s_{y y}=\left(\frac{1}{9 K}-\frac{1}{6 \mu}\right) \sigma_{z z} . \tag{7.45}
\end{gather*}
$$

Since the tensile stress is most common in engineering (and physical experiment) practice, both combinations of the elastic moduli participating in these two relations have deserved their own names. In particular, the constant in Eq. (44) is usually denoted as $1 / E$ (but in many texts, as $1 / Y$ ), where $E$ is called the Young's modulus:

Young's modulus

$$
\begin{equation*}
\frac{1}{E} \equiv \frac{1}{9 K}+\frac{1}{3 \mu}, \quad \text { i.e. } E \equiv \frac{9 K \mu}{3 K+\mu} \tag{7.46}
\end{equation*}
$$

As Fig. 6 shows, in the tensile stress geometry $s_{z z} \equiv \partial q_{z} / \partial z=\Delta L / L$, so that the Young's modulus scales the linear relation between the relative extension of the rod and the force applied per unit area: ${ }^{14}$

$$
\begin{equation*}
\frac{\Delta L}{L}=\frac{1}{E} \frac{F}{A} . \tag{7.47}
\end{equation*}
$$

[^101]The third column of Table 1 shows the values of this modulus for two well-known solids: diamond (with the highest known value of $E$ of all bulk materials ${ }^{15}$ ) and the steel (physically, a solid solution of $\sim 10 \%$ of carbon in iron) used in construction. Again, for fluids the Young's modulus vanishes - as it follows from Eq. (46) with $\mu=0$.

I am confident that the reader of these notes has been familiar with Eq. (44), in the form of Eq. (47), from his or her undergraduate studies. However, most probably this cannot be said about its counterpart, Eq. (45), which shows that at the tensile stress, rod's cross-section dimension also change. This effect is usually characterized by the following dimensionless Poisson's ratio:

$$
\begin{equation*}
-\frac{s_{x x}}{s_{z z}}=-\frac{s_{y y}}{s_{z z}}=-\left(\frac{1}{9 K}-\frac{1}{6 \mu}\right) /\left(\frac{1}{9 K}+\frac{1}{3 \mu}\right)=\frac{1}{2} \frac{3 K-2 \mu}{3 K+\mu} \equiv v \tag{7.48}
\end{equation*}
$$

According to this formula, for realistic materials with $K>0, \mu \geq 0$, values of $v$ may vary from (1) to $(+1 / 2)$, but for the vast majority of materials, ${ }^{16}$ they are between 0 and $1 / 2-$ see Table 1 . The lower limit is reached in porous materials like cork whose lateral dimensions almost do not change at the tensile stress. Some soft materials like rubber present the opposite case: $v \approx 1 / 2$. Since according to Eqs. (13), (44) and (45), the volume change is

$$
\begin{equation*}
\frac{\Delta V}{V}=s_{x x}+s_{y y}+s_{z z}=\frac{1}{E} \frac{F}{A}(1-2 v) \tag{7.49}
\end{equation*}
$$

such materials virtually do not change their volume at the tensile stress. The ultimate limit of this trend, $\Delta V / V=0$, is provided by fluids and gases, because their Poisson ratio $v$ is exactly equal to $1 / 2$. (This follows from Eq. (48) with $\mu=0$.) However, for most practicable construction materials such as steel (see Table 1) the change (49) of volume is as high as $\sim 40 \%$ of that of the length.

Due to the clear physical sense of coefficients $E$ and $v$, they are frequently used as a pair of independent elastic moduli, instead of $K$ and $\mu$. Solving Eqs. (46) and (48) for $K$ and $\mu$, we get

$$
\begin{equation*}
K=\frac{E}{3(1-2 v)}, \quad \mu=\frac{E}{2(1+v)} . \tag{7.50}
\end{equation*}
$$

Using these formulas, the two (equivalent) formulations of Hooke's law, expressed by Eqs. (34) and (36), may be rewritten as

$$
\begin{align*}
\sigma_{j j^{\prime}} & =\frac{E}{1+v}\left(s_{i j^{\prime}}+\frac{v}{1-2 v} \operatorname{Tr}(\mathrm{~s}) \delta_{i j^{\prime}}\right),  \tag{7.51a}\\
s_{i j^{\prime}} & =\frac{1+\sigma}{E}\left(\sigma_{j j^{\prime}}-\frac{v}{1+v} \operatorname{Tr}(\sigma) \delta_{i j^{\prime}}\right) . \tag{7.51b}
\end{align*}
$$

The linear relation between the strain and stress tensor allows one to calculate the potential energy $U$ of an elastic medium due to its elastic deformation. Indeed, to each infinitesimal part of this

[^102]strain increase, we may apply Eq. (32), with the work $\delta W$ of the surface forces equal to $-\delta U$. Let us slowly increase the deformation from a completely unstrained state (in which we may take $U=0$ ) to a certain strained state, in the absence of bulk forces $\mathbf{f}$, keeping the deformation type, i.e. the relation between the elements of the stress tensor intact. In this case, all elements of tensor $\sigma_{j j}$, are proportional to the same single parameter characterizing the stress (say, the total applied force), and according to Hooke's law, all elements of tensor $s_{j^{\prime} j}$ are proportional to that parameter as well. In this case, integration over the variation yields the final value ${ }^{17}$
\[

$$
\begin{equation*}
U=\int_{V} u(\mathbf{r}) d^{3} r, \quad u(\mathbf{r})=\frac{1}{2} \sum_{j, j^{\prime}=1}^{3} \sigma_{i j^{\prime}} S_{j^{\prime j}} \tag{7.52}
\end{equation*}
$$

\]

Evidently, $u(\mathbf{r})$ may be interpreted as the volume density of the potential energy of the elastic deformation.

### 7.4. Equilibrium

Now we are fully equipped to discuss dynamics of elastic deformations, but let us start with statics. The static (equilibrium) state may be described by requiring the right-hand part of Eq. (25) to vanish. In order to find the elastic deformation, we need to plug $\sigma_{i j}$, from the Hooke's law (51a), and then express elements $s_{j j}$, via the displacement distribution - see Eq. (9). For a uniform material, the result is ${ }^{18}$

$$
\begin{equation*}
\frac{E}{2(1+v)} \sum_{j^{\prime}=1}^{3} \frac{\partial^{2} q_{j}}{\partial r_{j^{\prime}}^{2}}+\frac{E}{2(1+v)(1-2 v)} \sum_{j^{\prime}=1}^{3} \frac{\partial^{2} q_{j^{\prime}}}{\partial r_{j} \partial r_{j^{\prime}}}+f_{j}=0 . \tag{7.53}
\end{equation*}
$$

Taking into account that the first sum in Eq. (53) is just the $j^{\text {th }}$ component of $\nabla^{2} \mathbf{q}$, while the second sum is the $j^{\text {th }}$ component of $\nabla(\nabla \cdot \mathbf{q})$, we see that all three equations (53) for three Cartesian components $(j=$ 1,2 and 3 ) of the deformation vector $\mathbf{q}$, may be conveniently merged into one vector equation

$$
\begin{equation*}
\frac{E}{2(1+v)} \nabla^{2} \mathbf{q}+\frac{E}{2(1+v)(1-2 v)} \nabla(\nabla \cdot \mathbf{q})+\mathbf{f}=0 \tag{7.54}
\end{equation*}
$$

Equation of elastic equilibrium

For some applications, it is more convenient to recast this equation to another form, using vector identity ${ }^{19} \nabla^{2} \mathbf{q}=\nabla(\nabla \cdot \mathbf{q})-\nabla \times(\nabla \times \mathbf{q})$. The result is

$$
\begin{equation*}
\frac{E(1-v)}{(1+v)(1-2 v)} \nabla(\nabla \cdot \mathbf{q})-\frac{E}{2(1+v)} \nabla \times(\nabla \times \mathbf{q})+\mathbf{f}=0 . \tag{7.55}
\end{equation*}
$$

It is interesting that in problems without volume-distributed forces $(\mathbf{f}=0)$, the Young's modulus $E$ cancels! Even more fascinating, in this case the equation may be re-written in a form not involving the Poisson ratio $v$ either. Indeed, acting by operator $\nabla$ on the remaining terms of Eq. (55), we get a surprisingly simple equation

[^103]\[

$$
\begin{equation*}
\nabla^{2}(\nabla \cdot \mathbf{q})=0 . \tag{7.56}
\end{equation*}
$$

\]

A natural question here is how do the elastic moduli affect the deformation distribution if they do not participate in the differential equation describing it. The answer is two-fold. If what is fixed at the body boundary are deformations, then the moduli are irrelevant, because the deformation distribution through the body does not depend on them. On the other hand, if the boundary conditions fix stress (or a combination of stress and strain), then the elastic constants creep into the solution via the recalculation of these conditions into the strain.

As a simple but representative example, let us find the deformation distribution in a (generally, thick) spherical shell under the effect of different pressures fixed inside and outside it (Fig. 7a).


Fig. 7.7. Spherical shell problem: (a) the general case and (b) the thin shell limit.

Due to the spherical symmetry of the problem, the deformation is obviously sphericallysymmetric and radial, $\mathbf{q}=q(r) \mathbf{n}_{r}$, i.e. is completely described by one scalar function $q(r)$. Since the curl of such a radial vector field is zero, ${ }^{20}$ Eq. (55) is reduced to

$$
\begin{equation*}
\nabla(\nabla \cdot \mathbf{q})=0 \tag{7.57}
\end{equation*}
$$

This equation means that the divergence of function $q(r)$ is constant within the shell. In spherical coordinates this means ${ }^{21}$

$$
\begin{equation*}
\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} q\right)=\text { const. } \tag{7.58}
\end{equation*}
$$

Naming this constant $3 a$ (with the numerical factor chosen for later notation convenience), and integrating Eq. (58), we get its solution,

$$
\begin{equation*}
q(r)=a r+\frac{b}{r^{2}} \tag{7.59}
\end{equation*}
$$

that also includes another integration constant $b$.
To complete the analysis, we have to determine constants $a$ and $b$ from the boundary conditions. According to Eq. (19),

$$
\sigma_{r r}= \begin{cases}-P_{1}, & r=R_{1},  \tag{7.60}\\ -P_{2}, & r=R_{2} .\end{cases}
$$

[^104]In order to relate this stress to strain, let us use Hooke's law, but for that, we first need to calculate the strain tensor components for the deformation distribution (59). Using Eqs. (16), we get

$$
\begin{equation*}
s_{r r}=\frac{\partial q}{\partial r}=a-2 \frac{b}{r^{3}}, \quad s_{\theta \theta}=s_{\varphi \varphi}=\frac{q}{r}=a+\frac{b}{r^{3}}, \tag{7.61}
\end{equation*}
$$

so that $\operatorname{Tr}(\mathrm{s})=3 a$. Plugging these relations into Eq. (51a) for $\sigma_{r r}$, we get

$$
\begin{equation*}
\sigma_{r r}=\frac{E}{1+v}\left[\left(a-2 \frac{b}{r^{3}}\right)+\frac{v}{1-2 v} 3 a\right] . \tag{7.62}
\end{equation*}
$$

Now plugging this relation into Eqs. (60), we get a system of two linear equations for coefficients $a$ and b. Solving this system, we get:

$$
\begin{equation*}
a=\frac{1-2 v}{E} \frac{P_{1} R_{1}^{3}-P_{2} R_{2}^{3}}{R_{2}^{3}-R_{1}^{3}}, \quad b=\frac{1+v}{2 E} \frac{\left(P_{1}-P_{2}\right) R_{1}^{3} R_{2}^{3}}{R_{2}^{3}-R_{1}^{3}} . \tag{7.63}
\end{equation*}
$$

Formulas (59) and (63) give a complete solution of our problem. It is rich in contents and deserves at least some analysis. First of all, note that according to Eq. (50), coefficient ( $1-2 \sigma$ )/E in the expression for $a$ is just $1 / 3 K$, so that the first term in Eq. (59) for deformation is just the hydrostatic compression. In particular, the second of Eqs. (63) shows that if $R_{1}=0$, then $b=0$. Thus for a solid sphere we have only the hydrostatic compression that was discussed in the previous section. Perhaps less intuitively, making two pressures equal gives the same result (hydrostatic compression) for arbitrary $R_{2}>R_{1}$.

However, in the general case $b \neq 0$, so that the second term in the deformation distribution (59), which describes the shear deformation, ${ }^{22}$ is also substantial. In particular, let us consider the important thin-shell limit $R_{2}-R_{1} \equiv t \ll R_{1,2} \equiv R$ - see Fig. 7b. In this case, $q\left(R_{1}\right) \approx q\left(R_{2}\right)$ is just the change of the shell radius $R$, for which Eqs. (59) and (63) (with $R_{2}{ }^{3}-R_{1}{ }^{3} \approx 3 R^{2} t$ ) give

$$
\begin{equation*}
\Delta R \equiv q(R) \approx a R+\frac{b}{R^{2}} \approx \frac{\left(P_{1}-P_{2}\right) R^{2}}{3 t}\left(\frac{1-2 v}{E}+\frac{1+v}{2 E}\right)=\left(P_{1}-P_{2}\right) \frac{R^{2}}{t} \frac{1-v}{2 E} . \tag{7.64}
\end{equation*}
$$

Naively, one could think that at least in this limit the problem could be analyzed by elementary means. For example, the total force exerted by the pressure difference $\left(P_{1}-P_{2}\right)$ on the diametrical crosssection of the shell (see, e.g., the dashed line in Fig. 7b) is $F=\pi R^{2}\left(P_{1}-P_{2}\right)$, giving the stress,

$$
\begin{equation*}
\sigma=\frac{F}{A}=\frac{\pi R^{2}\left(P_{1}-P_{2}\right)}{2 \pi R t}=\left(P_{1}-P_{2}\right) \frac{R}{2 t}, \tag{7.65}
\end{equation*}
$$

directed along shell's walls. One can check that this simple formula may be indeed obtained, in this limit, from the strict expressions for $\sigma_{\theta \theta}$ and $\sigma_{\varphi \varphi}$, following from the general treatment carried out above. However, if we try now to continue this approach by using the simple relation (47) to find the small change $R s_{z z}$ of sphere's radius, we would arrive at a result with the structure of Eq. (64), but without factor $(1-v)<1$ in the numerator. The reason for this error (which may be as significant as $\sim 30 \%$ for typical construction materials - see Table 1) is that Eq. (47), while being valid for thin rods of arbitrary cross-section, is invalid for thin broad sheets, and in particular the thin shell in our problem.

[^105]Indeed, while at the tensile stress both lateral dimensions of a thin rod may contract freely, in our problem all dimensions of the shell are under stress - actually, under much more tangential stress than the radial one. ${ }^{23}$

### 7.5. Rod bending

The general approach to the static deformation analysis, outlined in the beginning of previous section, may be simplified not only for symmetric geometries, but also for the uniform thin structures such as thin plates ("membranes" or "sheets") and thin rods. Due to the shortage of time, in this course I will demonstrate typical approaches to such systems only on the example of thin rods. (The theory of membrane deformation is very much similar.) Besides the tensile stress analyzed in Sec. 3, two other major deformations of rods are bending and torsion. Let us start from a "local" analysis of bending caused by a pair of equal and opposite external torques $\tau= \pm \mathbf{n}_{y} \tau_{y}$ perpendicular to the rod axis $z$ (Fig. 8), assuming that the rod is "quasi-uniform", i.e. that on the scale of this analysis (comparable with linear scale $a$ of the cross-section) its material parameters and cross-section $A$ do not change substantially.


Fig. 7.8. This rod bending, in a local reference frame (specific for each cross-section).

Just as in the tensile stress experiment (Fig. 6), at bending the components of the stress forces $d \mathbf{F}$, normal to the rod length, have to equal zero on the surface of the rod. Repeating the arguments made for the tensile stress discussion, we arrive at the conclusion that only one diagonal component of the tensor (in Fig. 8, $\sigma_{z z}$ ) may differ from zero:

$$
\begin{equation*}
\sigma_{i j j^{\prime}}=\delta_{j z} \sigma_{z z} . \tag{7.66}
\end{equation*}
$$

However, in contrast to the tensile stress, at pure static bending the net force along the rod has to vanish:

$$
\begin{equation*}
F_{z}=\int_{A} \sigma_{z z} d^{2} r=0, \tag{7.67}
\end{equation*}
$$

so that $\sigma_{z z}$ has to change sign at some point of axis $x$ (in Fig. 8, selected to lay in the plane of the bent rod). Thus, the bending deformation may be viewed as a combination of stretching some layers of the rod (bottom layers in Fig. 8) with compression of other (top) layers.

Since it is hard to find more about the stress distribution from these general considerations, let us turn over to strain, assuming that the rod's cross-section is virtually constant on the length of the order of its cross-section size. From the above presentation of bending as a combination of stretching and compression, it evident that the longitudinal deformation $q_{z}$ has to vanish along some neutral line on the

[^106]rod's cross-section - in Fig. 8, represented by the dashed line. ${ }^{24}$ Selecting the origin of coordinate $x$ on this line, and expanding the relative deformation in the Taylor series in $x$, due to the cross-section smallness, we may limit ourselves to the linear term:
\[

$$
\begin{equation*}
s_{z z} \equiv \frac{d q_{z}}{d z}=-\frac{x}{R} . \tag{7.68}
\end{equation*}
$$

\]

Here constant $R$ has the sense of the curvature radius of the bent rod. Indeed, on a small segment $d z$ the cross-section turns by a small angle $d \varphi_{y}=-d q_{z} / x$ (Fig. 8b). Using Eq. (68), we get $d \varphi_{y}=d z / R$, which is the usual definition of the curvature radius $R$ in the differential geometry, for our special choice of the coordinate axes. ${ }^{25}$

Expressions for other components of the strain tensor are harder to guess (like at the tensile stress, not all of them are equal to zero!), but what we already know about $\sigma_{z z}$ and $s_{z z}$ is already sufficient to start formal calculations. Indeed, plugging Eq. (66) into the Hooke's law in the form (51b), and comparing the result for $s_{z z}$ with Eq. (68), we find

$$
\begin{equation*}
\sigma_{z z}=-E \frac{x}{R} . \tag{7.69}
\end{equation*}
$$

From the same Eq. (51b), we could also find the transverse components of the strain tensor, and see that they are related to $s_{z z}$ exactly as at the tensile stress:

$$
\begin{equation*}
s_{x x}=s_{y y}=-v S_{z z}, \tag{7.70}
\end{equation*}
$$

and then, integrating these relations along the cross-section of the rod, find the deformation of the crosssection shape. More important for us, however, is the calculation of the relation between rod's curvature and the net torque acting on a given cross-section (of area $A$ and orientation $d A_{z}>0$ ):

$$
\begin{equation*}
\tau_{y} \equiv \int_{A}(\mathbf{r} \times d \mathbf{F})_{y}=-\int_{A} x \sigma_{z z} d^{2} r=\frac{E}{R} \int_{A} x^{2} d^{2} r=\frac{E I_{y}}{R}, \tag{7.71}
\end{equation*}
$$

where $I_{y}$ is a geometric constant defined as

$$
\begin{equation*}
I_{y} \equiv \int_{A} x^{2} d x d y \tag{7.72}
\end{equation*}
$$

Note that this factor, defining the bending rigidity of the rod, grows as fast as $a^{4}$ with the linear scale $a$ of the cross-section. ${ }^{26}$

In these expressions, $x$ has to be counted from the neutral line. Let us see where exactly does this line pass through rod's cross-section. Plugging result (69) into Eq. (67), we get the condition defining the neutral line:

[^107]\[

$$
\begin{equation*}
\int_{A} x d x d y=0 \tag{7.73}
\end{equation*}
$$

\]

This condition allows a simple interpretation. Imagine a thin sheet of some material, with a constant mass density $\sigma$ per unit area, cut in the form of rod's cross-section. If we place a reference frame into its center of mass, then, by its definition,

$$
\begin{equation*}
\sigma \int_{A} \mathbf{r} d x d y=0 \tag{7.74}
\end{equation*}
$$

Comparing this condition with Eq. (73), we see that one of neutral lines has to pass through the center of mass of the sheet, which may be called the "center of mass of the cross-section". Using the same analogy, we see that integral $I_{y}$ (72) may be interpreted as the moment of inertia of the same imaginary sheet of material, with $\sigma$ formally equal to 1 , for its rotation about the neutral line - see Eq. (6.24). This analogy is so convenient that the integral is usually called the moment of inertia of the cross-section and denoted similarly - just as has been done above. So, our basic result (71) may be re-written as

$$
\begin{equation*}
\frac{1}{R}=\frac{\tau_{y}}{E I_{y}} \tag{7.75}
\end{equation*}
$$

This relation is only valid if the deformation is small in the sense $R \gg a$. Still, since the deviations of the rod from its unstrained shape may accumulate along its length, Eq. (75) may be used for calculations of global deviations arbitrary on the scale of $a$. In order to describe such deformations, this equation has to be complemented by conditions of balance of the bending forces and torques. Unfortunately, this requires a bit more of differential geometry than I have time for, and I will only discuss this procedure for the simplest case of relatively small deviations $q \equiv q_{x}$ of the rod from its initial straight shape, which will be used for axis $z$ (Fig. 9a), by some bulk-distributed force $\mathbf{f}=\mathbf{n}_{x} f_{x}(z)$. (The simplest example is a uniform gravity field, for which $f_{x}=-\rho g=$ const.) Note that in the forthcoming discussion the reference frame will be global, i.e. common for the whole rod, rather than local (pertaining to each cross-section) as in the previous analysis - cf. Fig. 8.

(a)


Fig. 7.9. Global picture of rod bending: (a) forces acting on a small fragment of a rod and (b) two bending problem examples, each with two typical, different boundary conditions.

First of all, we may write an evident differential equation for the average vertical force $\mathbf{F}=$ $\mathbf{n}_{x} F_{x}(z)$ acting of the part of the rod located to the left of its cross-section located at point $z$. This equation expresses the balance of vertical forces acting on a small fragment $d z$ of the rod (Fig. 9a), necessary for the absence of its linear acceleration: $F_{x}(z+d z)-F_{x}(z)+f_{x}(z) A d z=0$, giving

$$
\begin{equation*}
\frac{d F_{x}}{d z}=-f_{x} A \tag{7.76}
\end{equation*}
$$

Note that this vertical component of the internal forces has been neglected at our derivation of Eq. (75), and hence our final results will be valid only if the ratio $F_{x} / A$ is much less than the magnitude of $\sigma_{z z}$ described by Eq. (69). However, these lateral forces create the very torque $\tau=\mathbf{n}_{y} \tau_{y}$ that causes the bending, and thus have to be taken into account at the analysis of the global picture. This re-calculation is expressed by the balance of torque components acting on the same rod fragment of length $d z$, necessary for the absence of its angular acceleration:

$$
\begin{equation*}
\frac{d \tau_{y}}{d z}=-F_{x} \tag{7.77}
\end{equation*}
$$

These two equations of dynamics (or rather statics) should be complemented by two geometric relations. The first of them is $d \varphi_{y} / d z=1 / R$, which has already been discussed. We may immediately combine it with the basic result (75) of the local analysis, getting:

$$
\begin{equation*}
\frac{d \varphi_{y}}{d z}=\frac{\tau_{y}}{E I_{y}} \tag{7.78}
\end{equation*}
$$

The final equation is the geometric relation evident from Fig. 9a:

$$
\begin{equation*}
\frac{d q_{x}}{d z}=\varphi_{y} \tag{7.79}
\end{equation*}
$$

which is (as all expressions of our simple analysis) only valid for small bending angles, $\left|\varphi_{y}\right| \ll 1$.
Four differential equations (76)-(79) are sufficient for the full solution of the weak bending problem, if complemented by appropriate boundary conditions. Figure $9 b$ shows four most frequently met conditions. Let us solve, for example, the problem shown on the top panel of Fig. 9 b : bending of a rod, clamped in a wall on one end, under its own weight. Considering, for the sake of simplicity, a uniform rod, ${ }^{27}$ we may integrate equations (70), (72)-(74) one by one, each time using the appropriate boundary conditions. To start, Eq. (76), with $f_{x}=-\rho g$, yields

$$
\begin{equation*}
F_{x}=\rho g A z+\text { const }=\rho g A(z-L), \tag{7.80}
\end{equation*}
$$

where the integration constant has been selected to satisfy the right-end boundary condition: $F_{x}=0$ at $z$ $=L$. As a sanity check, at the left wall $(z=0), F_{x}=-\rho g A L=-m g$, meaning that the whole weight of the rod is exerted on the wall - fine.

Next, plugging Eq. (80) into Eq. (77) and integrating, we get

$$
\begin{equation*}
\tau_{y}=-\frac{\rho g A}{2}\left(z^{2}-2 L z\right)+\mathrm{const}=-\frac{\rho g A}{2}\left(z^{2}-2 L z+L^{2}\right)=-\frac{\rho g A}{2}(z-L)^{2}, \tag{7.81}
\end{equation*}
$$

where the integration constant's choice ensures the second right-boundary condition: $\tau_{y}=0$ at $z=L$. Proceeding in the same fashion to Eq. (78), we get

[^108]\[

$$
\begin{equation*}
\varphi_{y}=-\frac{\rho g A}{2 E I_{y}} \frac{(z-L)^{3}}{3}+\text { const }=-\frac{\rho g A}{6 E I_{y}}\left[(z-L)^{3}+L^{3}\right] \tag{7.82}
\end{equation*}
$$

\]

where the integration constant is selected to satisfy the clamping condition at the left end of the rod: $\varphi_{y}$ $=0$ at $z=0$. (Note that this is different from the support condition, illustrated on the lower panel of Fig. 9 b , which allows the angle at $z=0$ to be finite but requires the torque to vanish.) Finally, integrating Eq. (79) with $\varphi_{y}$ given by Eq. (82), we get rod's global deformation law,

$$
\begin{equation*}
q_{x}(z)=-\frac{\rho g A}{6 E I_{y}}\left[\frac{(z-L)^{4}}{4}+L^{3} z+\text { const }\right]=-\frac{\rho g A}{6 E I_{y}}\left[\frac{(z-L)^{4}}{4}+L^{3} z-\frac{L^{4}}{4}\right] \tag{7.83}
\end{equation*}
$$

where the integration constant is selected to satisfy the second left-boundary condition: $q=0$ at $z=0$. So, the bending law is sort of complex even in this very simple problem. It is also remarkable how fast does the end's displacement grow with the increase of rod's length:

$$
\begin{equation*}
q_{x}(L)=-\frac{\rho g A L^{4}}{8 E I_{y}} \tag{7.84}
\end{equation*}
$$

To conclude the solution, let us discuss the validity of this result. First, the geometric relation (79) is only valid if $\left|\varphi_{y}(L)\right| \ll 1$, and hence if $\left|q_{x}(L)\right| \ll L$. Next, the local formula Eq. (78) is valid if $1 / R=\tau(L) / E I_{y} \ll 1 / a \sim A^{-1 / 2}$. Using results (81) and (84), we see that the latter condition is equivalent to $\left|q_{x}(L)\right| \ll L^{2} / a$, i.e. is weaker, because all our analysis has been based on the assumption that $L \gg a$.

Another point of concern may be that the off-diagonal stress component $\sigma_{x z} \sim F_{x} / A$, that is created by the vertical gravity forces, has been ignored in our local analysis. For that approximation to be, this component must be much smaller than the diagonal component $\sigma_{z z} \sim a E / R=a \tau / I_{y}$ taken into account in that analysis. Using Eqs. (80) and (81), we are getting the following estimates: $\sigma_{x z} \sim \rho g L, \sigma_{z z}$ $\sim a \rho g A L^{2} / I_{y} \sim a^{3} \rho g L^{2} / I_{y}$. According to its definition (72), $I_{y}$ may be crudely estimated as $a^{4}$, so that we finally get the following simple condition: $a \ll L$, which has been assumed from the very beginning.

### 7.6. Rod torsion

One more class of analytically solvable elasticity problems is torsion of quasi-uniform, straight rods by a couple of axially-oriented torques $\tau=\mathbf{n}_{z} \tau_{z}$ (Fig. 10).


Fig. 7.10. Rod torsion.

Here the main goal of the local analysis is to relate torque $\tau_{z}$ to parameter $\kappa$ in the relation

$$
\begin{equation*}
\frac{d \varphi_{z}}{d z}=\kappa \tag{7.85}
\end{equation*}
$$

If the deformation is elastic and small (in the sense $\kappa a \ll 1$, where $a$ is again the characteristic size of rod's cross-section), $\kappa$ is proportional to $\tau_{z}$, and their ratio,

Torsional rigidity $C$

$$
\begin{equation*}
C \equiv \frac{\tau_{z}}{\kappa}=\frac{\tau_{z}}{d \varphi_{z} / d z}, \tag{7.86}
\end{equation*}
$$

is called the torsional rigidity of the rod. Our task is to calculate the rigidity.
As the first guess (as we will see below, of a limited validity), one may assume that the torsion does not change the shape or size of the cross-section, but leads just to the mutual rotation of crosssections about certain central line. Using a reference frame with the origin on that line, this assumption immediately allows the calculation of components of the displacement vector $d \mathbf{q}$, by using Eq. (6) with $d \boldsymbol{\varphi}=\mathbf{n}_{\mathrm{z}} d \varphi_{z}:$

$$
\begin{equation*}
d q_{x}=-y d \varphi_{z}=-\kappa y d z, \quad d q_{y}=x d \varphi_{z}=\kappa x d z, \quad d q_{z}=0 \tag{7.87}
\end{equation*}
$$

From here, we can calculate all Cartesian components (9) of the strain tensor:

$$
\begin{equation*}
s_{x x}=s_{y y}=s_{z z}=0, \quad s_{x y}=s_{y x}=0, \quad s_{x z}=s_{z x}=-\frac{\kappa}{2} y, \quad s_{y z}=s_{z y}=\frac{\kappa}{2} x . \tag{7.88}
\end{equation*}
$$

The first of these equalities means that volume does not change, i.e. we are dealing with a pure shear deformation. As a result, all nonvanishing components of the stress tensor, calculated from Eqs. (34), ${ }^{28}$ are proportional to the shear modulus alone:

$$
\begin{equation*}
\sigma_{x x}=\sigma_{y y}=\sigma_{z z}=0, \quad \sigma_{x y}=\sigma_{y x}=0, \quad \sigma_{x z}=\sigma_{z x}=-\mu k y, \quad \sigma_{y z}=\sigma_{z y}=\mu \kappa x . \tag{7.89}
\end{equation*}
$$

Now it is straightforward to use this result to calculate the full torque as an integral over the cross-section area $A$ :

$$
\begin{equation*}
\tau_{z} \equiv \int_{A}(\mathbf{r} \times d \mathbf{F})_{z}=\int_{A}\left(x d F_{y}-y d F_{x}\right)=\int_{A}\left(x \sigma_{y z}-y \sigma_{x z}\right) d x d y . \tag{7.90}
\end{equation*}
$$

Using Eq. (89), we get $\tau_{\mathrm{z}}=\mu \kappa I_{z}$, i.e.

$$
\begin{equation*}
C=\mu I_{z}, \quad \text { where } \quad I_{z} \equiv \int_{A}\left(x^{2}+y^{2}\right) d x d y . \tag{7.91}
\end{equation*}
$$

Again, just as in the case of thin rod bending, we have got an integral similar to a moment of inertia, this time for rotation about axis $z$ passing through a certain point of the cross-section. For any axially-symmetric cross-section, this evidently should be the central point. Then, for example, for the practically important case of a round pipe with internal radius $R_{1}$ and external radius $R_{2}$, Eq. (91) yields

$$
\begin{equation*}
C=\mu 2 \pi \int_{R_{1}}^{R_{2}} \rho^{3} d \rho=\frac{\pi}{2} \mu\left(R_{2}^{4}-R_{1}^{4}\right) . \tag{7.92}
\end{equation*}
$$

In particular, for the solid rod of radius $R$ this gives torsional rigidity $C=(\pi / 2) \mu R^{4}$, while for a hollow pipe of small thickness $t \ll R$, Eq. (92) is reduced to

[^109]\[

$$
\begin{equation*}
C=2 \pi \mu R^{3} t \tag{7.93}
\end{equation*}
$$

\]

Note that per unit cross-section area $A$ (and hence per unit mass) this rigidity is twice higher that of a solid rod:

$$
\begin{equation*}
\left.\frac{C}{A}\right|_{\text {thin round pipe }}=\mu R^{2}>\left.\frac{C}{A}\right|_{\text {solid round rod }}=\frac{1}{2} \mu R^{2} . \tag{7.94}
\end{equation*}
$$

This fact is the basis of a broad use of thin pipes in construction.
However, for rods with axially-asymmetric cross-sections, Eq. (91) gives wrong results. For example, for a narrow rectangle of area $A=w t$ with $t \ll w$, it yields $C=\mu t w^{3} / 12$ [WRONG!], even functionally different from the correct result - cf. Eq. (106) below. The reason of the failure of the above analysis is that does not describe possible bending $q_{z}$ of rod's cross-section in the direction along the rod. (For axially-symmetric rods, such bending is evidently forbidden by the symmetry, so that Eq. (91) is valid, and results (92)-(94) are absolutely correct.) Let us describe ${ }^{29}$ this, rather counter-intuitive effect by taking

$$
\begin{equation*}
q_{z}=\kappa \psi(x, y) \tag{7.95}
\end{equation*}
$$

(where $\psi$ is some function to be determined), but still keeping Eq. (87) for two other components of the displacement vector. The addition of $\psi$ does not change the equality to zero of the diagonal components of the strain tensor, as well as of $s_{x y}=s_{y x}$, but contributes to other off-diagonal components:

$$
\begin{equation*}
s_{x z}=s_{z x}=\frac{\kappa}{2}\left(-y+\frac{\partial \psi}{\partial x}\right), \quad s_{y z}=s_{z y}=\frac{\kappa}{2}\left(x+\frac{\partial \psi}{\partial y}\right), \tag{7.96}
\end{equation*}
$$

and hence to the corresponding elements of the stress tensor:

$$
\begin{equation*}
\sigma_{x z}=\sigma_{z x}=\mu \kappa\left(-y+\frac{\partial \psi}{\partial x}\right), \quad \sigma_{y z}=\sigma_{z y}=\mu \kappa\left(x+\frac{\partial \psi}{\partial y}\right) . \tag{7.97}
\end{equation*}
$$

Now let us find the requirement imposed on function $\psi(x, y)$ by the fact that the stress force component parallel to rod's axis,

$$
\begin{equation*}
d F_{z}=\sigma_{z x} d A_{x}+\sigma_{z y} d A_{y}=\mu \kappa d A\left[\left(-y+\frac{\partial \psi}{\partial x}\right) \frac{d A_{x}}{d A}+\left(x+\frac{\partial \psi}{\partial y}\right) \frac{d A_{y}}{d A}\right] \tag{7.98}
\end{equation*}
$$

has to vanish at rod's surface(s), i.e. at each border of its cross-section. Coordinates $\{x, y\}$ of points at a border may be considered functions of the arc $l$ of that line - see Fig. 11. As this figure shows, the elementary area ratios participating in Eq. (98) may be readily expressed via derivatives of functions $x(l)$ and $y(l): d A_{x} / d A=\sin \alpha=d y / d l, d A_{y} / d A=\cos \alpha=-d x / d l$, so that we may write

$$
\begin{equation*}
\left[\left(-y+\frac{\partial \psi}{\partial x}\right)\left(\frac{d y}{d l}\right)+\left(x+\frac{\partial \psi}{\partial y}\right)\left(-\frac{d x}{d l}\right)\right]_{\mathrm{border}}=0 \tag{7.99}
\end{equation*}
$$

Introducing, instead of $\psi$, a new function $\chi(x, y)$, defined by its derivatives as

[^110]\[

$$
\begin{equation*}
\frac{\partial \chi}{\partial x} \equiv \frac{1}{2}\left(-x-\frac{\partial \psi}{\partial y}\right), \quad \frac{\partial \chi}{\partial y} \equiv \frac{1}{2}\left(-y+\frac{\partial \psi}{\partial x}\right), \tag{7.100}
\end{equation*}
$$

\]

we may rewrite condition (99) as

$$
\begin{equation*}
\left.2\left(\frac{\partial \chi}{\partial y} \frac{d y}{d l}+\frac{\partial \chi}{\partial x} \frac{d x}{d l}\right)_{\text {border }} \equiv 2 \frac{d \chi}{d l}\right|_{\text {border }}=0 \tag{7.101}
\end{equation*}
$$

so that function $\chi$ should be constant at each border of the cross-section.


Fig. 7.11. Deriving Eq. (101).

In particular, for a singly-connected cross-section, limited by just one continuous border line, the constant is arbitrary, because according to Eqs. (100), its choice does not affect the longitudinal deformation function $\psi(x, y)$ and hence the deformation as the whole. Now let use the definition (100) of function $\chi$ to calculate the 2D Laplace operator of this function:

$$
\begin{equation*}
\nabla_{x, y}^{2} \chi \equiv \frac{\partial^{2} \chi}{\partial^{2} x}+\frac{\partial^{2} \chi}{\partial^{2} y}=\frac{1}{2} \frac{\partial}{\partial x}\left(-x-\frac{\partial \psi}{\partial y}\right)+\frac{1}{2} \frac{\partial}{\partial y}\left(-y+\frac{\partial \psi}{\partial y}\right)=-1 . \tag{7.102}
\end{equation*}
$$

This a 2D Poisson equation (frequently met, for example, in electrostatics), but with a very simple, constant right-hand part. Plugging Eqs. (100) into Eqs. (97), and those into Eq. (90), we may express torque $\tau$, and hence the torsional rigidity $C$, via the same function:

$$
\begin{equation*}
C \equiv \frac{\tau_{z}}{\kappa}=-2 \mu \int_{A}\left(x \frac{\partial \chi}{\partial x}+y \frac{\partial \chi}{\partial y}\right) d x d y \tag{7.103a}
\end{equation*}
$$

Sometimes, it is easier to use this result in one of its two different forms. The first of them may be readily obtained from Eq. (103a) using integration by parts:

$$
\begin{align*}
C & =-2 \mu\left(\int d y \int x d \chi+\int d x \int y d \chi\right)=-2 \mu\left[\int d y\left(x \chi_{\text {border }}-\int \chi d x\right)+\int d x\left(y \chi_{\text {border }}-\int \chi d y\right)\right] \\
& =4 \mu\left[\int_{A} \chi d x d y-\chi_{\text {border }} \int_{A} d x d y\right], \tag{7.103b}
\end{align*}
$$

while the proof of one more form,

$$
\begin{equation*}
C=4 \mu \int_{A}\left(\nabla_{x, y} \chi\right)^{2} d x d y \tag{7.103c}
\end{equation*}
$$

is left for reader's exercise.
Thus, if we need to know rod's rigidity alone, it is sufficient to calculate function $\chi(x, y)$ from Eq. (102) with boundary condition (101), and plug it into any of Eqs. (103). Only if we are also curious about the longitudinal deformation (95) of the cross-section, we may continue by using Eq. (100) to find function $\psi(x, y)$. Let us see how does this general result work for the two examples discussed above. For the round cross-section of radius $R$, both the Poisson equation (102) and the boundary condition, $\chi=$ const at $x^{2}+y^{2}=R^{2}$, are evidently satisfied by the axially-symmetric function

$$
\begin{equation*}
\chi=-\frac{1}{4}\left(x^{2}+y^{2}\right)+\text { const. } \tag{7.104}
\end{equation*}
$$

For this case, either of Eqs. (103) yields

$$
\begin{equation*}
C=4 \mu \int_{A}\left[\left(-\frac{1}{2} x\right)^{2}+\left(-\frac{1}{2} y\right)^{2}\right] d x d y=\mu \int_{A}\left(x^{2}+y^{2}\right) d^{2} r \tag{7.105}
\end{equation*}
$$

i.e. the same result (91) that we had for $\psi=0$. Indeed, plugging Eq. (104) into Eqs. (100), we see that in this case $\partial \psi / \partial x=\partial \psi / \partial y=0$, so that $\psi(x, y)=$ const, i.e. the cross-section is not bent. (As we have discussed in Sec. 1, a uniform translation $d q_{z}=\kappa \psi=$ const does not give any deformation.)

Now, turning to a rod with a narrow rectangular cross-section wt with $t \ll w$, we may use this strong inequality to solve the Poisson equation (102) approximately, neglecting the derivative along the wider dimension (say, $y$ ). The remaining 1 D differential equation $d^{2} \chi / d^{2} x=-1$, with boundary conditions $\left.\chi\right|_{x=+t / 2}=\left.\chi\right|_{x=-t / 2}$ has an evident solution $\chi=-x^{2} / 2+$ const. Plugging this expression into any form of Eq. (103), we get the correct result for the torsional rigidity:

$$
\begin{equation*}
C=\frac{1}{6} \mu w t^{3} . \tag{7.106}
\end{equation*}
$$

Now let us have a look at the cross-section bending law (95) for this particular case. Using Eqs. (100), we get

$$
\begin{equation*}
\frac{\partial \psi}{\partial y}=-x-2 \frac{\partial \chi}{\partial x}=x, \quad \frac{\partial \psi}{\partial x}=y+2 \frac{\partial \chi}{\partial y}=y . \tag{7.107}
\end{equation*}
$$

Integrating these differential equations over the cross-section, and taking the integration constant (again, not contributing to the deformation) for zero, we get a beautifully simple result:

$$
\begin{equation*}
\psi=x y, \quad \text { i.e. } q_{z}=\kappa x y . \tag{7.108}
\end{equation*}
$$

It means that the longitudinal deformation of the rod has a "propeller bending" form: while the regions near the opposite corners (sitting on the same diagonal) of the cross-section bend toward one direction of axis $z$, corners on the other diagonal bend in the opposite direction. (This qualitative conclusion remains valid for rectangular cross-sections with any aspect ratio $t / w$.)

For rods with several surfaces, i.e. with cross-sections limited by several boundaries (say, hollow pipes), the boundary conditions for function $\chi(x, y)$ require a bit more care, and Eq. (103b) has to be modified, because the function may be equal to a different constant at each boundary. Let me leave the calculation of the torsional rigidity for this case for reader's exercise.

### 7.7. 3D acoustic waves

Now moving to elastic dynamics, we may start with Eq. (24) that may be transformed into the vector form exactly as this was done for the static case in the beginning of Sec. 4. Comparing Eqs. (24) and (54), we immediately see that the result may be presented as
 dynamics equation

$$
\begin{equation*}
\rho \frac{\partial^{2} \mathbf{q}}{\partial t^{2}}=\frac{E}{2(1+v)} \nabla^{2} \mathbf{q}+\frac{E}{2(1+v)(1-2 v)} \nabla(\nabla \cdot \mathbf{q})+\mathbf{f}(\mathbf{r}, t) \tag{7.109}
\end{equation*}
$$

Let us use this general equation for analysis of probably the most important type of timedependent deformations: elastic waves. First, let us address the simplest case of a virtually infinite, uniform elastic medium, without any external forces $\mathbf{f}$. In this case, due to the linearity and homogeneity of the resulting equation of motion, and in clear analogy with the 1 D case (see Sec. 5.3), we may look for a particular time-dependent solution in the form of a sinusoidal, linearly-polarized, plane wave

3D plane, sinusoidal wave

$$
\begin{equation*}
\mathbf{q}(\mathbf{r}, t)=\operatorname{Re}\left[\mathbf{a} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)}\right], \tag{7.110}
\end{equation*}
$$

where $\mathbf{a}$ is the constant complex amplitude of a wave (now a vector!), and $\mathbf{k}$ is the wave vector whose magnitude is equal to the wave number $k$. The direction of these two vectors should be clearly distinguished: while a determined wave's polarization, i.e. the direction of the particle displacements, vector $\mathbf{k}$ is directed along the spatial gradient of the full phase of the wave

$$
\begin{equation*}
\Psi \equiv \mathbf{k} \cdot \mathbf{r}-\omega t+\arg a, \tag{7.111}
\end{equation*}
$$

i.e. along the direction of the wave front propagation.

The importance of the angle between these two vectors may be readily seen from the following simple calculation. Let us point axis $z$ of an (inertial) reference frame along the direction of vector $\mathbf{k}$, and axis $x$ in such direction that vector $\mathbf{q}$, and hence a lie within the $\{x, z\}$ plane. In this case, all variables may change only along that axis, i.e. $\nabla=\mathbf{n}_{\mathrm{z}}(\partial / \partial z)$, while the amplitude vector may be presented as the sum of just two Cartesian components:

$$
\begin{equation*}
\mathbf{a}=a_{x} \mathbf{n}_{x}+a_{z} \mathbf{n}_{z} . \tag{7.112}
\end{equation*}
$$

Let us first consider a longitudinal wave, ${ }^{30}$ with the particle motion along the wave direction: $a_{x}$ $=0, a_{z}=a$. Then vector $\mathbf{q}$ in Eq. (109), describing that wave, has only one ( $z$ ) component, so that $\nabla \cdot \mathbf{q}=$ $d q_{z} / d z$ and $\nabla(\nabla \cdot \mathbf{q})=\mathbf{n}_{z}\left(\partial^{2} \mathbf{q} / \partial z^{2}\right)$, and the Laplace operator gives the same expression: $\nabla^{2} \mathbf{q}=\mathbf{n}_{z}\left(\partial^{2} \mathbf{q} / \partial z^{2}\right)$. As a result, Eq. (109), with $\mathbf{f}=0$, yields

$$
\begin{equation*}
\rho \frac{\partial^{2} q_{z}}{\partial t^{2}}=\left[\frac{E}{2(1+v)}+\frac{E}{2(1+v)(1-2 v)}\right] \frac{\partial^{2} q_{z}}{\partial z^{2}}=\frac{E(1-v)}{(1+v)(1-2 v)} \frac{\partial^{2} q_{z}}{\partial z^{2}} . \tag{7.113}
\end{equation*}
$$

Plugging the plane-wave solution (110) into this equation, we see that it is indeed satisfied if the wave number and wave frequency are related as

[^111]\[

$$
\begin{equation*}
\omega=v_{l} k, \quad v_{l}^{2}=\frac{E(1-v)}{(1+v)(1-2 v) \rho}=\frac{K+(4 / 3) \mu}{\rho} \tag{7.114}
\end{equation*}
$$

\]

This expression allows a simple interpretation. Let us consider a static experiment, similar to the tensile test experiment shown in Fig. 6, but with a sample much wider than $L$ in both directions perpendicular to the force. Then the lateral contraction is impossible, and we can calculate the only finite stress component, $\sigma_{z z}$, directly from Eq. (34) with $\operatorname{Tr}(\mathrm{s})=s_{z z}$ :

$$
\begin{equation*}
\sigma_{z z}=2 \mu\left(s_{z z}-\frac{1}{3} s_{z z}\right)+3 K\left(\frac{1}{3} s_{z z}\right)=\left(K+\frac{4}{3} \mu\right) s_{z z} . \tag{7.115}
\end{equation*}
$$

We see that the numerator in Eq. (114) is nothing more than the static elastic modulus for such a uniaxial deformation, and it is recalculated into the velocity exactly as the spring constant in the 1D waves considered in Sec. 5.3 - cf. Eq. (5.32). ${ }^{31}$ Thus, the longitudinal acoustic waves are just simple waves of uniaxial extension/compression along the propagation axis. Formula (114) becomes especially simple in fluids, where $\mu=0$, and the wave velocity is described by well-known expression

$$
\begin{equation*}
v_{l}=\left(\frac{K}{\rho}\right)^{1 / 2} \tag{7.116}
\end{equation*}
$$

Note, however, that for gases, with their high compressibility and temperature sensitivity, the value of $K$ participating in this formula may differ, at high frequencies, from that given by Eq. (42), because the fast compressions/extensions of gas are nearly adiabatic rather than isothermal. This difference is noticeable in Table 1 which, in particular, lists the values of $v_{l}$ for some representative materials.

Now let us consider an opposite case of transverse waves with $a_{x}=a, a_{z}=0$. In such a wave, the displacement vector is perpendicular to $z$, so that $\nabla \cdot \mathbf{q}=0$, and the second term in the right-hand part of Eq. (109) vanishes. On the contrary, the Laplace operator acting on such vector still gives the same nonzero contribution, $\nabla^{2} \mathbf{q}=n_{z}\left(\partial^{2} \mathbf{q} / \partial z^{2}\right)$, to Eq. (109), so that the equation yields

$$
\begin{equation*}
\rho \frac{\partial^{2} q_{x}}{\partial t^{2}}=\frac{E}{2(1+v)} \frac{\partial^{2} q_{x}}{\partial z^{2}} \tag{7.117}
\end{equation*}
$$

and instead of Eq. (114) we now get

$$
\begin{equation*}
\omega=v_{t} k, \quad v_{t}^{2}=\frac{E}{2(1+v) \rho}=\frac{\mu}{\rho} . \tag{7.118}
\end{equation*}
$$

Longitudinal waves: velocity in fluids

Longitudinal waves: velocity
the strain tensor $s_{j j}$, has no diagonal components, $\operatorname{Tr}(\mathrm{s})=0$, so that $\mu$ is the only elastic modulus actively participating in the Hooke's law (34).

In particular, fluids cannot carry transverse waves at all (formally, their velocity (118) vanishes), because they do not resist shear deformations. For all other materials, longitudinal waves are faster than the transverse ones. Indeed, for all known materials the Poisson ratio is positive, so that the velocity ratio that follows from Eqs. (114) and (118),

$$
\begin{equation*}
\frac{v_{l}}{v_{t}}=\left(\frac{2-2 v}{1-2 v}\right)^{1 / 2}, \tag{7.119}
\end{equation*}
$$

is above $\sqrt{ } 2 \approx 1.4$. For the most popular construction materials, with $\lambda \approx 0.3$, the ratio is about $2-$ see Table 1.

Let me emphasize again that for both longitudinal and transverse waves the relation between the wave number and frequency is linear: $\omega=v k$. As has already been discussed in Sec. 5.3, in this case of acoustic waves (or just "sound") there is no dispersion, i.e. a transverse or longitudinal wave of more complex form, consisting of several (or many) Fourier components of the type (110), preserves its form during propagation: ${ }^{33}$

$$
\begin{equation*}
\mathbf{q}(z, t)=\mathbf{q}(z-v t, 0) . \tag{7.120}
\end{equation*}
$$

As one may infer from the analysis in Sec. 5.3, the dispersion would be back at very high (hypersound) frequencies where the wave number $k$ becomes of the order of the reciprocal distance between the particles of the medium (e.g., atoms or molecules), and hence the approximation of the medium as a continuum, used through this chapter, became invalid.

As we already know from Sec. 5.3, besides the velocity, an important parameter characterizing waves of each type is the wave impedance $Z$ of the medium, for acoustic waves frequently called the acoustic impedance. Generalizing Eq. (5.44) to the 3D case, we may define the impedance as the ratio of the force per unit area (i.e. the corresponding component of the stress tensor) exerted by the wave, to particles' velocity. For example, for the longitudinal waves, propagating in the positive/negative direction along $z$ axis,

$$
\begin{equation*}
Z_{l} \equiv \mp \frac{\sigma_{z z}}{\partial q_{z} / \partial t}=\mp \frac{\sigma_{z z}}{s_{z z}} \frac{s_{z z}}{\partial q_{z} / \partial t}=\mp \frac{\sigma_{z z}}{s_{z z}} \frac{\partial q_{z} / \partial z}{\partial q_{z} / \partial t} . \tag{7.121}
\end{equation*}
$$

Plugging in Eqs. (110), (114), and (115), we get

$$
\begin{equation*}
Z_{l}=\left[\left(K+\frac{4}{3} \mu\right) \rho\right]^{1 / 2} \tag{7.122}
\end{equation*}
$$

in a clear analogy with Eq. (5.45). Similarly, for the transverse wave, the appropriately modified definition, $Z_{t} \equiv \mp \sigma_{x z} /\left(\partial q_{x} / \partial z\right)$, yields

$$
\begin{equation*}
Z_{t}=(\mu \rho)^{1 / 2} \tag{7.123}
\end{equation*}
$$

[^112]Just like in the 1D waves, one role of impedance is to scale the power carried by the wave. For plane 3D waves in infinite media, with their infinite wave front area, it is more appropriate to speak it is more appropriate to speak about power density, i.e. power $p=d \not \mathcal{P} d A$ per unit area of the front, and characterize it by not only its magnitude,

$$
\begin{equation*}
p=\frac{d \mathbf{F}}{d A} \cdot \frac{\partial \mathbf{q}}{\partial t} \tag{7.124}
\end{equation*}
$$

but also the direction of the energy propagation, that (for a plane wave in an isotropic medium) coincides with the direction of the wave vector $\mathbf{k}: \boldsymbol{p} \equiv \boldsymbol{\sim} \mathbf{n}_{\mathbf{k}}$. Using definition (18) of the stress tensor, we may present the Cartesian components of this Umov vector ${ }^{34}$ as

$$
\begin{equation*}
\boldsymbol{p}_{j}=\sum_{j^{\prime}} \sigma_{i j^{\prime}} \frac{\partial q_{j^{\prime}}}{\partial t} \tag{7.125}
\end{equation*}
$$

Returning to plane waves propagating along axis $z$, and acting exactly like in Sec. 5.3, for both the longitudinal and transverse waves we arrive at the following 3D analog Eq. (5.46),

$$
\begin{equation*}
p_{z}=\frac{\omega^{2} Z}{2} a a^{*} \tag{7.126}
\end{equation*}
$$

with $Z$ being the corresponding impedance - either $Z_{l}$ or $Z_{t}$.
Just as in 1D case, one more important effect in which the notion of impedance is crucial is wave reflection from at an interface between two media. The two boundary conditions, necessary for the analysis of these processes, may be obtained from the continuity of vectors $\mathbf{q}$ and $d \mathbf{F}$. (The former condition is evident, while the latter one may be obtained by applying the $2^{\text {nd }}$ Newton law to the infinitesimal volume $d V=d A d z$, where segment $d z$ straddles the boundary.) Let us start from the simplest case of the normal incidence on a plane interface between two uniform media with different elastic moduli and mass densities. Due to the symmetry, it is evident that the incident longitudinal/transverse wave may only excite longitudinal/transverse reflected and transferred waves, but not the counterpart wave type. Thus we can literally repeat all the calculations of Sec. 5.4, again arriving at the fundamental relations (5.53) and (5.54), with the only replacement of $Z$ and $Z$ ' with the corresponding values of either $Z_{l}(121)$ or $Z_{t}(123)$. Thus, at the normal incidence the wave reflection is determined solely by the acoustic impedances of the media, while the sound velocities are not involved.

The situation, however, becomes more involved at a nonvanishing incidence angle $\theta^{(i)}$ (Fig. 12), where the transmitted wave is generally also refracted, i.e. propagates under a different angle, $\theta^{(r)} \neq \theta^{(i)}$, to the interface. Moreover, at $\theta^{(i)} \neq 0$ the directions of particle motion (vector $\mathbf{q}$ ) and of the stress forces (vector $d \mathbf{F}$ ) in the incident wave are neither exactly parallel nor exactly perpendicular to the interface, and thus this wave serves as an actuator for reflected and refracted waves of both types - see Fig. 12. (It shows the particular case when the incident wave is transverse.) The corresponding four angles, $\theta_{t}^{(r)}$, $\theta_{t}^{(r)}, \theta_{l}^{\prime}$ ' $\theta_{t}^{\prime}$, may be readily related to $\theta^{(i)}$ by the "kinematic" condition that the incident wave, as well as

[^113]the reflected and refracted waves of both types should have the same spatial distribution along the interface plane, i.e. for the material particles participating in all five waves. According to Eq. (110), the necessary boundary condition is the equality of the tangential components (in Fig. 12, $k_{x}$ ), of all five wave vectors:
\[

$$
\begin{equation*}
k_{t} \sin \theta_{t}^{(r)}=k_{l} \sin \theta_{l}^{(r)}=k_{l}^{\prime} \sin \theta_{l}^{\prime}=k_{t}^{\prime} \sin \theta_{t}^{\prime}=k_{x} \equiv k_{t} \sin \theta_{t}^{(i)} . \tag{7.127}
\end{equation*}
$$

\]

Since the acoustic wave vectors, at fixed frequency, are inversely proportional to the corresponding wave velocities, we immediately get the following relations:

$$
\begin{equation*}
\theta_{t}^{(r)}=\theta_{t}^{(i)}, \quad \frac{\sin \theta_{l}^{(r)}}{v_{l}}=\frac{\sin \theta_{l}^{\prime}}{v_{l}^{\prime}}=\frac{\sin \theta_{t}^{\prime}}{v_{t}^{\prime}}=\frac{\sin \theta_{t}^{(i)}}{v_{t}} \tag{7.128}
\end{equation*}
$$

so that generally all 4 angles are different. (In optics, the latter relation, reduced to just one equality for the only possible, transverse waves, is known as the Snell law.) These relations show that, just like in optics, the direction of a wave propagating into a medium with lower velocity is closer to the normal (axis $z$ ). In particular, this means that if $v^{\prime}>v$, the acoustic waves, at larger angles of incidence, may exhibit the effect of total internal reflection, so well known from optics ${ }^{35}$, when the refracted wave vanishes. In addition, Eqs. (128) show that in acoustics, a reflected longitudinal wave, with velocity $v_{l}>$ $v_{t}$, may vanish at sufficiently large angles of transverse wave incidence.


Fig. 7.12. "Kinematic" condition of acoustic wave reflection and refraction.

All these fact automatically follow from general expressions for amplitudes of the reflected and refracted waves via the amplitude of the incident wave. These relations are straightforward to derive (again, from the continuity of vectors $\mathbf{q}$ and $d \mathbf{F}$ ), but since they are much more bulky then those in the electromagnetic wave theory (where they are called the Fresnel formulas ${ }^{36}$ ), I would not have time/space for spelling them up. Let me only note that, in contrast to the case of normal incidence, these relations involve 8 media parameters: the values of impedances $Z, Z^{\prime}$, and velocities $v, v$ ' on both sides of the interface, and for both the longitudinal and transverse waves.

There is another factor that makes boundary acoustic effects more complex. Within certain frequency ranges, interfaces (and in particular surfaces) of elastic solids may sustain so-called surface

[^114]acoustic waves (SAW), in particular, the Rayleigh waves and Love waves. ${ }^{37}$ The main feature that distinguishes such waves from their bulk (longitudinal and transverse) counterparts is that the particle displacement amplitude is maximal at the interface and decays exponentially into the bulk of both adjacent media. The characteristic depth of this penetration is of the order of, though not exactly equal to the wavelength.

In the Rayleigh waves, the particle displacement vector $\mathbf{q}$ has two components: one longitudinal (and hence parallel to the interface along which the wave propagates) and another transverse (perpendicular to the interface). In contrast to the bulk waves discussed above, the components are coupled (via their interaction with the interface) and as a result propagate with a single velocity $v_{\mathrm{R}}$. As a result, the trajectory of each particle in the Rayleigh wave is an ellipse in the plane perpendicular to the interface. A straightforward analysis ${ }^{38}$ of the Rayleigh waves on the surface of an elastic solid (i.e. its interface with vacuum) yields the following equation for $v_{R}$ :

$$
\begin{equation*}
\left(2-\frac{v_{R}^{2}}{v_{t}^{2}}\right)^{4}=16\left(1-\frac{v_{R}^{2}}{v_{t}^{2}}\right)^{2}\left(1-\frac{v_{R}^{2}}{v_{l}^{2}}\right)^{2} . \tag{7.129}
\end{equation*}
$$

According to this formula, and Eqs. (114) and (118), for realistic materials with $0<\sigma<1 / 2$, the Rayleigh waves are slightly (by 4 to 13\%) slower than the bulk transverse waves - and hence substantially slower than the bulk longitudinal waves.

In contrast, the Love waves are purely transverse, with vector $\mathbf{q}$ oriented parallel to the interface. However, the interaction of these waves with the interface reduces their velocity $v_{\mathrm{L}}$ in comparison with that $\left(v_{t}\right)$ of the bulk transverse waves, keeping it in the narrow interval between $v_{t}$ and $v_{\mathrm{R}}$ :

$$
\begin{equation*}
v_{\mathrm{R}}<v_{\mathrm{L}}<v_{t}<v_{l} \tag{7.130}
\end{equation*}
$$

The practical importance of surface acoustic waves is that their amplitude decays very slowly with distance $r$ from their point-like source: $a \propto 1 / r^{1 / 2}$, while any bulk waves decay much faster, as $a \propto$ $1 / r$. (Indeed, in the latter case power $\mathcal{P} \propto a^{2}$, emitted by such source, is distributed over a spherical surface area proportional to $r^{2}$, while in the former case all the power goes into a thin surface circle whose length scales as $r$.) At least two areas of applications of the surface acoustic waves have to be mentioned: in geophysics (for earthquake detection and Earth crust seismology), and electronics (for signal processing, with a focus on frequency filtering). Unfortunately, I cannot dwell on these interesting topics and I have to refer the reader to special literature. ${ }^{39}$

### 7.8. Elastic waves in restricted geometries

From what we have discussed in the end of the last section, it should be pretty clear that generally the propagation of acoustic waves in elastic bodies of finite size may be very complicated. There is, however, one important limit in which several important results may be readily obtained. This is the limit of (relatively) low frequencies, where the wavelength is much larger than at least one

[^115]dimension of a system. Let us consider, for example, various waves that may propagate along thin rods, in this case "thin" meaning that the characteristic size $a$ of rod's cross-section is much smaller than not only the length of the rod, but also the wavelength $\lambda=2 \pi / k$. In this case there is a considerable range of distances $z$ along the rod,
\[

$$
\begin{equation*}
a \ll \Delta z \ll \lambda \tag{7.131}
\end{equation*}
$$

\]

in which we can neglect the dynamic effects due to medium inertia, and apply results of our earlier static analyses.

For example, for a longitudinal wave of stress, which is essentially a wave of periodic tensile extensions and compressions of the rod, within range (131) we can use the static relation (44):

$$
\begin{equation*}
\sigma_{z z}=E s_{z z} . \tag{7.132}
\end{equation*}
$$

For what follows, it is easier to use the general equation of elastic dynamics not in its vector form (109), but rather in the precursor, Cartesian-component form (25), with $f_{j}=0$. For plane waves propagating along axis $z$, only one component (with $j^{\prime} \rightarrow z$ ) of the sum in the right-hand part of this equation is nonvanishing, and it is reduced to

$$
\begin{equation*}
\rho \frac{\partial^{2} q_{j}}{\partial^{2} t^{2}}=\frac{\partial \sigma_{j z}}{\partial z} . \tag{7.133}
\end{equation*}
$$

In our current case of longitudinal waves, all components of the stress tensor but $\sigma_{z z}$ are equal to zero. With $\sigma_{z z}$ from Eq. (132), and using the definition $s_{z z}=\partial q_{z} / \partial z=\partial q_{z} / \partial z$, Eq. (133) is reduced to a very simple wave equation,

$$
\begin{equation*}
\rho \frac{\partial^{2} q_{z}}{\partial^{2} t^{2}}=E \frac{\partial^{2} q_{z}}{\partial z^{2}} \tag{7.134}
\end{equation*}
$$

which shows that the velocity of such tensile waves is

Tensile waves: velocity

$$
\begin{equation*}
v=\left(\frac{E}{\rho}\right)^{1 / 2} \tag{7.135}
\end{equation*}
$$

Comparing this result with Eq. (114), we see that the tensile wave velocity, for any medium with $\sigma>0$, is lower than the velocity $v_{l}$ of longitudinal waves in the bulk of the same material. The reason for this difference in simple: in thin rods, the cross-section is free to oscillate (e.g., shrink in the longitudinal extension phase of the passing wave), ${ }^{40}$ so that the effective force resisting the longitudinal deformation is smaller than in a border-free space. Since (as clearly visible from the wave equation), the scale of the force gives the scale of $v^{2}$, this difference translates into slower waves in rods. Of course as wave frequency is increased, at $k a \sim 1$ there is a (rather complex and cross-section-depending) crossover from Eq. (135) to Eq. (114).

Proceeding to transverse waves in rods, let us first have a look at long bending waves, with vector $\mathbf{q}=\mathbf{n}_{x} q_{x}$ (with axis $x$ along the bending direction - see Fig. 8) being approximately constant in the whole cross-section. In this case, the only component of the stress tensor contributing to the net transverse force $F_{x}$ is $\sigma_{x z}$, so that the integral of Eq. (133) over the cross-section is

[^116]\[

$$
\begin{equation*}
\rho A \frac{\partial^{2} q_{x}}{\partial t^{2}}=\frac{\partial F_{x}}{\partial z}, \quad F_{x}=\int_{A} \sigma_{x z} d A . \tag{7.136}
\end{equation*}
$$

\]

Now, if Eq. (131) is satisfied, we again may use static local relations (77)-(79), with all derivatives $d / d z$ duly replaced with their partial form $\partial / \partial z$, to express force $F_{x}$ via the bending deformation $q_{x}$. Plugging these relations into each other one by one, we arrive at a very unusual differential equation

$$
\begin{equation*}
\rho A \frac{\partial^{2} q_{x}}{\partial t^{2}}=-E I_{y} \frac{\partial^{4} q_{x}}{\partial z^{4}} . \tag{7.137}
\end{equation*}
$$

Looking for its solution in the form of a sinusoidal wave (110), we get a nonlinear dispersion relation: ${ }^{41}$

$$
\begin{equation*}
\omega=\left(\frac{E I_{y}}{\rho A}\right)^{1 / 2} k^{2} \tag{7.138}
\end{equation*}
$$

Such relation means that the bending waves are not acoustic at any frequency, and cannot be characterized by a single velocity that would be valid for all wave numbers $k$, i.e. for all spatial Fourier components of a waveform. According to our discussion in Sec. 5.3, such strongly dispersive systems cannot pass non-sinusoidal waveforms too far without changing their waveform very considerably.

This situation changes, however, if the rod has an initial uniform longitudinal stress $\sigma_{z z}=T / A$ (where force $T$ is usually called tension), on whose background the transverse waves propagate. To analyze its effect, let us redraw Fig. 6, for a minute neglecting the bending stress - see Fig. 13.


Fig. 7.13. Additional forces in a thin rod ("string"), due to background tension $T$.

Still sticking to the limit of small angles $\varphi$, the additional vertical component $d \tau_{x}$ of the net force acting on a small rod fragment of length $d z$ is $\tau_{x}(z-d z)-T_{x}(z)=T \varphi_{y}(z+d z)-T \varphi_{y}(z) \approx T\left(\partial \varphi_{y} / \partial z\right) d z$, so that $\partial F_{x} / \partial z=T\left(\partial \varphi_{y} / \partial z\right)$. With the geometric relation (79) in its partial-derivative form $\partial q_{x} / \partial z=\varphi_{y}$, this additional term becomes $T\left(\partial^{2} q_{x} / \partial z^{2}\right)$. Adding it to the right-hand part of into Eq. (137), we get the following dispersion relation

$$
\omega^{2}=\frac{1}{\rho A}\left(E I_{y} k^{4}+7 k^{2}\right)
$$

[^117]At low $k$ (and hence low frequencies), it describes acoustic waves with the "guitar string" velocity that should be well known to the reader from undergraduate courses:

$$
\begin{equation*}
v^{2}=\frac{T}{\rho A} \tag{7.140}
\end{equation*}
$$

where the denominator is nothing else than the linear mass density. However, as the frequency grows, Eq. (139) describes a crossover to highly-dispersive bending waves (138).

Now let us consider the so-called torsional waves that are essentially the dynamic propagation of the torsional deformation discussed in Sec. 6. The easiest way to describe these waves, again within the limits given by Eq. (131), is to write the equation of rotation of a small segment $d z$ of the rod about axis $z$, passing through the "center of mass" of its cross-section, under the difference of torques $\tau=\mathbf{n}_{z} \tau_{z}$ applied on its ends - see Fig. 10:

$$
\begin{equation*}
\rho I_{z} d z \frac{\partial^{2} \varphi_{z}}{\partial t^{2}}=d \tau_{z} \tag{7.141}
\end{equation*}
$$

where $I_{z}$ is the "moment of inertia" defined by Eq. (91), which now, after its multiplication by $\rho d z$, i.e. by the mass per unit area, has turned into the real moment of inertia of a $d z$-thick slice of the rod. Dividing both parts by $d z$, using the static local relation (86), $\tau_{z}=C \kappa=C\left(\partial \varphi_{z} / \partial z\right)$, we get the following differential equation

$$
\begin{equation*}
\rho I_{z} \frac{\partial^{2} \varphi_{z}}{\partial t^{2}}=C \frac{\partial^{2} \varphi_{z}}{\partial z^{2}} . \tag{7.142}
\end{equation*}
$$

Just as Eqs. (114), (118), (135) and (140), this equation describes an acoustic (dispersion-free) wave that propagates with frequency-independent velocity

Torsional waves: velocity

$$
\begin{equation*}
v=\left(\frac{C}{\rho I_{z}}\right)^{1 / 2} \tag{7.143}
\end{equation*}
$$

As we have seen in Sec. 6, for rods with axially-symmetric cross-sections, the torsional rigidity $C$ is described by the simple equation (91), $C=\mu I_{z}$, so that expression (143) is reduced to Eq. (118) for the transverse waves in infinite media. The reason for this similarity is simple: in a torsional wave, particles oscillate along small arcs (Fig. 14a), so that if the rod's cross-section is round, the stress-free surface does not perturb or modify the motion in any way, and hence does not affect the transverse velocity.

(b)

Fig. 7.14. Particle trajectories in two different transverse waves with the same velocity: (a) torsional waves in a thin round rod and (b) circularly-polarized waves in an infinite (or very broad) sample.

This fact raises an interesting issue of the relation between the torsional and circularly-polarized waves. Indeed, in Sec. 7, I have not emphasized enough that Eq. (118) is valid for a transverse wave polarized in any direction perpendicular to vector $\mathbf{k}$ (in our notation, directed along axis $z$ ). In particular, this means that such waves are doubly-degenerate: any isotropic elastic medium can carry simultaneously two non-interacting transverse waves propagating in the same direction with the same velocity (118), with mutually perpendicular linear polarizations (directions of vector a), for example, directed along axes $x$ and $y$. If both waves are sinusoidal (110), with the same frequency, each point of the medium participates in two simultaneous sinusoidal motions within the $[x, y]$ plane:

$$
\begin{equation*}
q_{x}=\operatorname{Re}\left[a_{x} e^{i(k z-\omega t)}\right]=A_{x} \cos \Psi, \quad q_{y}=\operatorname{Re}\left[a_{y} e^{i(k z-\omega t)}\right]=A_{y} \cos (\Psi+\varphi), \tag{7.144}
\end{equation*}
$$

where $\Psi \equiv k z-\omega t+\varphi_{x}$, and $\varphi \equiv \varphi_{y}-\varphi_{x}$. Trigonometry tells us that the trajectory of such motion on the $[x, y]$ plane is an ellipse (Fig. 15), so that such waves are called elliptically-polarized. The most important particular cases of such polarization are:
(i) $\varphi=0$ or $\pi$. a linearly-polarized wave, with vector a turned by angle $\theta=\tan ^{-1}\left(A_{y} / A_{x}\right)$ from axis $x$; and
(ii) $\varphi= \pm \pi / 2$ and $A_{x}=A_{y}$ : circularly polarized waves, with the right or left polarization, respectively.

The circularly polarized waves play an important role in quantum mechanics, where such waves may be most naturally quantized, with elementary excitations (in the case of mechanical waves we are discussing, called phonons) having either positive or negative angular momentum $L_{z}= \pm \hbar$.

Now comparing the trajectories of particles in the torsional wave in a thin round rod (or pipe) and the circularly-polarized wave in a broad sample (Fig. 14), we see that, despite the same wave propagation velocity, these transverse waves are rather different. In the former case (Fig. 14a) each particle moves back and forth along an arc, with the arc length different for different particles (and vanishing at rod's center). On the other hand, in a circularly-polarized, plane wave all particles move along similar, circular trajectories.


Fig. 7.15. Trajectory of a particle of an infinite medium with elliptically-polarized transverse wave, within the plane perpendicular to the direction of wave propagation.

In conclusion, let me briefly mention the opposite limit, when the size of the body, from whose boundary are completely reflected, ${ }^{42}$ is much larger than the wavelength. In this case, the waves

[^118]propagate almost as in an infinite 3D medium (Sec. 7), and the most important new effect is the finite numbers of wave modes in the body. Repeating 1D analysis of Sec. 5.4 for each dimension of a 3D cuboid of volume $V=L_{1} L_{2} L_{3}$ (for example, using the Born-Karman boundary conditions in each dimension), we obtain Eq. (5.59) for the spectrum of components of wave vector $\mathbf{k}$ along each side. This means that all possible wave vectors are located in nodes of a rectangular 3D mesh with steps $2 \pi / L_{j}$ in each direction, and hence with the $k$-space ("reciprocal space") volume

Reciprocal volume per wave vector

$$
\begin{equation*}
V_{k}=\frac{2 \pi}{L_{1}} \frac{2 \pi}{L_{2}} \frac{2 \pi}{L_{3}}=\frac{(2 \pi)^{3}}{V} \tag{7.145}
\end{equation*}
$$

per each vector. It is possible (though not quite as straightforward as it is sometimes assumed) to prove that this relation is valid regardless of the shape of volume $V$. Hence the number of different wave vectors within the reciprocal space volume $d^{3} k \gg V_{k}$ is

$$
\begin{equation*}
d N=\frac{d^{3} k}{V_{k}}=\frac{V}{(2 \pi)^{3}} d^{3} k \gg 1 \tag{7.146a}
\end{equation*}
$$

In quantum mechanics, this relation takes the form of the density of quantum states in $k$-space:

$$
\begin{equation*}
g_{k} \equiv g \frac{d N}{d^{3} k}=\frac{g V}{(2 \pi)^{3}} \tag{7.146b}
\end{equation*}
$$

where $g$ is the number of possible different quantum states with the same de Broglie wave vector $\mathbf{k}$. In this form, Eq. (146) is ubiquitous in physics. ${ }^{43}$ For phonons, formed from quantization of one longitudinal mode, and two transverse modes with different polarizations, $g=3$.

### 7.9. Exercise problems

7.1. A uniform thin sheet of an isotropic, elastic material is compressed, along its thickness $t$, by two plane, parallel, broad (of area $A \gg t^{2}$ ) rigid surfaces - see Fig. on the right. Assuming no slippage between the sheet and the surfaces, calculate the relative compression ($\Delta t / t)$ as a function of the compressing force. Compare the result with
 that for the tensile stress, given by Eq. (47).
7.2. A thin, wide sheet of an isotropic, elastic material is clamped in two rigid, plane, parallel surfaces that are pulled apart with force $F$. Find the relative extension $\Delta L / L$ of the sheet in the direction of the force, and its relative compression $\Delta t / t$ in the perpendicular direction, and compare the results with Eqs. (47)-(48) for the tensile stress, and the solution of Problem 1.
the impedance of a longitudinal wave in a typical metal (say, steel) is almost two orders of magnitude higher than that in air, ensuring their virtually full reflection from the surface.
${ }^{43}$ See, e.g., EM Secs. 7.7 and 7.9, and QM Sec. 1.5.
7.3. Calculate the radial extension $\Delta R$ of a thin, long, round cylindrical pipe under the effect of its rotation with a constant angular velocity $\omega$ about its symmetry axis (see Fig. on the right), in terms of the elastic moduli $E$ and $\nu$, assuming that pressure both inside and outside the pipe is negligible.

7.4. A long, uniform rail with the cross-section shown in Fig. on the right, is being bent with the same (small) torque twice: first within plane $x z$ and then within plane $y z$. Assuming that $t \ll L$, find the ratio of rail deformations in these two cases.

7.5. Two thin rods of the same length and mass have been made of the same elastic, isotropic material. The crosssection of one of them is a circle, while another one is an equilateral triangle - see Fig. on the right. Which of the rods is more stiff for bending along its length? Quantify the relation. Does the result depend on the bending plane
 orientation?
7.6. A thin, elastic, uniform, initially straight beam is placed on two point supports at the same height - see Fig. on the right. What support point placement minimizes the largest deviation of the beam from the horizontal line, under its own weight?
7.7. Calculate the largest compression force $T$ that may be withstood by a thin, straight, elastic rod without bucking (see Figs. on the right) for two shown cases:
(i) rod's ends are clamped, and
(ii) the rod it free to rotate about the support points.
(i)

(ii)

7.8. Calculate the potential energy of a small and slowly changing, but otherwise arbitrary bending deformation of a uniform, elastic, initially straight rod. Can the result be used to derive the dispersion relation (7.138)?
7.9.* Calculate the spring constant $d F / d L$ of a coil spring made of a uniform, elastic wire, with circular crosssection of diameter $d$, wound as a dense round spiral of $N$ $\gg 1$ turns of diameter $D \gg d$ - see Fig. on the right. Comment on the type of material's deformation.

7.10. The coil discussed in Problem 9 is now used as what is sometimes called the torsion spring - see Fig. on the right. Find the corresponding spring constant $d \tau / d \varphi$, where $\tau$ is the torque of external forces $\mathbf{F}$ relative the center of the coil (point $O$ ).

7.11. Use Eqs. (101) and (102) to recast Eq. (103b) for the torsional rigidity $C$ into the form given by Eq. (103c).
7.12. ${ }^{*}$ Generalize Eq. (103b) to the case of rods with more than one cross-section boundary. Use the result to calculate the torsional rigidity of a thin round pipe, and compare it with Eq. (93).
7.13. Calculate the potential energy of a small but otherwise arbitrary torsional deformation $\varphi_{z}(z)$ of a uniform, straight, elastic rod.
7.14. A steel wire with the circular cross-section of a $3-\mathrm{mm}$ diameter is stretched with a constant force of 10 N and excited at frequency 1 kHz by an actuator that excites all modes of longitudinal and transverse waves. Which wave has the highest group velocity? Accept the following parameters for steel (see Table 7.1): $E=170 \mathrm{GPa}, \sigma=0.30, \rho=7.8 \mathrm{~g} / \mathrm{cm}^{3}$.
7.15. Define and calculate appropriate wave impedances for (i) tensile and (ii) torsional waves in a thin rod. Use the results to calculate what fraction of each wave's power is reflected from the connection of a long rod with round cross-section to a similar rod, but with twice larger diameter - see Fig.
 on the right.


## Chapter 8. Fluid Mechanics

This chapter describes the basic notions of mechanics of fluids, discusses a few core problems of statics and dynamics of ideal and viscous fluids, and gives a very brief review of such a complex phenomenon as turbulence. Also, the viscous fluid flow is used to give an elementary introduction to numerical methods of partial differential equation solution - whose importance extends well beyond this particular field.

### 8.1. Hydrostatics

The mechanics of fluids (the class of materials that includes both liquids and gases) is both more simple and more complex than that of the elastic solids, with the simplicity falling squarely to the domain of statics - often called hydrostatics, because water has always been the main fluid for the human race and hence for science and engineering. Indeed, fluids are, by definition, the media that cannot resist static shear deformations. There are two ways to express this fact. First, we can formally take the shear modulus $\mu$, describing this resistance, to be equal zero. Then the Hooke's law (7.34) shows that the stress tensor is diagonal:

$$
\begin{equation*}
\sigma_{i j^{\prime}}=\delta_{j j^{\prime}} \sigma_{i j} . \tag{8.1}
\end{equation*}
$$

Alternatively, the same conclusion may be reached by looking at the stress tensor definition (7.19) and saying that in the absence of shear stress, the elementary interface $d \mathbf{F}$ has to be perpendicular to the area element $d A$, i.e. parallel to vector $d \mathbf{A}$.

Moreover, in fluids at equilibrium, all three diagonal components $\sigma_{j j}$ of the stress tensor have to be equal. To prove that, it is sufficient to single out (mentally rather than physically) from a fluid a small volume in the shape of a right prism, with mutually perpendicular faces normal to the two directions we are interested in (Fig. 1, along axes $x$ and $y$ ).


The prism is in equilibrium if each Cartesian component of the total force acting on all its faces nets to zero. For the $x$-component this balance is $\sigma_{x x} d A_{x}-\left(\sigma_{\alpha \alpha} d A\right) \cos \alpha=0$. However, from the geometry (Fig. 1), $d A_{x}=d A \cos \alpha$, and the above balance condition yields $\sigma_{\alpha \alpha}=\sigma_{x x}$. A similar argument for the vertical forces gives $\sigma_{\alpha \alpha}=\sigma_{y y}$, so that $\sigma_{x x}=\sigma_{y y}$. Since such equality holds for any pair of diagonal components of the stress tensor, $\sigma_{j j}$, all three of them have to be equal. This common component is usually represented as $(-P)$, because in the vast majority of cases, parameter $P$, called pressure, is positive. Thus we arrive at the key relation (which has already been mentioned in Ch .7 ):

$$
\begin{equation*}
\sigma_{i j^{\prime}}=-P \delta_{i j^{\prime}} \tag{8.2}
\end{equation*}
$$

In the absence of bulk forces, pressure should be constant through the volume of fluid, due to symmetry. Let us see how this result is affected by bulk forces. With the simple stress tensor (2), the general condition of equilibrium of a continuous medium, expressed by Eq. (7.25) with zero left-hand part, becomes just

$$
\begin{equation*}
-\frac{\partial P}{\partial r_{j}}+f_{j}=0 \tag{8.3}
\end{equation*}
$$

and may be re-written in a convenient vector form:

$$
\begin{equation*}
-\nabla P+\mathbf{f}=0 \tag{8.4}
\end{equation*}
$$

In the simplest case of a heavy fluid, with mass density $\rho$, in a uniform gravity field, $\mathbf{f}=\rho \mathbf{g}$, and the equation of equilibrium becomes,

$$
\begin{equation*}
-\nabla P+\rho \mathbf{g}=0 \tag{8.5}
\end{equation*}
$$

with only one nonvanishing component (vertical, near the Earth surface). If, in addition, the fluid may be considered incompressible, with its density $\rho$ constant, ${ }^{1}$ this equation may be readily integrated to give the so-called Pascal equation: ${ }^{2}$

$$
\begin{equation*}
P+\rho g y=\text { const } \tag{8.6}
\end{equation*}
$$

where $y$ is the vertical coordinate, with the direction opposite to that of vector $\mathbf{g}$.
Let me hope that this equation, and its simple applications (including buoyant force calculations using the Archimedes principle), are well familiar to the reader from his or her undergraduate physics courses, so that I may save time by skipping their discussion. I would only like to note, that the integration of Eq. (4) may be more complex in the case if the bulk forces $\mathbf{f}$ depend on position, ${ }^{3}$ and/or if the fluid is substantially compressible. In the latter case, Eq. (4) should be solved together with the media-specific equation of state $\rho=\rho(P)$ describing the compressibility law - whose example is given by Eq. (7.40) for ideal gases: $\rho \equiv m N / V=m P / k_{\mathrm{B}} T$, where $m$ is the mass of one gas molecule.

### 8.2. Surface tension effects

Besides the bulk (volume-distributed) forces, one more possible source of pressure is surface tension. This effect results from the difference between the potential energy of atomic interactions on the interface between two different fluids and that in their bulks, and thus may be described by an additional potential energy

$$
\begin{equation*}
U_{i}=\gamma A, \tag{8.7}
\end{equation*}
$$

[^119]where $A$ is the interface area, and $\gamma$ is called the surface tension constant (or just the "surface tension"), evidently of the dimensionality of $\mathrm{J} / \mathrm{m}^{2}$, i.e. $\mathrm{N} / \mathrm{m}$. For a stable interface of any two fluids, $\gamma$ is always positive. ${ }^{4}$ In the absence of other forces, the surface tension makes a liquid drop spherical to minimize its surface area at fixed volume.

For the analysis of the surface tension effects in the presence of other forces, it is convenient to reduce it to a certain additional effective pressure drop $\Delta P_{\text {ef }}$ at the interface. In order to calculate $\Delta P_{\text {ef }}$, let us consider the condition of equilibrium of a small part $d A$ of a smooth interface between two fluids (Fig. 2), in the absence of bulk forces.


Fig. 8.2. Deriving the Young-Laplace formula (10).

If pressures $P_{1,2}$ on two sides of the interface are different, the work of stress forces on fluid 1 at a small virtual displacement $\delta \mathbf{r}=\mathbf{n} \delta r$ of the interface (where $\mathbf{n}=d \mathbf{A} / d A$ is the unit vector normal to the interface) equals ${ }^{5}$

$$
\begin{equation*}
\delta W=d A \delta r\left(P_{1}-P_{2}\right) . \tag{8.8}
\end{equation*}
$$

For equilibrium, this work has to be compensated by an equal change of the interface energy, $\delta U_{i}=$ $\gamma \delta(d A)$. Differential geometry tells us that in the linear approximation in $\delta r$, the relative change of the elementary surface area, corresponding to a fixed solid angle $d \Omega$, may be expressed as

$$
\begin{equation*}
\frac{\delta(d A)}{d A}=\frac{\delta r}{R_{1}}+\frac{\delta r}{R_{2}} \tag{8.9}
\end{equation*}
$$

where $R_{1,2}$ are the so-called principal radii of the interface curvature. ${ }^{6}$ Combining Eqs. (7)-(9), we get the Young-Laplace formula ${ }^{7}$

[^120]\[

$$
\begin{equation*}
P_{1}-P_{2}=\Delta P_{\mathrm{ef}} \equiv \gamma\left(\frac{1}{R_{1}}+\frac{1}{R_{2}}\right) . \tag{8.10}
\end{equation*}
$$

\]

In particular, this formula shows that the additional pressure created by surface tension inside a spherical drop of a liquid, of radius $R$, equals $2 \gamma / R$, i.e. decreases with $R$. In contrast, according to Eqs. (5)-(6), the effects of bulk forces, for example gravity, grow as $\rho g R$. The comparison of these two pressure components shows that if the drop radius (or more generally, the characteristic linear size of a fluid sample) is much larger than the so-called capillary length

$$
\begin{equation*}
a_{c} \equiv\left(\frac{2 \gamma}{\rho g}\right)^{1 / 2} \tag{8.11}
\end{equation*}
$$

the surface tension may be safely ignored - as will be done in the following sections of this chapter, besides a brief discussion of Eq. (48). For the water surface, or more exactly its interface with air at ambient conditions, $\gamma \approx 0.073 \mathrm{~N} / \mathrm{m}$, while $\rho \approx 1,000 \mathrm{~kg} / \mathrm{m}^{3}$, so that $a_{c} \approx 4 \mathrm{~mm}$.

On the other hand, in very narrow tubes, such as blood capillary vessels with radius $a \sim 1 \mu \mathrm{~m}$, i.e. $a \ll a_{c}$, the surface tension effects are very important. The key notion for the analysis of these effects is the equilibrium contact angle $\theta_{\mathrm{c}}$ (also called the "wetting angle") at the edge of a liquid wetting a solid - see Fig. 3.


Fig. 8.5. Contact angles for (a) hydrophilic and (b) hydrophobic surfaces.

According to its definition (7), constant $\gamma$ may be interpreted as a force (per unit length of the interface boundary) directed along the interface and trying to reduce its area. As a result, the balance of horizontal components of the three such forces, shown in Fig. 3, immediately yields

$$
\begin{equation*}
\gamma_{\mathrm{sl}}+\gamma_{\mathrm{lg}} \cos \theta_{\mathrm{c}}=\gamma_{\mathrm{sg}}, \tag{8.12}
\end{equation*}
$$

where the indices at constants $\gamma$ correspond to three possible interfaces between the liquid, solid and gas. For the so-called hydrophilic surfaces that "like to be wet" by this particular liquid (not necessarily water), meaning that $\gamma_{\mathrm{sl}}<\gamma_{\mathrm{sg}}$, this relation yields $\cos \theta_{\mathrm{c}}>0$, i.e. $\theta_{\mathrm{c}}<\pi / 2-$ the situation shown in Fig. 3a. On the other hand, for hydrophobic surfaces with $\gamma_{\mathrm{sl}}>\gamma_{\mathrm{sg}}$, Young's equation (12) yields larger contact angles, $\theta_{\mathrm{c}}>\pi / 2-$ see Fig. 3b.

Let us use this notion to solve the simplest but perhaps the most important problem of this field find the height $h$ of the fluid column in a narrow vertical tube made of a hydrophilic material, lifted by the surface tension forces, assuming its internal surface to be a round cylinder of radius $a-$ see Fig. 4. Inside an incompressible fluid, pressure drops with height according to the Pascal equation (6), so that just below the surface, $P \approx P_{0}-\rho g h$, where $P_{0}$ is the background (e.g., atmospheric) pressure. This means that at $a \ll h$ the pressure variation along the concave surface (called the meniscus) of the liquid
is negligible, so that according to the Young-Poisson equation (10) the sum $\left(1 / R_{1}+1 / R_{2}\right)$ has to be virtually constant along the surface. Due to the axial symmetry of the problem, this means that the surface has to be a part of a sphere. ${ }^{8}$ From the contact angle definition, radius $R$ of the sphere is equal to $a / \cos \theta_{\mathrm{c}}-$ see Fig. 4.


Fig. 8.4. Liquid rise in a vertical capillary tube.

Plugging this relation into Eq. (10) with $P_{1}-P_{2}=\rho g h$, we get the following equation for $h$ :

$$
\begin{equation*}
\rho g h=\frac{2 \gamma \cos \theta_{\mathrm{c}}}{a} . \tag{8.13a}
\end{equation*}
$$

In hindsight, this result might be obtained more directly - by requiring the total weight $\rho g V=\rho g\left(\pi a^{2} h\right)$ of the lifted liquid's column to be equal to the vertical component $F \cos \theta_{\mathrm{c}}$ of the full surface tension force $F=\gamma p$ acting on the perimeter $p=2 \pi a$ of the meniscus. Using the definition (11) of the capillary length $a_{c}$, Eq. (13a) may be presented as the so-called Jurin rule:

$$
\begin{equation*}
h=\frac{a_{c}^{2}}{a} \cos \theta_{\mathrm{c}} \leq \frac{a_{c}^{2}}{a} \tag{8.13b}
\end{equation*}
$$

according to our initial assumption $h \gg a$, Eq. (13) is only valid for narrow tubes, with radius $a \ll a_{c}$. This capillary rise is the basic mechanism of lifting water with nutrients from roots to the branches and leaves of plants, so that the tallest tree height is practically established by the Jurin rule (13), with $\cos \theta_{c}$ $\approx 1$ and the pore radius $a$ limited from below by a few microns, because of the viscosity effects restricting the fluid discharge - see Sec. 5 below and in particular the Poiseuille formula (60).

### 8.3. Kinematics

In contrast to the stress tensor, which is useful and simple - see Eq. (2), the strain tensor is not a very useful notion in fluid mechanics. Indeed, besides a very few situations, ${ }^{9}$ typical problems of this field involve fluid flow, i.e. a state when velocity of fluid particles has some nonzero time average. This means that the trajectory of each individual particle is a long line, and the notion of its displacement $\mathbf{q}$

[^121]becomes impracticable. However, particle's velocity $\mathbf{v} \equiv d \mathbf{q} / d t$ is a much more useful notion, especially if it is considered as a function the observation point $\mathbf{r}$ and (generally) time $t$. In an important class of fluid dynamics problem, the so-called stationary (or "steady", or "static") flow, the velocity defined in this way does not depend on time, $\mathbf{v}=\mathbf{v}(\mathbf{r})$.

There is, however, a price to pay for the convenience of this notion: namely, due to the difference between vectors $\mathbf{q}$ and $\mathbf{r}$, particle's acceleration $\mathbf{a}=d^{2} \mathbf{q} / d t^{2}$ (that participates, in particular, in the $2^{\text {nd }}$ Newton law) cannot be calculated just as a time derivative of velocity $\mathbf{v}(\mathbf{r}, t)$. This fact is evident, for example, for the static flow case, in which the acceleration of individual fluid particles may be very significant even if $\mathbf{v}(\mathbf{r})$ does not depend on time - just think about the acceleration of a drop of water flowing over the Niagara Falls rim, first accelerating fast and then virtually stopping below, while the water velocity $\mathbf{v}$ at every particular point, as measured from a bank-based reference frame, is nearly constant. Thus the main task of fluid kinematics is to express a via $\mathbf{v}(\mathbf{r}, t)$; let us do this.

Since each Cartesian component $v_{j}$ of the velocity has to be considered as a function of four independent scalar variables, three Cartesian components $r_{j^{\prime}}$ of vector $\mathbf{r}$ and time $t$, its full time derivative may be presented as

$$
\begin{equation*}
\frac{d v_{j}}{d t}=\frac{\partial v_{j}}{\partial t}+\sum_{j^{\prime}=1}^{3} \frac{\partial v_{j}}{\partial r_{j^{\prime}}} \frac{d r_{j^{\prime}}}{d t} \tag{8.14}
\end{equation*}
$$

Let us apply this general relation to a specific set of infinitesimal changes $\left\{d r_{1}, d r_{2}, d r_{3}\right\}$ that follows a small displacement $d \mathbf{q}$ of a certain particular particle of the fluid, $d \mathbf{r}=d \mathbf{q}=\mathbf{v} d t$, i.e.

$$
\begin{equation*}
d r_{j}=v_{j} d t \tag{8.15}
\end{equation*}
$$

In this case $d v_{j} / d t$ is the $j$-th component $a_{j}$ of the particle's acceleration a, so that Eq. (14) yields the following key relation of fluid kinematics:

$$
\begin{equation*}
a_{j}=\frac{\partial v_{j}}{\partial t}+\sum_{j^{\prime}=1}^{3} v_{j^{\prime}} \frac{\partial v_{j}}{\partial r_{j^{\prime}}} \tag{8.16a}
\end{equation*}
$$

Using operator $\nabla$, this result may be rewritten in the following compact vector form: ${ }^{10}$

$$
\begin{equation*}
\mathbf{a}=\frac{\partial \mathbf{v}}{\partial t}+(\mathbf{v} \cdot \nabla) \mathbf{v} \tag{8.16b}
\end{equation*}
$$

This relation already signals the main technical problem of the fluid dynamics: many equations involving particle's acceleration are nonlinear in velocity, excluding such a powerful tool the linear superposition principle from the applicable mathematical arsenal.

One more basic relation of the fluid kinematics is the so-called continuity equation, which is essentially just the differential version of the mass conservation law. Let us mark, inside a fluid flow, an arbitrary volume $V$ limited by stationary (time-independent) surface $S$. The total mass of the fluid inside the volume may change only due to its flow though the boundary:

[^122]\[

$$
\begin{equation*}
\frac{d M}{d t} \equiv \frac{d}{d t} \int_{V} \rho d^{3} r=-\int_{S} \rho v_{n} d^{2} r \equiv-\int_{S} \rho \mathbf{v} \cdot d \mathbf{A}, \tag{8.17a}
\end{equation*}
$$

\]

where the elementary area vector $d \mathbf{A}$ is defined just as in Sec. 7.2 - see Fig. 5.


Fig. 8.5. Deriving the continuity equation.

Using the same the same divergence theorem that has been used several times in this course, ${ }^{11}$ the surface integral in Eq. (17a) may be transformed into the integral of $\nabla(\rho \mathbf{v})$ over volume $V$, so that this relation may be rewritten as

$$
\begin{equation*}
\int_{V}\left(\frac{\partial \rho}{\partial t}+\nabla \cdot \mathbf{j}\right) d^{3} r=0 \tag{8.17b}
\end{equation*}
$$

where vector $\mathbf{j} \equiv \rho \mathbf{v}$ defined is called either the mass flux density or the mass current. Since Eq. (17b) is valid for an arbitrary volume, the function under the integral has to vanish at any point:

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}+\nabla \cdot \mathbf{j}=0 \tag{8.18}
\end{equation*}
$$

Note that such continuity equation is valid not only for mass, but for other conserved physics quantities (e.g., the electric charge, quantum-mechanical probability, etc.), with the proper re-definition of $\rho$ and $\mathbf{j} .{ }^{12}$

### 8.4. Dynamics: Ideal fluids

Let us start our discussion of fluid dynamics from the simplest case when the stress tensor obeys the simple expression (2) even at the fluid motion. Physically, this means that fluid viscosity effects, including mechanical energy loss, are negligible. (We will discuss the conditions of this assumption in the next section.) Then the equation of motion of such an ideal fluid (essentially the $2^{\text {nd }}$ Newton law for its unit volume) may be obtained from Eq. (7.25) using the simplifications of its right-hand part, discussed in Sec. 1:

$$
\begin{equation*}
\rho \mathbf{a}=-\nabla P+\mathbf{f} . \tag{8.19}
\end{equation*}
$$

Now using the basic kinematic relation (16), we arrive at the following Euler equation: ${ }^{13}$

[^123]\[

$$
\begin{equation*}
\rho \frac{\partial \mathbf{v}}{\partial t}+\rho(\mathbf{v} \cdot \nabla) \mathbf{v}=-\nabla P+\mathbf{f} \tag{8.20}
\end{equation*}
$$

\]

Generally this equation has to be solved together with the continuity equation (11) and equation of state of the particular fluid, $\rho=\rho(P)$. However, as we have already discussed, in many situations the compressibility of water and other important fluids is very low and may be ignored, so that $\rho$ may be treated as a given constant. Moreover, in many cases the bulk forces $\mathbf{f}$ are conservative and may be presented as a gradient of a certain potential function $u(\mathbf{r})$ - the potential energy per unit volume:

$$
\begin{equation*}
\mathbf{f}=-\nabla u \tag{8.21}
\end{equation*}
$$

for example, for a uniform gravity field, $u=\rho g h$. In this case the right-hand part of Eq. (20) becomes $\nabla(P+u)$. For these cases, it is beneficial to recast the left-hand of that equation as well, using the following well-know identity of vector algebra ${ }^{14}$

$$
\begin{equation*}
(\mathbf{v} \cdot \nabla) \mathbf{v}=\nabla\left(\frac{v^{2}}{2}\right)-\mathbf{v} \times(\nabla \times \mathbf{v}) \tag{8.22}
\end{equation*}
$$

As a result, the Euler equation takes the form

$$
\begin{equation*}
\rho \frac{\partial \mathbf{v}}{\partial t}-\rho \mathbf{v} \times(\nabla \times \mathbf{v})+\nabla\left(P+u+\rho \frac{v^{2}}{2}\right)=0 . \tag{8.23}
\end{equation*}
$$

In a stationary flow, the first term of this equation vanishes. If the second term, describing fluid's vorticity, is zero as well, then Eq. (23) has the first integral of motion,

$$
\begin{equation*}
P+u+\frac{\rho}{2} v^{2}=\text { const } \tag{8.24}
\end{equation*}
$$

called the Bernoulli equation. Numerous examples of application of Eq. (24) to simple problems of stationary flow in pipes, in the Earth gravity field (giving $u=\rho g h$ ), should be well known to the reader, so I hope I can skip their discussion without much harm.

In the general case an ideal fluid may have vorticity, so that Eq. (24) is not always valid. Moreover, due to absence of viscosity in an ideal fluid, the vorticity, once created, does not decrease along the streamline - the fluid particle's trajectory, to which the velocity is tangential in every point. ${ }^{15}$ Mathematically, this fact ${ }^{16}$ is expressed by the following Kelvin theorem: $(\nabla \times \mathbf{v}) \cdot d \mathbf{A}=$ const along any small contiguous group of streamlines crossing an elementary area $d A .{ }^{17}$

In many important cases the vorticity of fluid is negligible. For example, if a solid body of arbitrary shape is embedded into an ideal fluid that is uniform (meaning, by definition, that $\mathbf{v}(\mathbf{r}, t)=\mathbf{v}_{0}=$

[^124]const) at large distances, its vorticity is zero everywhere. (Indeed, since $\nabla \times \mathbf{v}$ at the uniform flow, the vorticity is zero at distant points of any streamline, and according to the Kelvin theorem, should equal zero everywhere.) In this case the velocity, as any curl-free vector field, may be presented as a gradient of some effective potential function,
\[

$$
\begin{equation*}
\mathbf{v}=-\nabla \phi \tag{8.25}
\end{equation*}
$$

\]

Such potential flow may be described by a simple differential equation. Indeed, the continuity equation (18) for a steady flow of an incompressible fluid is reduced to $\nabla \cdot \mathbf{v}=0$. Plugging Eq. (25) into this relation, we get the scalar Laplace equation,

$$
\begin{equation*}
\nabla^{2} \phi=0 \tag{8.26}
\end{equation*}
$$

which should be solved with appropriate boundary conditions. For example, the fluid flow may be limited by solid bodies inside which that the fluid cannot penetrate. Then the fluid velocity at these boundaries should not have a normal component:

$$
\begin{equation*}
\frac{\partial \phi}{\partial n}=0 . \tag{8.27}
\end{equation*}
$$

On the other hand, at large distances from the body in question the fluid flow is known, e.g., uniform:

$$
\begin{equation*}
\nabla \phi=-\mathbf{v}_{0}, \quad \text { at } r \rightarrow \infty . \tag{8.28}
\end{equation*}
$$

As the reader may already know (for example, from a course of electrodynamics ${ }^{18}$ ), the Laplace equation (26) is readily solvable analytically in several simple (symmetric) but important situations. Let us consider, for example, the case of a round cylinder, with radius $R$, immersed into a flow with the initial velocity $\mathbf{v}_{0}$ perpendicular to the cylinder axis (Fig. 6). ${ }^{19}$

For this problem, it is natural to use cylindrical coordinates with axis $z$ parallel to cylinder's axis. In this case the velocity distribution is evidently independent of $z$, so that we may simplify the general expression of the Laplace operator in cylindrical coordinates ${ }^{20}$ by taking $\partial / \partial \mathrm{z}=0$. As a result, Eq. (26) is reduced to ${ }^{21}$

$$
\begin{equation*}
\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial \phi}{\partial r}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2} \phi}{\partial \theta^{2}}=0, \quad \text { at } \rho \geq R . \tag{8.29}
\end{equation*}
$$

The general solution of this equation may be obtained using the variable separation method: ${ }^{22}$

$$
\begin{equation*}
\phi=a_{0}+b_{0} \ln \rho+\sum_{n=1}^{\infty}\left(c_{n} \cos n \varphi+s_{n} \sin n \varphi\right)\left(a_{n} \rho^{n}+b_{n} \rho^{-n}\right), \tag{8.30}
\end{equation*}
$$

[^125]where coefficients $a_{n}$ and $b_{n}$ have to be found from the boundary conditions (27) and (28). Choosing axis $x=r \cos \varphi$ to be parallel to vector $\mathbf{v}_{0}$ (Fig. 6a) we may rewrite these the conditions in the form
\[

$$
\begin{gather*}
\frac{\partial \phi}{\partial \rho}=0, \text { at } \rho=R,  \tag{8.31}\\
\phi \rightarrow-v_{0} \rho \cos \varphi+\phi_{0}, \text { at } \rho \gg R, \tag{8.32}
\end{gather*}
$$
\]

where $\phi_{0}$ is an arbitrary constant, which does not affect the velocity distribution, and may be taken for zero. The latter condition is incompatible with all terms of Eq. (30) except the term with $n=1$ (with $s_{1}=$ 0 and $c_{1} a_{1}=-v_{0}$ ), so it is reduced to

$$
\begin{equation*}
\phi=\left(-v_{0} \rho+\frac{c_{1} b_{1}}{\rho}\right) \cos \varphi \tag{8.33}
\end{equation*}
$$

Now, plugging this solution into Eq. (31), we get $c_{1} b_{1}=-v_{0} R^{2}$, so that, finally,

$$
\begin{equation*}
\phi=-v_{0}\left(\rho+\frac{R^{2}}{\rho}\right) \cos \varphi \tag{8.34}
\end{equation*}
$$


(a)
(b)

Fig. 8.6. Flow of ideal, incompressible fluid around a round cylinder: (a) equipotential surfaces and (b) streamlines.

Figure 6a shows the surfaces of constant velocity potential $\phi$. In order to find the fluid velocity, it is easier to rewrite result (34) in the Cartesian coordinates $x=\rho \cos \varphi, y=\rho \sin \varphi$ :

$$
\begin{equation*}
\phi=-v_{0} x\left(1+\frac{R^{2}}{\rho^{2}}\right)=-v_{0} x\left(1+\frac{R^{2}}{x^{2}+y^{2}}\right) . \tag{8.35}
\end{equation*}
$$

From this equation, we may readily calculate the Cartesian components $v_{x}=-\partial \phi / \partial x$ and $v_{y}=-\partial \phi / \partial y$ of the fluid velocity. Figure 6 b shows particle streamlines. ${ }^{23}$ One can see that the largest potential gradient, and hence the maximum speed, is achieved at points near the vertical diameter ( $\rho=R, \varphi= \pm \pi / 2$ ), where

$$
\begin{equation*}
v=v_{x}=-\left.\frac{\partial \phi}{\partial x}\right|_{\substack{R=r, x=0}}=2 v_{0} . \tag{8.36}
\end{equation*}
$$

Now the pressure distribution may now be found from the Bernoulli equation (24). For $u(\mathbf{r})=0$, it shows that the pressure reaches maximum at the ends of the longitudinal diameter $y=0$, while at the ends of the transverse diameter $x=0$, where the velocity is largest, it is less by $2 \rho v_{0}{ }^{2}$ (where $\rho$ is the fluid density again - sorry for the notation jitters!) Note that the distributions of both velocity and pressure are symmetric about the transverse axis $x=0$, so that the fluid flow does not create any net drag force in its direction. This result, which stems from the conservation of the mechanical energy of an ideal fluid, remains valid for a solid body of arbitrary shape moving inside an infinite volume of such ideal fluid - the so-called D'Alambert paradox. However, if a body moves near ideal fluid's surface, its energy may be transformed into that of surface waves, and the drag becomes possible.

Speaking about the surface waves in a gravity field ${ }^{24}$, their description is one more classical problem of the ideal fluid dynamics. Let us consider an open surface of an ideal fluid of density $\rho$ in a uniform gravity field $\mathbf{f}=\rho \mathbf{g}=-\rho g \mathbf{n}_{y}-$ see Fig. 7. If the wave amplitude $A$ is sufficiently small, we can neglect the nonlinear term $(\mathbf{v} \cdot \nabla) \mathbf{v} \propto A^{2}$ in the Euler equation (20) in comparison with the first term, $\partial \mathbf{v} / \partial t$, that is linear in $A$. For a wave with frequency $\omega$ and wavenumber $k$, particle's velocity $\mathbf{v}=d \mathbf{q} / d t$ is of the order of $\omega A$, so that this approximation is legitimate if $\omega^{2} A \gg k(\omega A)^{2}$, i.e. when

$$
\begin{equation*}
k A \ll 1 \tag{8.37}
\end{equation*}
$$

i.e. when the wave amplitude is much smaller than its wavelength $\lambda=2 \pi / k$. By this assumption, we may neglect the fluid vorticity effects, and again use Eq. (25) and (for an incompressible fluid) Eq. (26).


Fig. 8.7. Small "plane" surface wave on a deep fluid. Dashed lines show fluid particle trajectories. (For clarity, the displacement amplitude $A \equiv(k / \omega) \Phi_{0}$ is strongly exaggerated.)
ion (26) in the natural form of a 1D sinusoidal
wave, ${ }^{25}$

[^126]\[

$$
\begin{equation*}
\phi=\operatorname{Re}\left[\Phi(y) e^{i(k z-\omega t)}\right], \tag{8.38}
\end{equation*}
$$

\]

we get a simple equation

$$
\begin{equation*}
\frac{d^{2} \Phi}{d y^{2}}-k^{2} \Phi=0 \tag{8.39}
\end{equation*}
$$

with an exponential solution (decaying, as it has to, at $y \rightarrow-\infty$ ) $\Phi=\Phi_{0} \exp \{k y\}$, so that Eq. (38) becomes

$$
\begin{equation*}
\phi=\operatorname{Re}\left[\Phi_{0} e^{k y} e^{i(k z-\omega t)}\right]=\Phi_{0} e^{k y} \cos (k z-\omega t) \tag{8.40}
\end{equation*}
$$

where the last form is valid if $\Phi_{0}$ is real - which may be always arranged by a proper selection of origins of $z$ and/or $t$. Note that the rate of wave decay with depth is exactly equal to the wavenumber of its propagation along the surface. Because of that, the trajectories of fluid particles are exactly circular. Indeed, using Eqs. (25) and (40) (with amplitude) to calculate velocity components,

$$
\begin{equation*}
v_{x}=0, \quad v_{y}=-\frac{\partial \phi}{\partial y}=-k \Phi_{0} e^{k y} \cos (k z-\omega t), \quad v_{z}=-\frac{\partial \phi}{\partial z}=k \Phi_{0} e^{k y} \sin (k z-\omega t) \tag{8.41}
\end{equation*}
$$

we see that they have equal real amplitudes, and are phase-shifted by $\pi / 2$. This result becomes even more clear if we use the velocity definition $\mathbf{v}=d \mathbf{q} / d t$ to integrate Eqs. (41) over time to recover the particle displacement law $\mathbf{q}(t)$. Due to the strong inequality (37), the integration may be done at fixed $y$ and $z$ :

$$
\begin{equation*}
q_{y}=\frac{k}{\omega} \Phi_{0} e^{k y} \sin (k z-\omega t), \quad q_{z}=\frac{k}{\omega} \Phi_{0} e^{k y} \cos (k z-\omega t) . \tag{8.42}
\end{equation*}
$$

Note that the phase of oscillations of $v_{z}$ coincides with that of $q_{y}$. It means, in particular, that at wave's top ("crest"), fluid particles are moving in the direction of wave's propagation - see arrows in Fig. 7.

It is remarkable that all this picture follows from the Laplace equation alone! The "only" remaining feature to calculate is the dispersion law $\omega(k)$, and for that we need to combine Eq. (40) with what remains, in our linear approximation, of the Euler equation (23). In this approximation, and with the bulk force potential $u=\rho g y$, this equation is reduced to

$$
\begin{equation*}
\nabla\left(-\rho \frac{\partial \phi}{\partial t}+P+\rho g y\right)=0 \tag{8.43}
\end{equation*}
$$

This equation means that the function in the parentheses is constant in space; at the surface, it should equal to pressure $P_{0}$ above the surface (say, the atmospheric pressure), that we assume to be constant. This means that on the surface, the contributions to $P$ that come from the first and the third term in Eq. (43), should compensate each other. Let us take the average surface position for $y=0$; then the surface with waves is described by relation $y=q_{y}-$ see Fig. 7. Due to the strong relation (37), which means $k\left|q_{y}\right|$ $\ll 1$, we can use Eqs. (40) and (42) with $y=0$, so that the above compensation condition yields

$$
\begin{equation*}
-\rho \omega \Phi_{0} \sin (k z-\omega t)+\rho g \frac{k}{\omega} \Phi_{0} \sin (k z-\omega t)=0 \tag{8.44}
\end{equation*}
$$

This condition is identically satisfied on the whole surface (and for any $\Phi_{0}$ ) as soon as

$$
\begin{equation*}
\omega^{2}=g k \tag{8.45}
\end{equation*}
$$

this equality giving the dispersion relation we were looking for.
Looking at this surprisingly simple result (which includes just one constant, g), note, first of all, that it does not involved fluid's density. This is not too much surprising, because due to the weak equivalence principle, particle masses always drop out of the results of problems involving gravitational forces alone. Second, the dispersion law (45) is strongly nonlinear, and in particular does not have the acoustic wave limit. This means that the surface wave propagation is strongly dispersive, with the phase velocity $\omega / k \propto 1 / \omega$ diverging at $\omega \rightarrow 0$. This divergence is an artifact of our assumption of the infinite fluid thickness. A rather straightforward generalization of the above calculations to a layer of finite thickness $h$, using the additional boundary condition $\left.v_{y}\right|_{y=-h}=0$, yields the following modified dispersion relation,

$$
\begin{equation*}
\omega^{2}=g k \tanh k h . \tag{8.46}
\end{equation*}
$$

It shows that relatively long waves, with $\lambda \gg h$, i.e. with $k h \ll 1$, propagate without dispersion (i.e. have $\omega / k=$ const $\equiv v$ ), with velocity

$$
\begin{equation*}
v=(g h)^{1 / 2} . \tag{8.47}
\end{equation*}
$$

For the Earth oceans, this velocity is rather high, approaching $300 \mathrm{~m} / \mathrm{s}$ (!) for $h=10 \mathrm{~km}$. This result explains, in particular, the very fast propagation of tsunami waves.

In the opposite limit of very short waves (large $k$ ), Eq. (45) also does not give a good description of experimental data, due to the effects of surface tension (see Sec. 2 above). Using Eq. (8.10), it is easy (and hence left for the reader :-) to show that their account leads (at $k h \gg 1$ ) to the following modification of Eq. (45):

$$
\begin{equation*}
\omega^{2}=g k+\frac{\gamma k^{3}}{\rho} . \tag{8.48}
\end{equation*}
$$

According to this formula, the surface tension is important at wavelengths smaller than the capillary constant $a_{s}$ given by Eq. (11). Much shorter waves, for whom Eq. (48) yields $\omega \propto k^{3 / 2}$, are called the capillary waves - or just "ripples".

All these generalizations are still limited to potential forces, and do not allow one to describe energy loss, in particular the attenuation of either bulk or surface waves in fluids. For that, as well as for the drag force description, we need to proceed to the effects of viscosity.

### 8.5. Dynamics: Viscous fluids

Fluid viscosity of many fluids, at not too high velocities, may be described surprisingly well by adding, to the static stress tensor (2), additional components proportional to velocity $\mathbf{v} \equiv d \mathbf{q} / d t$ :

$$
\begin{equation*}
\sigma_{j j^{\prime}}=-P \delta_{i j j^{\prime}}+\widetilde{\sigma}_{j j^{\prime}}(\mathbf{v}) \tag{8.49}
\end{equation*}
$$

Since the Hooke law (7.34) has taught us about the natural structure of such a tensor in the case of stress proportional to displacement $\mathbf{q}$, we may expect a similar expression with replacement $\mathbf{q} \rightarrow \mathbf{v}=d \mathbf{q} / d t$ :

$$
\begin{equation*}
\tilde{\sigma}_{i j j^{\prime}}=2 \eta\left(e_{i j}-\frac{1}{3} \delta_{i j j^{\prime}} \operatorname{Tr}(\mathrm{e})\right)+3 \varsigma\left(\frac{1}{3} \delta_{i j j^{2}} \operatorname{Tr}(\mathrm{e})\right), . \tag{8.50a}
\end{equation*}
$$

where $e_{i j}$ are the elements of the symmetrized strain derivative tensor:

$$
\begin{equation*}
e_{i j j^{\prime}} \equiv \frac{d s_{i j^{\prime}}}{d t}=\frac{1}{2}\left(\frac{\partial v_{j}}{\partial r_{j^{\prime}}}+\frac{\partial v_{j^{\prime}}}{\partial r_{j}}\right) . \tag{8.50b}
\end{equation*}
$$

Experiment confirms that Eq. (50) gives a good description of the viscosity effects in a broad range of isotropic fluids. Coefficient $\eta$ is called either the shear viscosity, or the dynamic viscosity, or just viscosity, while $\zeta$ is called the second (or bulk) viscosity.

In the most frequent case of a virtually incompressible fluid, $\operatorname{Tr}(\mathrm{u})=d[\operatorname{Tr}(\mathrm{~s})] / d t=(d V / d t) / V=0$, so that the term proportional to $\zeta$ vanishes, and $\eta$ is the only important viscosity parameter. ${ }^{26}$ Table 1 shows the approximate values of the viscosity, together with the mass density $\rho$, for several common fluids. One can see that $\eta$ may vary in extremely broad limits; the extreme cases are glasses (somewhat counter-intuitively, these amorphous materials are not stable solids even at room temperature, but rather may "flow", though extremely slowly, until they eventually crystallize) and liquid helium. ${ }^{27}$

Table 8.1. Important parameters of several representative fluids (approximate values)

| Fluid (all at 300 K , besides the helium) | $\eta(\mathrm{mPa} \cdot \mathrm{s})$ | $\rho\left(\mathrm{kg} / \mathrm{m}^{3}\right)$ |
| :--- | :---: | :---: |
| Glasses | $10^{21}-10^{24}$ | $2,200-2,500$ |
| Machine oils (SAE 10W - 40 W) | $65-320$ | 900 |
| Water | 0.89 | 1,000 |
| Mercury | 1.53 | 13,530 |
| Liquid helium 4 (at 4.2K, $\left.10^{5} \mathrm{~Pa}\right)$ | 0.019 | 130 |
| Air $\left(\right.$ at $\left.10^{5} \mathrm{~Pa}\right)$ | 0.018 | 1.3 |

Incorporating the additional components of $\sigma_{j j}$, to the equation (20) of fluid motion, absolutely similarly to how it was done at the derivation of Eq. (7.109) of the elasticity theory, with the account of Eq. (16) we arrive at the famous Navier-Stokes equation: ${ }^{28}$

$$
\begin{equation*}
\rho \frac{\partial \mathbf{v}}{\partial t}+\rho(\mathbf{v} \cdot \nabla) \mathbf{v}=-\nabla P+\mathbf{f}+\eta \nabla^{2} \mathbf{v}+\left(\varsigma+\frac{\eta}{3}\right) \nabla(\nabla \cdot \mathbf{v}) \tag{8.51}
\end{equation*}
$$

The apparent simplicity of this equation should not mask an enormous range of phenomena, notably including turbulence (see the next section), that are described by it, and the complexity of its

[^127]solutions even for some simple geometries. In most problems interesting for practice the only option is to use numerical methods, but due to the large number of parameters ( $\rho, \eta, \zeta$, plus geometrical parameters of the involved bodies, plus the distribution of bulk forces $\mathbf{f}$, plus boundary conditions), this way is strongly plagued by the "curse of dimensionality" that was discussed in Sec. 4.8.

Let us see how does the Navier-Stokes equation work, on several simple examples. As the simplest case, let us consider the so-called Couette flow caused in an incompressible fluid layer between two wide, horizontal plates (Fig. 8) by mutual sliding of the plates with a constant relative velocity $\mathbf{v}_{0}$.


Fig. 8.8. The simplest problem of the viscous fluid flow.

Let us assume a laminar (vorticity-free) fluid flow. (As will be discussed in the next section, this assumption is only valid within certain limits.) Then we may use the evident symmetry of the problem, to take, in the reference frame shown in Fig. $8, \mathbf{v}=\mathbf{n}_{z} v(y)$. Let the bulk forces be vertical, $\mathbf{f}=\mathbf{n}_{y} f$, so they do not give an additional drive to fluid flow. Then for the stationary flow $(\partial \mathbf{v} / \partial t=0)$, the vertical, $y$-component of the Navier-Stokes equation is reduced to the static Pascal equation (3), showing that the pressure distribution is not affected by the plate (and fluid) motion. In the horizontal, $z$-component of the equation only one term, $\nabla^{2} v$, survives, so that for the only Cartesian component of velocity we get the 1D Laplace equation

$$
\begin{equation*}
\frac{d^{2} v}{d y^{2}}=0 \tag{8.52}
\end{equation*}
$$

In contract to the ideal fluid (see, e.g., Fig. 6b), the relative velocity of a viscous fluid and a solid wall it flows by should approach zero at the wall, ${ }^{29}$ so that Eq. (52) should be solved with boundary conditions

$$
v= \begin{cases}0, & \text { at } y=0  \tag{8.53}\\ v_{0}, & \text { at } y=d\end{cases}
$$

Using the evident solution of this boundary problem, $v(y)=(y / d) v_{0}$, illustrated by arrows in Fig. 8, we can now calculate the horizontal drag force acting on a unit area of each plate. For the bottom plate,

$$
\begin{equation*}
\frac{F_{z}}{A_{y}}=\left.\sigma_{z y}\right|_{y=0}=\left.\eta \frac{\partial v}{\partial y}\right|_{y=0}=\eta \frac{v_{0}}{d} . \tag{8.54}
\end{equation*}
$$

(For the top plate, the derivative $\partial v / \partial y$ has the same value, but the sign of $d A_{y}$ has to be changed to reflect the direction of the outer normal to the solid surface, so that we get a similar force but with the

[^128]negative sign.) The well-known result (54) is often used, in undergraduate courses, for a definition of the dynamic viscosity $\eta$, and indeed shows its physical meaning very well.

As the next, slightly less trivial example let us consider the so-called Poiseuille problem ${ }^{30}$ of the relation between the constant external pressure gradient $\chi \equiv-\partial P / \partial z$ applied along a round pipe with internal radius $R$ (Fig. 9) and the so-called discharge $Q$ - defined as the mass of fluid flowing through pipe's cross-section per unit time.


Fig. 8.9. The Poiseuille problem.

Again assuming a laminar flow, we can involve the problem uniformity along the $z$ axis and its axial symmetry to infer that $\mathbf{v}=\mathbf{n}_{z} v(\rho)$, and $P=-\chi z+f(\rho, \varphi)+$ const (where $\rho=\{\rho, \varphi\}$ is the 2D radiusvector rather than fluid density), so that the Navier-Stokes equation (51) for an incompressible fluid (with $\nabla \cdot \mathbf{v}=0$ ) is reduced to a 2D Poisson equation

$$
\begin{equation*}
\eta \nabla_{2}^{2} v=-\chi . \tag{8.55}
\end{equation*}
$$

After spelling out the 2D Laplace operator in polar coordinates for our axially-symmetric case $\partial / \partial \varphi=0$, Eq. (55) becomes a simple ordinary differential equation,

$$
\begin{equation*}
\eta \frac{1}{\rho} \frac{d}{d \rho}\left(\rho \frac{d v}{d \rho}\right)=-\chi \tag{8.56}
\end{equation*}
$$

that has to be solved at the segment $0 \leq \rho \leq R$, with the following boundary conditions:

$$
\begin{array}{ll}
v=0, & \text { at } \rho=R \\
\frac{d v}{d \rho}=0, & \text { at } \rho=0 \tag{8.57}
\end{array}
$$

(The latter condition is required by the axial symmetry.) A straightforward double integration yields:

$$
\begin{equation*}
v=\frac{\chi}{4 \eta}\left(R^{2}-\rho^{2}\right) \tag{8.58}
\end{equation*}
$$

so that the integration of the mass flow density over the cross-section of the pipe,

$$
\begin{equation*}
Q \equiv \int_{A} \rho v d^{2} r=2 \pi \rho \frac{\chi}{4 \eta} \int_{0}^{R}\left(R^{2}-\rho^{\prime 2}\right) \rho^{\prime} d \rho^{\prime}, \tag{8.59}
\end{equation*}
$$

immediately gives us the so-called Poiseuille (or "Hagen-Poiseuille") law for the fluid discharge:

$$
\begin{equation*}
Q=\frac{\pi}{8} \rho \frac{\chi}{\eta} R^{4} \tag{8.60}
\end{equation*}
$$

[^129]where (sorry!) $\rho$ is the mass density again.


Fig. 8.10. Application of the finitedifference method with a very coarse mesh (with step $h=a / 2$ ) to the problem of viscous fluid flow in a pipe with a square cross-section.

Of course, not for each cross-section shape the 2D Poisson equation (55) is so readily solvable. For example, consider a very simple, square-shape cross-section with side $a$ (Fig. 10). For it, it is natural to use the Cartesian coordinates, so that Eq. (55) becomes

$$
\begin{equation*}
\frac{\partial^{2} v}{\partial x^{2}}+\frac{\partial^{2} v}{\partial y^{2}}=-\frac{\chi}{\eta}=\mathrm{const}, \quad \text { for } 0 \leq x, y \leq a \tag{8.61}
\end{equation*}
$$

and has to be solved with boundary conditions

$$
\begin{equation*}
v=0, \quad \text { at } x, y=0, a . \tag{8.62}
\end{equation*}
$$

For this boundary problem, analytical methods ${ }^{31}$ give answers in the form of infinite sums (series) that ultimately require computers for their plotting and comprehension. Let me use this pretext to discuss how explicitly numerical methods may be used for such problems - or any partial differential equations involving the Laplace operator. The simplest of them is the finite-difference method ${ }^{32}$ in which the function to be calculated, $f\left(r_{1}, r_{2}, \ldots\right)$, is represented by its values in discrete points of a rectangular grid (frequently called mesh) of the corresponding dimensionality (Fig. 11).

## (a)


(b)


Fig. 8.11. Idea of the finitedifference method in (a) one and (b) two dimensions.

In Sec. 4.7, we have already discussed how to use such a grid to approximate the first derivative - see Eq. (4.98). Its extension to the second derivative is straightforward - see Fig. 11a:

[^130]\[

$$
\begin{equation*}
\frac{\partial^{2} f}{\partial r_{j}^{2}}=\frac{\partial}{\partial r_{j}}\left(\frac{\partial f}{\partial r_{j}}\right) \approx \frac{1}{h}\left(\frac{\partial f}{\partial r_{j \rightarrow}}-\frac{\partial f}{\partial r_{j_{\leftarrow}}}\right) \approx \frac{1}{h}\left[\frac{f_{\rightarrow}-f}{h}-\frac{f-f_{\leftarrow}}{h}\right]=\frac{f_{\rightarrow}+f_{\leftarrow}-2 f}{h^{2}} . \tag{8.63}
\end{equation*}
$$

\]

The relative error of this approximation is of the order of $h^{2} \partial^{4} / \partial r_{j}^{4}$, quite acceptable in many cases. As a result, the left-hand part of Eq. (61), treated on a square mesh with step $h$ (Fig. 11b), may be presented as the so-called 5-point scheme:

$$
\begin{equation*}
\frac{\partial^{2} v}{\partial x^{2}}+\frac{\partial^{2} v}{\partial y^{2}} \approx \frac{v_{\rightarrow}+v_{\leftarrow}-2 v}{h^{2}}+\frac{v_{\uparrow}+v_{\downarrow}-2 v}{h^{2}}=\frac{v_{\rightarrow}+v_{\leftarrow}+v_{\uparrow}+v_{\downarrow}-4 v}{h^{2}} . \tag{8.64}
\end{equation*}
$$

(The generalization to the 7-point scheme, appropriate for 3D problems, is straightforward.)
Let us apply this scheme to the pipe with the square cross-section, using an extremely coarse mesh with step $h=a / 2$ (Fig. 10). In this case the fluid velocity $v$ should equal zero on the walls, i.e. in all points of the five-point scheme (Fig. 11b) except for the central point (in which velocity is evidently the largest), so that Eqs. (61) and (64) yield ${ }^{33}$

$$
\begin{equation*}
\frac{0+0+0+0-4 v_{\max }}{(a / 2)^{2}} \approx-\frac{\chi}{\eta}, \quad \text { i.e. } v_{\max } \approx \frac{1}{16} \frac{\chi a^{2}}{\eta} \tag{8.65}
\end{equation*}
$$

The resulting expression for the maximal velocity is only $\sim 20 \%$ different from the exact value. Using a slightly finer mesh with $h=a / 4$, which gives a readily solvable system of 3 linear equations for 3 different velocity values (the exercise highly recommended to the reader), brings us within a couple percent from the exact result. This shows that such "numerical" methods may be more efficient practically than the "analytical" ones, even if the only available tool is a calculator app on your smartphone rather than an advanced computer.

Of course, many practical problems of fluid dynamics do require high-performance computing, especially in conditions of turbulence (see the next section) with its complex, irregular spatial-temporal structure. In these conditions, the finite-difference approach may become unsatisfactory, because is implies the same accuracy of derivative approximation through the whole volume. A more powerful (but also much more complex for implementation) approach is the finite-element method in which the discrete point mesh is based on triangles with uneven sides, and is (in most cases, automatically) generated in accordance with the system geometry - see Fig. 12. Unfortunately I do not have time for going into the details of that method, so the reader is referred to the special literature on this subject. ${ }^{34}$

Before proceeding to our next topic, let me note one more important problem that is analytically solvable using the Navier-Stokes equation (51): a slow motion of a solid sphere of radius $R$, with a constant velocity $\mathbf{v}_{0}$, through an incompressible viscous fluid - or equivalently, a slow flow of the fluid (uniform at large distances) around an immobile sphere. Indeed, in the limit $v \rightarrow 0$, the second term in the left-hand part of this equation is negligible (just as at the surface wave analysis in Sec. 3), and the equation takes the form

[^131]\[

$$
\begin{equation*}
-\nabla P+\eta \nabla^{2} \mathbf{v}=0 \tag{8.66}
\end{equation*}
$$

\]

which should be complemented with the incompressibility condition $\nabla \cdot \mathbf{v}=0$ and boundary conditions

$$
\begin{align*}
& \mathbf{v}=0, \text { at } r=R, \\
& \mathbf{v} \rightarrow \mathbf{v}_{0}, \text { at } r \rightarrow \infty . \tag{8.67}
\end{align*}
$$

In spherical coordinates, with the polar axis directed along vector $\mathbf{v}_{0}$, this boundary problem has the axial symmetry (so that $\partial \mathbf{v} / \partial \varphi=0$ and $v_{\varphi}=0$ ), and allows the following analytical solution:

$$
\begin{equation*}
v_{r}=v_{0} \cos \theta\left(1-\frac{3 R}{2 r}+\frac{R^{3}}{2 r^{2}}\right), \quad v_{\theta}=-v_{0} \sin \theta\left(1-\frac{3 R}{4 r}-\frac{R^{3}}{4 r^{2}}\right) . \tag{8.68}
\end{equation*}
$$



Fig. 8.12. Typical finite-element mesh generated automatically for an object of complex geometry in this case, a plane wing's cross-section. (Figure adapted from www.mathworks.com.)

Calculating pressure from Eq. (66), and integrating it over the surface of the sphere it is now straightforward to obtain the famous Stokes formula for the drag force acting on the sphere:

$$
\begin{equation*}
F=6 \pi \eta R v_{0} \tag{8.69}
\end{equation*}
$$

Historically, this formula has played an important role in the first precise (with accuracy better than 1\%) calculation of the fundamental electric charge $e$ by R. Millikan and H. Fletcher from their famous oil drop experiments in 1909-1913.

### 8.6. Turbulence

The Stokes formula (69), whose derivation is limited to low velocities at that the nonlinear term $(\mathbf{v} \cdot \nabla) \mathbf{v}$ could be neglected, become invalid if the fluid velocity is increased. For example, Fig. 13 shows the drag coefficient defined as

$$
\begin{equation*}
C_{D} \equiv \frac{F}{\rho v_{0}^{2} A / 2} \tag{8.70}
\end{equation*}
$$

where $A$ is the cross-section of the body as seen from the fluid flow direction, for a sphere of radius $R$ (so that $A=\pi R^{2}$ ), as a function of the so-called Reynolds number, ${ }^{35}$ for this particular geometry defined as

$$
\begin{equation*}
R e \equiv \frac{\rho v_{0}(2 R)}{\eta}=\frac{\rho v_{0} D}{\eta} \tag{8.71}
\end{equation*}
$$



Fig. 8.13. The drag coefficient for a sphere and a round thin disk as functions of the Reynolds number.
Adapted from F. Eisner, Das Widerstandsproblem, Proc. $3^{\text {rd }}$ Int. Cong. On Appl. Mech., Stockholm, 1931.

In this notation, the Stokes formula (69) reads $C_{D}=24 / R e$. One can see this formula is only valid at $R e \ll 1$, while at larger velocities the drag force becomes substantially higher than that prediction, and its dependence on velocity very complicated, so that only its general, semi-quantitative features may be readily understood from simple arguments. ${ }^{36}$

The reason for this complexity is a gradual development of very intricate, time-dependent fluid patterns, called turbulence, rich with vortices - for an example, see Fig. 14. These vortices are especially pronounced in the region behind the moving body (so-called wake), while the region before the body is virtually unperturbed. Figure 14 indicates that turbulence exhibits rather different behaviors in an extremely broad range of velocities (i.e. values of $R e$ ), and sometimes changes rather abruptly see, for example, the significant drag drop at $R e \approx 5 \times 10^{5}$.
${ }^{35}$ This notion was introduced in 1851 by the same G. Stokes, but eventually named after O. Reynolds who popularized it three decades later.
${ }^{36}$ For example, Fig. 13 shows that, within a very broad range of Reynolds numbers, from $\sim 10^{2}$ to $\sim 3 \times 10^{5}, C_{D}$ for sphere is of the order of (and for a flat disk, remarkably close to) unity. This level, i.e., the approximate equality $F$ $\approx \rho v_{0}{ }^{2} A / 2$, may be understood (in the picture where the object is moved by an external force $F$ with velocity $\mathrm{v}_{0}$ through a fluid which is initially at rest) as the equality of force's power $F v_{0}$ and fluid's kinetic energy $\left(\rho v_{0}{ }^{2} / 2\right) V$ created in volume $V=v_{0} A$ in unit time. This relation would be exact if the object gave velocity $v_{0}$ to each and every fluid particle its cross-section runs into, for example by dragging all such particles behind itself. In reality, much of this kinetic energy goes into vortices - see Fig. 14 and its discussion below.


Fig. 8.14. Snapshot of the turbulent tail (wake) behind a sphere moving in a fluid with a high Reynolds number, showing the so-called von Kármán vortex street. A nice animation of such a pattern may be found at http://en.wikipedia.org/wiki/Reynolds number.

In order to understand the conditions of this phenomenon, let us estimate the scale of various terms in the Navier-Stokes equation (51) for the generic case of a body with characteristic size $l$ moving in an otherwise static, incompressible fluid, with velocity $v$. In this case the characteristic time scale of possible non-stationary phenomena is given by the ratio $l / v,{ }^{37}$ so that we arrive at the following estimates:

$$
\begin{array}{lcccc}
\text { Equation term: } & \rho \frac{\partial \mathbf{v}}{\partial t} & \rho(\mathbf{v} \cdot \nabla) \mathbf{v} & \mathbf{f} & \eta \nabla^{2} \mathbf{v} \\
\text { Order of magnitude: } & \rho \frac{v^{2}}{l} & \rho \frac{v^{2}}{l} & \rho g & \eta \frac{v}{l^{2}} \tag{8.72}
\end{array}
$$

(I have skipped term $\nabla P$, because as we saw in the previous section, in typical fluid flow problems it balances the viscosity term, and hence is of the same order of magnitude.) This table shows that relative importance of the terms may be characterized by two dimensionless ratios. ${ }^{38}$

The first of them is the so-called Froude number

$$
\begin{equation*}
F \equiv \frac{\rho v^{2} / l}{\rho g}=\frac{v^{2}}{l g}, \tag{8.73}
\end{equation*}
$$

[^132]which characterizes the relative importance of bulk gravity - or, upon an appropriate modification, other bulk forces. In most practical problems (with the important exception of surface waves, see Sec. 4 above) $F \gg 1$, so that the gravity effects may be neglected.

Much more important is another ratio, the Reynolds number (71), in the general case defined as

$$
\begin{equation*}
R e \equiv \frac{\rho v^{2} / l}{\eta v / l^{2}}=\frac{\rho v l}{\eta} \tag{8.74}
\end{equation*}
$$

Reynolds number
which is a measure of the relative importance of the fluid particle's inertia in comparison with the viscosity effects. ${ }^{39}$ Thus, it is not quite surprising that for a sphere, the role of the vorticity-creating term $(\mathbf{v} \cdot \nabla) \mathbf{v}$ becomes noticeable already at $R e \sim 1-$ see Fig. 13. Much more surprising is the onset of turbulence in systems where the laminar (turbulence-free) flow is formally an exact solution to the Navier-Stokes equation for any $R e$. For example, at $R e>R e_{t} \approx 2,100$ (with $l=2 R$ and $v=v_{\max }$ ) the laminar flow in a round pipe, described by Eq. (58), becomes unstable, and the resulting turbulence decreases the fluid discharge $Q$ in comparison with the Poiseuille law (60). Even more strikingly, the critical value of $R e$ is rather insensitive to the pipe wall roughness.

Since $R e \gg 1$ in many real-life situations, ${ }^{40}$ turbulence is very important for practice. However, despite nearly a century of intensive research, there is no general, quantitative analytical theory of this phenomenon, ${ }^{41}$ and most results are still obtained either by rather approximate analytical treatments, or by the numerical solution of the Navier-Stokes equations using the approaches discussed in the previous section, or in experiments (e.g., on scaled models ${ }^{42}$ in wind tunnels).

Unfortunately, due to the time/space restrictions, for a more detailed discussion of these results I have to refer the reader to more specialized literature, ${ }^{43}$ and will conclude the chapter with a brief discussion of just one issue: can the turbulence be "explained by a singe mechanism"? (In other words, can it be reduced, at least on a semi-quantitative level, to a set of simpler phenomena that are commonly considered "well understood"?) Apparently the answer in no, ${ }^{44}$ though nonlinear dynamics of simpler systems may provide some useful insights.

At the middle of the past century, the most popular qualitative explanation of turbulence had been the formation of an "energy cascade" that would transfer energy from larger to smaller vortices. With our background, it is easier to retell that story in the time-domain language (with velocity $v$ serving

[^133]as the conversion factor), using the fact that in a rotating vortex each component of the particle radiusvector oscillates in time, so that to some extent the vortex plays the role of an oscillatory motion mode. Let us consider the passage of a solid body between the two, initially close, small parts of fluid. The body pushes them apart, but after its passage these partial volumes are free to return to their initial positions. However, the domination of inertia effects at motion with $R e \gg 1$ means that the volumes continue to "oscillate" for a while about those equilibrium positions. (Since elementary volumes of an incompressible fluid cannot merge, these oscillations take the form of rotating vortices.)

Now, from Sec. 4.8 we know that intensive oscillations in a system with quadratic nonlinearity, in this case provided by the convective term $(\mathbf{v} \cdot \nabla) \mathbf{v}$, are equivalent, for small perturbations, to the oscillation of the system parameters at the corresponding frequency. On the other hand, the discussion in Sec. 5.5 shows that in a system with two oscillatory degrees of freedom, a periodic parameter change with frequency $\omega_{p}$ may lead to non-degenerate parametric excitation of oscillations with frequencies $\omega_{1,2}$ satisfying relation $\omega_{1}+\omega_{2}=\omega_{p}$. Moreover, the spectrum of oscillations in such system also has higher combinational frequencies such as $\left(\omega_{p}+\omega_{1}\right)$, thus pushing the oscillation energy up the frequency scale. In the presence of other oscillatory modes, these oscillations may in turn produce, via the same nonlinearity, even higher frequencies, etc. In a fluid, the spectrum of these "oscillatory modes" (actually, vortex structures) is essentially continuous, so that the above arguments make very plausible a sequential transfer of energy to a broad spectrum of modes - whose frequency spectrum is limited from above by the energy dissipation due to viscosity. When excited, these modes interact (in particular, phase-lock) through system's nonlinearity, creating the complex motion we call turbulence.

Though not having much quantitative predictive power, such handwaving explanations, which are essentially based on the excitation of a large number of effective degrees of freedom, had been dominating the fluid dynamics reviews until the mid-1960s. At that point, the discovery (or rather rediscovery) of quasi-random motion in classical dynamic systems with just a few degrees of freedom altered the discussion substantially. Since this phenomenon, called the deterministic chaos, extends well beyond the fluid dynamics, and I will devote to it a separate (albeit short) next chapter, and in its end briefly return to the discussion of turbulence.

### 8.7. Exercise problems

8.1. A solid round cylinder of radius $r$ is let to float in a water inside the glass, also of a round cylindrical form with radius $R$ - see Fig. on the right, which shows the water levels before and after the submersion, and some vertical dimensions of the system. Calculate the buoyant force $F$ exerted by water on the floating body.

Hint: This is just a fast check whether the reader understands the Archimedes principle correctly.

8.2. Pressure $P$ under a free water surface crudely obeys the Pascal law, Eq. (6). Find the firstorder corrections to this result, due to small compressibility of water.

8.3. Find the stationary shape of the open surface of an incompressible, heavy fluid rotated about a vertical axis with a constant angular velocity $\omega$ - see Fig. on the right.
8.4.* Calculate the shape of the surface of an incompressible fluid of density $\rho$ near a vertical plane wall, in a uniform gravity field - see Fig. on the right. In particular, find the height $h$ of liquid's rise at the wall surface as a function of the contact angle $\theta_{c}$.

8.5.* A soap film with surface tension $\gamma$ is stretched between two similar, coaxial, thin, round rings of radius $R$, separated by distance $d$-see Fig. on the right. Neglecting gravity, calculate the equilibrium shape of the film, and the force needed for keeping it stretched.

8.6. A solid sphere of radius $R$ is kept in a steady, vorticity-free flow of an ideal incompressible fluid, with velocity $v_{0}$. Find the spatial distribution of velocity and pressure, and in particular their extremal values. Compare the results with those obtained in Sec. 4 for a round cylinder.
8.7.* A small source, located at distance $d$ from a plane wall of a container filled with an ideal, incompressible fluid of density $\rho$, injects additional fluid isotropically, at a constant mass current ("discharge") $Q \equiv d M / d t$ - see Fig. on the right. Calculate fluid's velocity distribution, and its pressure on the wall, created by the flow.

Hint: Recall the charge image method in electrostatics, ${ }^{45}$ and contemplate its possible analog.

8.8. Derive Eq. (46) for surface waves on a finite-thickness layer of a heavy liquid.
8.9. Derive Eq. (48) for the capillary waves ("ripples").
8.10.* Derive a 2D differential equation describing propagation of waves on the surface of a broad layer, of constant thickness $h$, of an ideal, incompressible fluid, and use it to calculate the longest standing wave modes and frequencies in a layer covering a spherical planet of radius $R \gg h$.

[^134]Hint: The second assignment requires some familiarity with the basic properties of spherical harmonics. ${ }^{46}$
8.11. Calculate the velocity distribution and dispersion relation of waves propagating along the horizontal interface of two ideal, incompressible fluids of different densities.
8.12. Calculate the energy of a monochromatic, plane surface wave on an, ideal, incompressible, deep fluid, and the power it carries (per unit width of wave's front).
8.13. Use the finite-difference approximation for the Laplace operator, with mesh $h=a / 4$, to find the maximum velocity and total mass flow $Q$ of a viscous, incompressible fluid through a long pipe with a square-shaped cross-section of side $a$. Compare the results with those described in Sec. 4 for:
(i) the same problem with mesh $h=a / 2$, and
(ii) a pipe with circular cross-section of the same area.
8.14. A layer, of thickness $h$, of a heavy, viscous, incompressible fluid flows down a long and wide incline plane, under its own weight - see Fig. on the right. Find the stationary velocity distribution profile, and the total fluid discharge (per unit width.)

8.15. Calculate the drag torque exerted on a unit length of a solid round cylinder of radius $R$ that rotates about its axis, with angular velocity $\omega$, inside an incompressible fluid with viscosity $\eta$.
8.16. Calculate the tangential force (per unit area) exerted by incompressible fluid, with density $\rho$ and viscosity $\eta$, on a broad solid plane placed over its surface and forced to oscillate, along the surface, with amplitude $a$ and frequency $\omega$.
8.17. A massive barge, with a flat bottom of area $A$, floats in shallow water, with clearance $h \ll A^{1 / 2}$ (see Fig. on the right). Calculate the time dependence of barge's velocity $V(t)$, and the water velocity profile, after the barge's engine has been turned off. Discuss the limits of large and
 small values of the dimensionless parameter $M / \rho A h$.
8.18.* Derive a general expression for mechanical energy loss rate in a viscous incompressible fluid that obeys the Navier-Stokes equation, and use this expression to calculate the attenuation coefficient of surface waves, assuming that the viscosity is small (quantify this condition).

[^135]8.19. Use the Navier-Stokes equation to calculate the attenuation coefficient for a plane, sinusoidal acoustic wave.

## Chapter 9. Deterministic Chaos

This chapter gives a very brief review of chaotic phenomena in deterministic maps and dynamic systems with and without dissipation, and an even shorter discussion of the possible role of chaos in fluid turbulence.

### 9.1. Chaos in maps

Chaotic behavior of dynamic systems ${ }^{1}$ (sometimes called the deterministic chaos) has become broadly recognized ${ }^{2}$ after the publication of a 1963 paper by E. Lorenz who was examining numerical solutions of the following system of three nonlinear, ordinary differential equations,

Lorenz system

$$
\begin{align*}
& \dot{q}_{1}=a_{1}\left(q_{2}-q_{1}\right), \\
& \dot{q}_{2}=a_{2} q_{1}-q_{2}-q_{1} q_{3},  \tag{9.1}\\
& \dot{q}_{3}=q_{1} q_{2}-a_{3} q_{3},
\end{align*}
$$

as a rudimentary model for heat transfer through a horizontal liquid layer between two solid plates. (Experiment shows that if the bottom plate is kept hotter than the top one, the liquid may exhibit turbulent convection.) He has found that within a certain range of constants $a_{1,2,3}$, the solutions of Eq. (1) follow complex, unpredictable, non-repeating trajectories in the 3D $q$-space. Moreover, the resulting functions $q_{j}(t)$ (where $j=1,2,3$ ) are so sensitive to initial conditions $q_{j}(0)$ that at sufficiently large times $t$, solutions corresponding to slightly different initial conditions are completely different.

Very soon it was realized that such behavior is typical for even simpler mathematical objects called maps, so that I will start my discussion of chaos from these objects. A 1D map is essentially a rule for finding the next number $q_{n+1}$ of a sequence, in the simplest case using only its last known value $q_{n}$, in a discrete series numbered by integer index $n$. The most famous example is the so-called logistic map: ${ }^{3}$

Logistic
map

$$
\begin{equation*}
q_{n+1}=f\left(q_{n}\right) \equiv r q_{n}\left(1-q_{n}\right) \tag{9.2}
\end{equation*}
$$

The basic properties of this map may be understood using the (hopefully, self-explanatory) graphical presentation shown in Fig. 1.4 One can readily see that at $r<1$ (Fig. 1a) the sequence rapidly converges to the trivial fixed point $q^{(0)}=0$, because each next value of $q$ is less than the previous one. However, if $r$ is increased above 1 (as in the example shown in Fig. 1b), fixed point $q^{(0)}$ becomes unstable. Indeed, at $q_{n} \ll 1$, map (2) yields $q_{n+1}=r q_{n}$, so that at $r>1$, values $q_{n}$ grow with each iteration. Instead of the unstable point $q^{(0)}=0$, in the range $1<r<r_{1}$, where $r_{1} \equiv 3$, the map has a stable fixed point, $q^{(1)}$, that may be found by plugging this value into both parts of Eq. (2):

[^136]\[

$$
\begin{equation*}
q^{(1)}=r q^{(1)}\left(1-q^{(1)}\right), \tag{9.3}
\end{equation*}
$$

\]

giving $q^{(1)}=(1-1 / r)-$ see the left branch of the plot shown in Fig. 2.



Fig. 9.1. Graphical analysis of the logistic map for: (a) $r<1$ and (b) $r>1$.


Fig. 9.2. Fixed points and chaotic regions of the logistic map. The plot is adapted from http://en.wikipedia.org/wiki/Lo gistic map; a very nice live simulation of the map is also available on this Web site.

At $r>r_{1}=3$, the plot gets thicker: here the fixed point $q^{(1)}$ also becomes unstable. To prove that, let us take $q_{n}=q^{(1)}+\tilde{q}_{n}$, assume that deviation $\tilde{q}_{n}$ from the fixed point $q^{(1)}$ is small, and linearize map (3) in $\widetilde{q}_{n}$, just as we repeatedly did for differential equations earlier in this course. The result is

$$
\begin{equation*}
\widetilde{q}_{n+1}=\left.\frac{d f}{d q}\right|_{q=q^{(1)}} \widetilde{q}_{n}=r\left(1-2 q^{(1)}\right) \widetilde{q}_{n}=(2-r) \widetilde{q}_{n} . \tag{9.4}
\end{equation*}
$$

It shows that $0<2-r<1$, i.e. $1<r<2$, deviations $\widetilde{q}_{n}$ decrease monotonically. At $-1<2-r<0$, i.e. in the range $2<r<3$, the deviation signs alternate but the magnitude still decreases (as in a stable focus - see Sec. 4.6). However, at $-1<2-r$, i.e. $r>r_{1}=3$, the deviations are growing by magnitude, while still changing sign, at each step. Since Eq. (2) has no other fixed points, this means that at $n \rightarrow \infty$, values
$q_{n}$ do not converge to one point; rather, within the range $r_{1}<r<r_{2}$, they approach a limit cycle of alternation of two points, $q_{+}^{(2)}$ and $q_{-}^{(2)}$ that satisfy the following system of algebraic equations

$$
\begin{equation*}
q_{+}^{(2)}=f\left(q_{-}^{(2)}\right), q_{-}^{(2)}=f\left(q_{+}^{(2)}\right) \tag{9.5}
\end{equation*}
$$

(These points are also plotted in Fig. 2, as functions of parameter $r$.) What has happened at point $r_{1}$ is called the period-doubling bifurcation. The story repeats at $r=r_{2}=1+\sqrt{ } 6 \approx 3.45$ where the system goes from the 2-point limit cycle to a 4-point cycle, then at point $r=r_{3} \approx 3.54$ at that the limit cycle becomes consisting of 8 alternating points, etc. Most remarkably, the period-doubling bifurcation points $r_{n}$, at that the number of points in the limit cycle doubles from $2^{n-1}$ points to $2^{n}$ points, become closer and closer. Numerical calculations have shown that these points obey the following asymptotic behavior: sequence

$$
\begin{equation*}
r_{n} \rightarrow r_{\infty}-\frac{C}{\delta^{n}}, \quad \text { where } r_{\infty}=3.5699 \ldots, \quad \delta=4.6692 \ldots \tag{9.6}
\end{equation*}
$$

Parameter $\delta$ is called the Feigenbaum constant; for other maps, and some dynamic systems (see the next section), period-doubling sequences follow a similar law, but with different parameter $\delta$.

More important for us, however, is what happens at $r>r_{\infty}$. Numerous numerical experiments, repeated with increasing precision, ${ }^{5}$ have confirmed that here the system is fully disordered, with no reproducible limit cycle, though (as Fig. 2 shows) at $r \approx r_{\infty}$, all sequential values $q_{n}$ are still confined to a few narrow regions. ${ }^{6}$ However, as parameter $r$ is increased well beyond $r_{\infty}$, these regions broaden and merge. This the so-called full, or well-developed chaos, with no apparent order at all. ${ }^{7}$

The most important feature of chaos (in this and any other system) is the exponential divergence of trajectories. For a 1 D map, this means that even if the initial conditions $q_{1}$ in two map implementations differ by a very small amount $\Delta q_{1}$, the difference $\Delta q_{n}$ between the corresponding sequences $q_{n}$ is growing (on the average) exponentially with $n$. Such exponents may be used to characterize chaos. Indeed, let us assume that $\Delta q_{1}$ is so small that $N$ first values $q_{n}$ are relatively close to each other. Then an evident generalization of the first of Eqs. (4) to an arbitrary point $q_{n}$ is

$$
\begin{equation*}
\Delta q_{n+1}=e_{n} \Delta q_{n},\left.\quad e_{n} \equiv \frac{d f}{d q}\right|_{q=q_{n}} . \tag{9.7}
\end{equation*}
$$

Using this result iteratively for $N$ steps, we get

$$
\begin{equation*}
\Delta q_{N}=\Delta q_{1} \prod_{n=1}^{N} e_{n}, \quad \text { so that } \ln \left|\frac{\Delta q_{N}}{\Delta q_{1}}\right|=\sum_{n=1}^{N} \ln \left|e_{n}\right| . \tag{9.8}
\end{equation*}
$$

[^137]Numerical experiments show that in most chaotic regimes, at $N \rightarrow \infty$ such a sum fluctuates about an average, which grows as $\lambda N$, with parameter

$$
\begin{equation*}
\lambda=\lim _{\Delta q_{1} \rightarrow 0} \lim _{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^{N} \ln \left|e_{n}\right|, \tag{9.9}
\end{equation*}
$$

Lyapunov exponent
called the Lyapunov exponent, ${ }^{8}$ being independent on the initial conditions. The bottom panel in Fig. 3 shows it as a function of the parameter $r$ for the logistic map (2).


Fig. 9.3. The Lyapunov exponent for the logistic map. Adapted from the monograph by Schuster and Just (cited below). © WileyVCH Verlag GmbH \& Co. KGaA.

Note that at $r<r_{\infty}, \lambda$ is negative, indicating trajectory's stability, besides points $r_{1}, r_{2}, \ldots$ where $\lambda$ would become positive if the limit cycle change had not brought it back to the negative territory. However, at $r>r_{\infty}, \lambda$ becomes positive, returning the negative values only in limited intervals of stable limit cycles. It is evident that in numerical experiments (which dominate the studies of the deterministic chaos) the Lyapunov exponent may be used as a good measure of chaos' "depth". ${ }^{9}$

Despite all the abundance of results published for particular maps, ${ }^{10}$ and several interesting general observations (like the existence of the Feigenbaum bifurcation sequences), to the best of my knowledge nobody can yet predict the patterns like those shown in Fig. 2 and 3, from just looking at the map rule itself, i.e. without carrying out actual numerical experiments with in. Unfortunately the situation with chaos in other systems is not much better.

[^138]
### 9.2. Chaos in dynamic systems

Proceeding to the discussion of chaos in dynamic systems, it is more natural, with our background, to illustrate this discussion not with the Lorenz' system Eqs. (1), but with the system of equations describing a dissipative pendulum driven by a sinusoidal external force, which was repeatedly discussed in Chapter 4. Introducing two new variables, the normalized momentum $p \equiv \dot{q} / \omega_{0}$ and the external force's full phase $\psi \equiv \omega t$, we may rewrite Eq. (4.42) describing the pendulum,

$$
\begin{equation*}
\ddot{q}+2 \delta \ddot{q}+\omega_{0}^{2} \sin q=f_{0} \cos \omega t \tag{9.10a}
\end{equation*}
$$

in a form similar to Eq. (1), i.e. as a system of three first-order ordinary differential equations:

$$
\begin{align*}
\dot{q} & =\omega_{0} p, \\
\dot{p} & =-\omega_{0} \sin q-2 \delta p+\left(f_{0} / \omega_{0}\right) \cos \psi,  \tag{9.10b}\\
\dot{\psi} & =\omega .
\end{align*}
$$

Figure 4 several results of numerical solution of Eq. (10). ${ }^{11}$ In all cases, the internal parameters $\delta$ and $\omega_{0}$ of the system, and the external force amplitude $f_{0}$ are fixed, while the external frequency $\omega$ is gradually changed. For the case shown on the top panel, the system still tends to a stable periodic solution, with low contents of higher harmonics. If the external force frequency is reduced by a just few percent, the $3^{\text {rd }}$ subharmonic may be excited. (This effect has already been discussed in Sec. $4.8-$ see, e.g., Fig. 4.15.) The next panel shows that just a very small further reduction of frequency leads to a new tripling of the period, i.e. the generation of a complex waveform with the $9^{\text {th }}$ subharmonic. Finally, even a minor further change of parameters leads to oscillations without any visible period, e.g., chaos.

In order to trace this transition, direct observation of the oscillation waveforms $q(t)$ is not very convenient, and trajectories on the phase plane $[q, p]$ also become messy if plotted for many periods of the external frequency. In situations like this, the Poincaré (or "stroboscopic") plane, already discussed in Sec. 4.6, is much more useful. As a reminder, this is essentially just the phase plane [ $q, p$ ], but with the points highlighted only once a period, e.g., at $\psi=2 \pi n$, with $n=1,2, \ldots$ On this plane, periodic oscillations of frequency $\omega$ are presented just as one fixed point - see, e.g. the top panel in the right column of Fig. 4. The beginning of the $3^{\text {rd }}$ subharmonic generation, shown on the next panel, means tripling of the oscillation period, and is reflected on the Poincare plane by splitting the fixed point into three. It is evident that this transition is similar to the period-doubling bifurcation in the logistic map, besides the fact (already discussed in Sec. 4.8) that in systems with an asymmetric nonlinearity, such as the pendulum (10), the $3^{\text {rd }}$ subharmonic is easier to excite. From this point, the $9^{\text {th }}$ harmonic generation (shown on the $3^{\text {rd }}$ panel of Fig. 4), i.e. one more splitting of the points on the Poincaré plane, may be understood as one more step on the Feigenbaum-like route to chaos - see the bottom panel of that figure.

So, the transition to chaos in dynamic systems may be at least qualitatively similar to than in 1D maps, with the similar law (6) for the critical values of some parameter $r$ of the system (in Fig. 4, frequency $\omega$ ), though generally with a different value of exponent $\delta$. Moreover, it is evident that we can always consider the first two differential equations of system (10b) as a 2D map that relates the vector $\left\{q_{n+1}, p_{n+1}\right\}$ of the coordinate and velocity, measured at $\psi=2 \pi(n+1)$, with the previous value $\left\{q_{n}, p_{n}\right\}$

[^139]of that vector (reached at $\psi=2 \pi n$ ). Unfortunately this similarity also implies that chaos in dynamical systems is at least as complex, and it as little understood, as in maps.


Fig. 9.4. Oscillations in a pendulum with weak damping, $\delta / \omega_{0}=0.1$, driven by a sinusoidal external force with a fixed effective amplitude $f_{0} / \omega_{0}{ }^{2}=1$, and several close values of the frequency (listed on the panels). Left column: oscillation waveforms $q(t)$ recorded after certain initial transient intervals. Right column: representations of the same processes on the Poincaré plane of variables $[p, q]$.

For example, Fig. 5 shows (a part of) the state diagram of the externally-driven pendulum, with the red bar marking the route to chaos traced in Fig. 4, and shading/hatching styles marking different regimes. One can that the pattern is at least as complex as that shown in Figs. 2 and 3, and besides a few features, ${ }^{12}$ is equally unpredictable from the form of the equation.


Fig. 9.5. Phase diagram of an externally-driven pendulum with $\delta / \omega_{0}=0.1$. Regions of oscillations with the basic period are not shaded. The notation for other regions is as follows. Doted: subharmonic generation; cross-hatched: chaos; hatched: chaos or basic period (depending on the initial conditions); hatchdotted: basic period or subharmonics. Solid lines show boundaries of single-regime regions, while dashed lines are boundaries of regions in which several types of motion are possible, depending on history. (Figure courtesy V. Kornev.)

Are there any valuable general results concerning chaos in dynamic systems? The most important (though an almost evident) result is that this phenomenon is impossible in any system described by one or two first-order differential equations with right-hand parts independent of time. Indeed, let us start with a single equation

$$
\begin{equation*}
\dot{q}=f(q) \tag{9.11}
\end{equation*}
$$

where $f(q)$ is any single-valued function. This equation may be directly integrated to give

$$
\begin{equation*}
t=\int^{q} \frac{d q^{\prime}}{f\left(q^{\prime}\right)}+\text { const } \tag{9.12}
\end{equation*}
$$

showing that the relation between $q$ and $t$ is unique and hence does not leave place for chaos.
Now, let us explore the system of two such equations:

$$
\begin{align*}
& \dot{q}_{1}=f_{1}\left(q_{1}, q_{2}\right)  \tag{9.13}\\
& \dot{q}_{2}=f_{2}\left(q_{1}, q_{2}\right)
\end{align*}
$$

Consider its phase plane shown schematically in Fig. 6. In a "usual" system, the trajectories approach either some fixed point (Fig. 6a) describing static equilibrium, or a limit cycle (Fig. 6b) describing periodic oscillations. (Both notions are united by the term attractor, because they "attract" trajectories launched from various initial conditions.) However, phase plane trajectories of a chaotic system of

[^140]equations that describe real physical variables (which cannot tend to infinity), should be confined to a limited phase plane area, and simultaneously cannot start repeating each other. (This topology is frequently called the strange attractor.) For that, 2D trajectories need to cross - see, e.g., point $A$ in Fig. $6 c$.


Fig. 9.6. Attractors in dynamical systems: (a) a fixed point, (b) a limit cycle, and (c) a strange attractor.
However, in the case described by Eqs. (13), this is clearly impossible, because according to these equations, the tangent slope on the phase plane is a unique function of point coordinates $\left\{q_{1}, q_{2}\right\}$ :

$$
\begin{equation*}
\frac{d q_{1}}{d q_{2}}=\frac{f_{1}\left(q_{1}, q_{2}\right)}{f_{2}\left(q_{1}, q_{2}\right)} \tag{9.14}
\end{equation*}
$$

Thus, in this case the deterministic chaos is impossible. ${ }^{13}$ It becomes, however, readily possible if the right-hand parts of a system similar to Eq. (13) depend either on other variables of the system or time. For example, if we consider the first two differential equations of system (10b), in the case $f_{0}=0$ they have the structure of the system (13) and hence chaos is impossible, even at $\delta<0$ when (as we know from Sec. 4.4) the system allows self-excitation of oscillations - leading to a limit-cycle attractor. However, if $f_{0} \neq 0$, this argument does not work any longer and (as we have already seen) the system may have a strange attractor - which is, for dynamic systems, a synonym for the deterministic chaos. Thus, chaos is possible in dynamic systems that may be described by three or more differential equations of the first order. ${ }^{14}$

### 9.3. Chaos in Hamiltonian systems

The last analysis is of course valid for Hamiltonian systems, which are just a particular type of dynamic systems. However, one may wonder whether these systems, that feature at least one first integral of motion, $H=$ const, and hence are more "ordered" than the systems discussed above, can exhibit chaos at all. The question is yes, because such systems still can have mechanisms for an exponential growth of a small initial perturbation.

[^141]As the simplest way to show it, let us consider a so-called mathematical billiard, i.e. a ballistic particle (a "ball") moving freely by inertia on a horizontal plane surface ("table") limited by rigid impenetrable walls. In this idealized model of the usual game of billiards, ball's velocity $\mathbf{v}$ is conserved when it moves on the table, and when it runs into a wall, the ball is elastically reflected from it as from a mirror, ${ }^{15}$ with the reversal of the sign of the normal velocity $v_{n}$, and conservation of the tangential velocity $v_{\tau}$, and hence without any loss of its kinetic (and hence the full) energy

$$
\begin{equation*}
E=H=T=\frac{m}{2} v^{2}=\frac{m}{2}\left(v_{n}^{2}+v_{\tau}^{2}\right) \tag{9.15}
\end{equation*}
$$

This model, while being a legitimate 2D dynamic system, ${ }^{16}$ allows geometric analyses for several simple table shapes. The simplest case is a rectangular billiard of area $a \times b$ (Fig. 7), whose analysis may be readily carried out by the replacement of each ball reflection event with the mirror reflection of the table in that wall - see dashes lines in panel (a).


Fig. 9.7. Ball motion on a rectangular billiard at (a) a commensurate, and (b) an incommensurate launch angle.

Such analysis (left for reader' pleasure :-) shows that if the tangent of the ball launching angle $\varphi$ is commensurate with the side length ratio,

$$
\begin{equation*}
\tan \varphi= \pm \frac{m}{n} \frac{b}{a} \tag{9.16}
\end{equation*}
$$

where $n$ and $m$ are non-negative integers without common integer multipliers, the ball returns exactly to the launch point $O$, after bouncing $m$ times from each wall of length $a$, and $n$ times from each wall of length $b$. (Red lines in Fig. 7a show an example of such trajectory for $n=m=1$, while blue lines, for $m$ $=3, n=1$.) Thus the larger is the sum $(m+n)$, the more complex is such closed trajectory - "orbit".

Finally, if $(n+m) \rightarrow \infty$, i.e. $\tan \varphi$ and $b / a$ are incommensurate (meaning that their ratio is an irrational number), the trajectory covers all the table area, and the ball never returns exactly into the launch point. Still, this is not the real chaos. Indeed, a small shift of the launch point shifts all the trajectory fragments by the same displacement. Moreover, at any time $t$, each of Cartesian components $v_{j}(t)$ of the ball's velocity (with coordinate axes parallel to the table sides) may take only two values, $\pm v_{j}(0)$, and hence may vary only as much as the initial velocity is being changed.

[^142]In 1963, Ya. Sinai showed that the situation changes completely if an additional wall, in the shape of a circle, is inserted into the rectangular billiard (Fig. 8). For most initial conditions, ball's trajectory eventually runs into the circle (see the red line on panel (a) as an example), and the further trajectory becomes essentially chaotic. Indeed, let us consider ball's reflection from the circle-shaped wall - Fig. 8 b . Due to the conservation of the tangential velocity, and the sign change of the normal velocity component, the reflection obeys the mechanical analog of the Snell law (cf. Fig. 7.12 and its discussion): $\theta_{r}=\theta_{i}$. Figure 8 b shows that as the result, a small difference $\delta \varphi$ between the angles of two close trajectories (as measured in the lab system), doubles by magnitude at each reflection from the curved wall. This means that the small deviation grows along the ball trajectory as

$$
\begin{equation*}
|\delta \varphi(N)| \sim|\delta \varphi(0)| \times 2^{N}=|\delta \varphi(0)| e^{N \ln 2} \tag{9.17}
\end{equation*}
$$

where $N$ is the number of reflections from the convex wall. ${ }^{17}$ As we already know, such exponential divergence of trajectories, with a positive Lyapunov exponent, is the sign of deterministic chaos. ${ }^{18}$

(a)

(b)

Fig. 9.8. (a) Motion on a Sinai billiard table, and (b) the mechanism of the exponential divergence of close trajectories.

The most important new feature of the dynamic chaos in Hamiltonian systems is its dependence on initial conditions. (In the systems discussed in the previous two previous sections, that lack the integrals of motion, the initial conditions are rapidly "forgotten", and the chaos is usually characterized after cutting out the initial transient period - see, e.g., Fig. 4.) Indeed, even a Sinai billiard allows periodic motion, along closed orbits, at certain initial conditions - see the blue and green lines in Fig. 8a as examples. Thus the chaos "depth" in such systems may be characterized by the "fraction" 19 of the phase space of initial parameters (for a 2D billiard, the 3D space of initial values of $x, y$, and $\varphi$ ) resulting in chaotic trajectories.

This conclusion is also valid for Hamiltonian systems that are met in experiments more frequently than the billiards, for example, coupled nonlinear oscillators without damping. Perhaps, the

[^143]earliest and the most popular example is the so-called Hénon-Heiles system, ${ }^{20}$ which may be descrbed by the following Lagrangian function:
\[

$$
\begin{equation*}
L=\frac{m_{1}}{2}\left(\dot{q}_{1}^{2}-\omega_{1}^{2} q_{1}^{2}\right)+\frac{m_{2}}{2}\left(\dot{q}_{2}^{2}-\omega_{2}^{2} q_{2}^{2}\right)-\varepsilon\left(q_{1}^{2}-\frac{1}{3} q_{2}^{2}\right) q_{2} . \tag{9.18}
\end{equation*}
$$

\]

HénonHeiles system

It is straightworward to use Eq. (18) to derive the Lagrangian equations of motion,

$$
\begin{align*}
& m_{1}\left(\ddot{q}_{1}+\omega_{1}^{2} q_{1}\right)=-2 \varepsilon q_{1} q_{2}, \\
& m_{2}\left(\ddot{q}_{2}+\omega_{2}^{2} q_{2}\right)=-\varepsilon\left(q_{1}^{2}-q_{2}^{2}\right), \tag{9.19}
\end{align*}
$$

and find its first integral of motion (physically, the energy conservation law):

$$
\begin{equation*}
H=E=\frac{m_{1}}{2}\left(\dot{q}_{1}^{2}+\omega_{1}^{2} q_{1}^{2}\right)+\frac{m_{2}}{2}\left(\dot{q}_{2}^{2}+\omega_{2}^{2} q_{2}^{2}\right)+\varepsilon\left(q_{1}^{2}-\frac{1}{3} q_{2}^{2}\right) q_{2}=\text { const } . \tag{9.20}
\end{equation*}
$$

In the conext of our discussions in Chapter 4 and 5, Eqs. (19) may be readily interpreted as those describing two oscillators, with small-oscillation eigenfrequencies $\omega_{1}$ and $\omega_{2}$, nonlinearly coupled only as described by the terms in the right-hand parts of the equations. This means that as the oscillation amplitudes $A_{1,2}$, and hence the total energy $E$ of the system, tend to zero, the oscillator subsystems are virtually independent, each performing sinusoidal oscillations at its own frequency. This observation suggestes a convenient way to depict the system motion. ${ }^{21}$ Let us consider a Poincaré plane for one of the oscillators (say, with coordinate $q_{2}$ ), similar to that discussed in Sec. 2 above, with the only difference is that (because of the absence of an explicit function of time in system's equations), the trajectory on the $\left[q_{2}, \dot{q}_{2}\right]$ plane is highlighted at the moments when $q_{1}=0$.

Let us start from the limit $A_{1,2} \rightarrow 0$, when oscillations of $q_{2}$ are virtually sinusoidal. As we already know (see Fig. 4.9 and its discussion), if the representation point highlighting was perfectly synchronous with frequency $\omega_{2}$ of the oscillations, there would be only one point on the Poincaré plane - see, e.g. the right top plane in Fig. 4. However, at the $q_{1}$ - initiated highlighting, there is not such synchronism, so that each period, a different point of the elliptical (at the proper scaling of the velocity, circular) trajectory is highlighted, so that the resulting points, for certain initial conditions, reside on a circle of radius $A_{2}$. If we now vary the initial conditions, i.e. redistribute the initial energy between the oscillators, but keep the total energy $E$ constant, on the Poincaré plane we get a series of ellipses.

Now, if the initial energy is increased, nonlinear interaction of the oscillations start to deform these ellipses, causing also their crossings - see, e.g., the top left panel of Fig. 9. Still, below a certain threshold value of $E$, all Poincaré points belonging to a certain initial condition sit on a single closed

[^144]contour. Moreover, these contours may be calculated approximately, but with a pretty good accuracy, using a straighforward generalization of the small parameter method discussed in Sec. 4.2.22


However, starting from some value of energy, certain initial conditions lead to series of points scattered over final-area parts of the Poincaré plane - see the top right panel of Fig. 9. This means that the corresponding oscillations $q_{2}(t)$ do not repeat from one (quasi-) period to the next one -cf . Fig. 4 for the dissipative, forced pendulum. This is chaos. ${ }^{23}$ However, some other initial conditions still lead to closed contours. This feature is similar to Sinai billiards, and is typical for Hamiltonian systems. As the energy is increased, the larger and larger part of the Poincare plane belongs to the chaotic motion, signifying deeper and deeper chaos.

[^145]
### 9.4. Chaos and turbulence

This extremely short section consists of essentially just one statement, extending the discussion in Sec. 8.5. The (re-) discovery of the deterministic chaos in systems with just a few degrees of freedom in the 1960s changed the tone of debates concerning origins of turbulence very considerably. At first, an extreme point of view that equated the notions of chaos and turbulence, became the debate's favorite. ${ }^{24}$ However, after an initial excitement, a significant evidence of the Landau-style mechanisms, involving many degrees of freedom, has been rediscovered and could not be ignored any longer. To the best knowledge of this author, who is a very distant albeit interested observer of that field, most experimental and numerical-simulation data carry features of both mechanisms, so that the debate continues. ${ }^{25}$ Due to the age difference, most readers of these notes have much better chances than the author to see where will this discussion end (if it does :-). ${ }^{26}$

### 9.5. Exercise problems

9.1. Generalize the reasoning of Sec. 1 to an arbitrary 1 D map $q_{n+1}=f\left(q_{n}\right)$, with function $f(q)$ differentiable at all points of interest. In particular, derive the condition of stability of an $N$-point limit cycle $q^{(1)} \rightarrow q^{(2)} \rightarrow \ldots \rightarrow q^{(N)} \rightarrow q^{(1)}$.
9.2. Use the stability condition, derived in Problem 9.1, to analyze chaos excitation in the socalled tent map:

$$
f(q)=\left\{\begin{array}{ll}
r q, & \text { for } 0 \leq q \leq 1 / 2, \\
r(1-q), & \text { for } 1 / 2 \leq q \leq 1,
\end{array} \quad \text { with } 0 \leq r \leq 2\right.
$$

9.3. A dynamic system is described by the following system of ordinary differential equations:

$$
\begin{aligned}
& \dot{q}_{1}=-q_{1}+a_{1} q_{2}^{3}, \\
& \dot{q}_{2}=a_{2} q_{2}-a_{3} q_{2}^{3}+a_{4} q_{2}\left(1-q_{1}^{2}\right) .
\end{aligned}
$$

Can it exhibit chaos at some set of constant parameters $a_{1-} a_{4}$ ?
9.4. A periodic function of time has been added to the right-hand part of the first equation of the system considered in the previous problem. Is chaos possible now?

[^146]

## Chapter 10. A Bit More of Analytical Mechanics

This concluding chapter reviews two alternative approaches to analytical mechanics, whose main advantage is a closer parallel to quantum mechanics in general and to its quasiclassical (WKB) approximation in particular. One of them, the Hamiltonian formalism, is also used to derive an important asymptotic result, the adiabatic invariance, for classical systems with slowly changing parameters.

### 10.1. Hamilton equations

Throughout this course we have seen how useful the analytical mechanics, in its Lagrangian form, may be invaluable for solving various particular problems of classical mechanics. Now let us discuss several alternative formulations ${ }^{1}$ that may not be much more useful for this purpose, but shed light on possible extensions of classical mechanics, most importantly to quantum mechanics.

As was already discussed in Sec. 2.3, the partial derivative $p_{j} \equiv \partial L / \partial \dot{q}_{j}$ participating in the Lagrange equations (2.19)

$$
\begin{equation*}
\frac{d}{d t} \frac{\partial L}{\partial \dot{q}_{j}}-\frac{\partial L}{\partial q_{j}}=0, \tag{10.1}
\end{equation*}
$$

may be considered as the generalized momentum corresponding to generalized coordinate $q_{j}$, and the full set of this momenta may be used to define the Hamiltonian function (2.32):

$$
\begin{equation*}
H \equiv \sum_{j} p_{j} \dot{q}_{j}-L \tag{10.2}
\end{equation*}
$$

Now let us rewrite the full differential of this function ${ }^{2}$ in the following form:

$$
\begin{align*}
d H & =d\left(\sum_{j} p_{j} \dot{q}_{j}-L\right)=\sum_{j}\left[d\left(p_{j}\right) \dot{q}_{j}+p_{j} d\left(\dot{q}_{j}\right)\right]-d L \\
& =\sum_{j}\left[d\left(p_{j}\right) \dot{q}_{j}+p_{j} d\left(\dot{q}_{j}\right)\right]-\left[\frac{\partial L}{\partial t} d t+\sum_{j}\left(\frac{\partial L}{\partial q_{j}} d\left(q_{j}\right)+\frac{\partial L}{\partial \dot{q}_{j}} d\left(\dot{q}_{j}\right)\right)\right] . \tag{10.3}
\end{align*}
$$

According to the definition of the generalized momentum, the second terms of each sum over $j$ cancel, while according to the Lagrange equation (1), the derivative $\partial L / \partial q_{j}$ is just $\dot{p}_{j}$, so that

$$
\begin{equation*}
d H=-\frac{\partial L}{\partial t} d t+\sum_{j}\left(\dot{q}_{j} d p_{j}-\dot{p}_{j} d q_{j}\right) . \tag{10.4}
\end{equation*}
$$

So far, this is just a universal identity. Now comes the main trick of Hamilton's approach: let us consider $H$ a function of the following independent arguments: time $t$, the generalized coordinates $q_{j}$,

[^147]and the generalized momenta $p_{j}$ (rather than generalized velocities). With this commitment, the general rule of differentiation of a function of several arguments gives
\[

$$
\begin{equation*}
d H=\frac{\partial H}{\partial t} d t+\sum_{j}\left(\frac{\partial H}{\partial q_{j}} d q_{j}+\frac{\partial H}{\partial p_{j}} d p_{j}\right) \tag{10.5}
\end{equation*}
$$

\]

where $d t, d q_{j}$, and $d p_{j}$ are independent differentials. Since Eq. (5) should be valid for any choice of these argument differentials, it should hold in particular if the differentials correspond to the real law of motion, for which Eq. (4) is valid as well. The comparison of Eqs. (4) and (5) gives us three relations:

$$
\begin{align*}
& \frac{\partial H}{\partial t}=-\frac{\partial L}{\partial t} .  \tag{10.6}\\
& \dot{q}_{j}=\frac{\partial H}{\partial p_{j}}, \\
& \dot{p}_{j}=-\frac{\partial H}{\partial q_{j}} . \tag{10.7}
\end{align*}
$$

Comparing the first of them with Eq. (2.35), we see that

$$
\begin{equation*}
\frac{d H}{d t}=\frac{\partial H}{\partial t}, \tag{10.8}
\end{equation*}
$$

meaning that function $H\left(t, q_{j}, p_{j}\right)$ can change in time only via its explicit dependence on $t$. Eqs. (7) are even more substantial: provided that such function $H\left(t, q_{j}, p_{j}\right)$ has been calculated, they give us two firstorder differential equations (called the Hamilton equations) for the time evolution of the generalized coordinate and generalized momentum of each degree of freedom of the system. ${ }^{3}$

Let us have a look at these equations for the simplest case of a system with one degree of freedom, with the simple Lagrangian function (3.3):

$$
\begin{equation*}
L=\frac{m_{\mathrm{ef}}}{2} \dot{q}^{2}-U_{\mathrm{ef}}(q, t) \tag{10.9}
\end{equation*}
$$

In this case, $p \equiv \partial L / \partial \dot{q}=m_{\text {ef }} \dot{q}$, and $H \equiv p \dot{q}-L=m_{\text {ef }} \dot{q}^{2} / 2+U_{\text {ef }}(q, t)$. In order to honor our new commitment, we need to express the Hamiltonian function explicitly via $t, q$ and $p$ (rather than $\dot{q}$ ):

$$
\begin{equation*}
H=\frac{p^{2}}{2 m_{\mathrm{ef}}}+U_{\mathrm{ef}}(q, t) . \tag{10.10}
\end{equation*}
$$

Now we can spell out Eqs. (7) for this particular case:

$$
\begin{equation*}
\dot{q}=\frac{\partial H}{\partial p}=\frac{p}{m_{\mathrm{ef}}} \tag{10.11}
\end{equation*}
$$

[^148]\[

$$
\begin{equation*}
\dot{p}=-\frac{\partial H}{\partial q}=-\frac{\partial U_{\mathrm{ef}}}{\partial q} . \tag{10.12}
\end{equation*}
$$

\]

While the first of these equations just repeats the definition of the generalized momentum corresponding to coordinate $q$, the second one gives the equation of momentum change. Differentiating Eq. (11) over time, and plugging Eq. (12) into the result, we get:

$$
\begin{equation*}
\ddot{q}=\frac{\dot{p}}{m_{\mathrm{ef}}}=-\frac{1}{m_{\mathrm{ef}}} \frac{\partial U_{\mathrm{ef}}}{\partial q} . \tag{10.13}
\end{equation*}
$$

So, we have returned to the same equation (3.4) that had been derived from the Lagrangian approach.
Thus, the Hamiltonian formalism does not give much new for the solution of most problems of classical mechanics. (This is why I have postponed its discussion until the very end of this course.) Moreover, since the Hamiltonian function $H\left(t, q_{j}, p_{j}\right)$ does nor include generalized velocities explicitly, the phenomenological introduction of dissipation in this approach is less straightforward than that in the Lagrangian equations whose precursor form (2.17) is valid for dissipative forces as well. However, the Hamilton equations (7), which treat the generalized coordinates and momenta in a manifestly symmetric way, are aesthetically appealing and heuristically fruitful. This is especially true in the cases where these arguments participate in $H$ in a similar way. For example, for the very important case of a dissipationfree harmonic oscillator, for which $U_{\text {ef }}=\kappa_{\text {ef }} q^{2} / 2$, Eq. (10) gives the famous symmetric form

$$
\begin{equation*}
H=\frac{p^{2}}{2 m_{\mathrm{ef}}}+\frac{\kappa_{\mathrm{ef}} x^{2}}{2}=\frac{p^{2}}{2 m_{\mathrm{ef}}}+\frac{m_{\mathrm{ef}} \omega_{0}^{2} x^{2}}{2}, \quad \text { where } \omega_{0}^{2} \equiv \frac{\kappa_{\mathrm{ef}}}{m_{\mathrm{ef}}} . \tag{10.14}
\end{equation*}
$$

The Hamilton equations (7) for this system preserve the symmetry, especially evident if we introduce the normalized momentum $\rho \equiv p / m_{\text {ef }} \omega_{0}$ (already used in Secs. 4.3 and 9.2):

$$
\begin{equation*}
\frac{d q}{d t}=\omega_{0} \rho, \quad \frac{d \rho}{d t}=-\omega_{0} q . \tag{10.15}
\end{equation*}
$$

More practically, the Hamilton approach gives additional tools for the search for the integrals of motion. In order to see that, let us consider the full time derivative of an arbitrary function $f\left(t, q_{j}, p_{j}\right)$ :

$$
\begin{equation*}
\frac{d f}{d t}=\frac{\partial f}{\partial t}+\sum_{j}\left(\frac{\partial f}{\partial q_{j}} \dot{q}_{j}+\frac{\partial f}{\partial p_{j}} \dot{p}_{j}\right) \tag{10.16}
\end{equation*}
$$

Plugging in $\dot{q}_{j}$ and $\dot{p}_{j}$ from the Hamilton equations (7), we get

Dynamics of arbitrary variable

$$
\begin{equation*}
\frac{d f}{d t}=\frac{\partial f}{\partial t}+\sum_{j}\left(\frac{\partial H}{\partial p_{j}} \frac{\partial f}{\partial q_{j}}-\frac{\partial H}{\partial q_{j}} \frac{\partial f}{\partial p_{j}}\right)=\frac{\partial f}{\partial t}+\{H, f\} \tag{10.17}
\end{equation*}
$$

where the last term in the right-hand part is the so-called Poisson bracket ${ }^{4}$ that is defined, for two arbitrary functions $f\left(t, q_{j}, p_{j}\right)$ and $g\left(t, q_{j}, p_{j}\right)$, as

Poisson bracket

$$
\begin{equation*}
\{g, f\} \equiv \sum_{j}\left(\frac{\partial g}{\partial p_{j}} \frac{\partial f}{\partial q_{j}}-\frac{\partial f}{\partial p_{j}} \frac{\partial g}{\partial q_{j}}\right) \tag{10.18}
\end{equation*}
$$

[^149]From this definition, one can readily verify that besides evident relations $\{f, f\}=0$ and $\{f, g\}=-\{g, f\}$, the Poisson brackets obey the following important Jacobi identity:

$$
\begin{equation*}
\{f,\{g, h\}\}+\{g,\{h, f\}\}+\{h,\{f, g\}\}=0 . \tag{10.19}
\end{equation*}
$$

Now let us use these relations for a search for integrals of motion. First, equation (17) shows that if a function $f$ does not depend on time explicitly, and

$$
\begin{equation*}
\{H, f\}=0 \tag{10.20}
\end{equation*}
$$

then $d f / d t=0$, i.e. function $f$ is an integral of motion.
Moreover, if we already know two integrals of motion, say $f$ and $g$, then function

$$
\begin{equation*}
F \equiv\{f, g\} \tag{10.21}
\end{equation*}
$$

is also an integral of motion - the so-called Poisson theorem. In order to prove it, we may use the Jacobi identity (19) with $h=H$. Now using Eq. (17) to express the Poisson brackets $\{g, H\},\{H, g\}$, and $\{H$, $\{f$, $g\}\}=\{H, F\}$ via the full and partial time derivatives of functions $f, g$, and $F$, we get

$$
\begin{equation*}
\left\{f, \frac{\partial g}{\partial t}-\frac{d g}{d t}\right\}+\left\{g, \frac{d f}{d t}-\frac{\partial f}{\partial t}\right\}+\frac{d F}{d t}-\frac{\partial F}{\partial t}=0 \tag{10.22}
\end{equation*}
$$

so that if $f$ and $g$ are indeed integrals of motion, i.e., $d f / d t=d g / d t=0$, then

$$
\begin{equation*}
\frac{d F}{d t}=\frac{\partial F}{\partial t}+\left\{g, \frac{\partial f}{\partial t}\right\}-\left\{f, \frac{\partial g}{\partial t}\right\}=\frac{\partial F}{\partial t}-\left[\left\{\frac{\partial f}{\partial t}, g\right\}+\left\{f, \frac{\partial g}{\partial t}\right\}\right] \tag{10.23}
\end{equation*}
$$

Plugging Eq. (21) into the first term of the right-hand part of this equation, and differentiating it by parts, we get $d F / d t=0$, i.e. $F$ is indeed an integral of motion as well.

Finally, one more important role of the Hamilton formalism is that it allows one to trace the close connection between the classical and quantum mechanics. Indeed, using Eq. (18) to calculate the Poisson brackets of the generalized coordinates and momenta, we readily get

$$
\begin{equation*}
\left\{q_{j}, q_{j^{\prime}}\right\}=0, \quad\left\{p_{j}, p_{j^{\prime}}\right\}=0, \quad\left\{q_{j}, p_{j^{\prime}}\right\}=-\delta_{i j^{\prime}} \tag{10.24}
\end{equation*}
$$

In quantum mechanics, ${ }^{5}$ operators of these quantities ("observables") obey commutation relations

$$
\begin{equation*}
\left[\hat{q}_{j}, \hat{q}_{j^{\prime}}\right]=0, \quad\left[\hat{p}_{j}, \hat{p}_{j^{\prime}}\right]=0, \quad\left[\hat{q}_{j}, \hat{p}_{j^{\prime}}\right]=i \hbar \delta_{j j^{\prime}}, \tag{10.25}
\end{equation*}
$$

where the definition of the commutator, $[\hat{g}, \hat{f}] \equiv \hat{g} \hat{f}-\hat{f} \hat{g}$, is to a certain extent ${ }^{6}$ similar to that (18) of the Poisson bracket. We see that the classical relations (24) are similar to quantum-mechanical relations (25) if we following parallel has been made:

$$
\begin{equation*}
\{g, f\} \leftrightarrow \frac{i}{\hbar}[\hat{g}, \hat{f}] . \tag{10.26}
\end{equation*}
$$

[^150]This analogy extends well beyond Eqs. (24)-(25). For example, making replacement (26) in Eq. (17), we get

$$
\begin{equation*}
\frac{d \hat{f}}{d t}=\frac{\partial \hat{f}}{\partial t}+\frac{i}{\hbar}[\hat{H}, \hat{f}], \quad \text { i.e. } i \hbar \frac{d \hat{f}}{d t}=i \hbar \frac{\partial \hat{f}}{\partial t}+[\hat{f}, \hat{H}] \tag{10.27}
\end{equation*}
$$

which is the correct equation of operator evolution in the Heisenberg picture of quantum mechanics. ${ }^{7}$
This analogy implies, in particular, that the quantum-mechanical operators (and the matrices used for their representation in a particular basis) should satisfy the same identities including Eq. (17).

### 10.2. Adiabatic invariance

One more application of the Hamiltonian formalism in classical mechanics is the solution of the following problem. ${ }^{8}$ Earlier in the course, we already studied some effects of time variation of parameters of a single oscillator (Sec. 4.5) and coupled oscillators (Sec. 5.5). However, those discussions were focused on the case when the parameter variation frequency is comparable with the initial oscillation frequency (or frequencies) of the system. Another practically important case is when some system's parameter (let us call it $\lambda$ ) is changed much more slowly (adiabatically ${ }^{9}$ ),

$$
\begin{equation*}
\left|\frac{\lambda}{\lambda}\right| \ll \frac{1}{\tau} \tag{10.28}
\end{equation*}
$$

where $\tau$ is a typical time period of oscillations in the system. Let us consider a 1 D system whose Hamiltonian $H(q, p, \lambda)$ depends on time only via the slow (28) evolution of parameter $\lambda=\lambda(t)$, and whose initial energy restricts system's motion to a finite coordinate interval - see Fig. 3.2c.

Then, as we know from Sec. 3.3, if parameter $\lambda$ is constant, the system performs a periodic (though not necessarily sinusoidal) motion back and forth axis $q$, or, in a different language, along a closed trajectory on the phase plane $[q, p]$ - see Fig. $1 .{ }^{10}$ According to Eq. (8), in this case $H$ is constant on the trajectory. (In order to distinguish this particular value from the Hamiltonian function as such, I will assume that this constant coincides with the full mechanical energy $E$, like is does for Hamiltonian (10), though this assumption is not necessary for the calculation made below.)

The oscillation period $\tau$ may be calculated as a contour integral along this closed trajectory:

$$
\begin{equation*}
T \equiv \int_{0}^{\tau} d t=\oint \frac{d t}{d q} d q=\oint \frac{1}{\dot{q}} d q . \tag{10.29}
\end{equation*}
$$

Using the first of the Hamilton equations (7), we may now present this integral as

[^151]\[

$$
\begin{equation*}
\tau=\oint \frac{1}{\partial H / \partial p} d q \tag{10.30}
\end{equation*}
$$

\]

At each given point $q, H=E$ is a function of $p$ alone, so that we may flip the partial derivative in the denominator just as a full derivative, and rewrite Eq. (30) as

$$
\begin{equation*}
\tau=\oint \frac{\partial p}{\partial E} d q . \tag{10.31}
\end{equation*}
$$

For the particular Hamiltonian (10), this relation is immediately reduced to Eq. (3.27) in the form of a contour integral:

$$
\begin{equation*}
\tau=\left(\frac{m_{\mathrm{ef}}}{2}\right)^{1 / 2} \oint \frac{1}{\left[E-U_{\mathrm{ef}}(q)\right]^{1 / 2}} d q \tag{10.32}
\end{equation*}
$$



Fig. 10.1. Phase-plane representation of periodic oscillations of a 1D Hamiltonian system, for two values of energy (schematically).

Superficially, it looks that these formulas may be also used to find the motion period change when parameter $\lambda$ is being changed adiabatically, for example, by plugging known functions $m_{\mathrm{ef}}(\lambda)$ and $U_{\text {ef }}(q, \lambda)$ into Eq. (32). However, there is no guarantee that energy $E$ in that integral would stay constant as the parameter change, and indeed we will see below that this is not necessarily the case. Even more interestingly, in the most important case of the harmonic oscillator ( $U_{\mathrm{ef}}=\kappa_{\mathrm{e} f} q^{2} / 2$ ), whose oscillation period $\tau$ does not depend on $E$ (see Eq. (3.29) and its discussion), its variation in the adiabatic limit (28) may be readily predicted: $T(\lambda)=2 \pi / \omega_{0}(\lambda)=2 \pi\left[m_{\mathrm{ef}}(\lambda) / \kappa_{\mathrm{ef}}(\lambda)\right]^{1 / 2}$, but the dependence of the oscillation energy $E$ (and hence the oscillation amplitude) on $\lambda$ is not immediately obvious.

In order to address this issue, let us use Eq. (8) (with $E=H$ ) to present the energy change with $\lambda(t)$, i.e. in time, as

$$
\begin{equation*}
\frac{d E}{d t}=\frac{\partial H}{\partial t}=\frac{\partial H}{\partial \lambda} \frac{d \lambda}{d t} . \tag{10.33}
\end{equation*}
$$

Since we are interested in a very slow (adiabatic) time evolution of energy, we can average Eq. (33) over fast oscillations in the system, for example over one oscillation period $\tau$, treating $d \lambda / d t$ as a constant during this averaging. ${ }^{11}$ The averaging yields

[^152]\[

$$
\begin{equation*}
\frac{\overline{d E}}{d t} \approx \frac{d \lambda}{d t} \frac{\overline{\partial H}}{\partial \lambda}=\frac{d \lambda}{d t} \frac{1}{T} \int_{0}^{\tau} \frac{\partial H}{\partial \lambda} d t . \tag{10.34}
\end{equation*}
$$

\]

Transforming the time integral to the contour one, just as we did at the transition from Eq. (29) to Eq. (30), and using Eq. (31) for $T$, we get

$$
\begin{equation*}
\frac{\overline{d E}}{d t}=\frac{d \lambda}{d t} \frac{\oint \frac{\partial H / \partial \lambda}{\partial H / \partial p} d q}{\oint \frac{\partial p}{\partial E} d q} \tag{10.35}
\end{equation*}
$$

At each point $q$ of the contour, $H$ is a function of not only $\lambda$, but also of $p$, which may be also $\lambda$ dependent, so that if $E$ is fixed, the partial differentiation of relation $E=H$ over $\lambda$ yields

$$
\begin{equation*}
\frac{\partial H}{\partial \lambda}+\frac{\partial H}{\partial p} \frac{\partial p}{\partial \lambda}=0, \quad \text { i.e. } \frac{\partial H / \partial \lambda}{\partial H / \partial p}=-\frac{\partial p}{\partial \lambda} . \tag{10.36}
\end{equation*}
$$

Plugging the last relation into Eq.(35), we get

$$
\begin{equation*}
\frac{\overline{d E}}{d t}=-\frac{d \lambda}{d t} \frac{\oint \frac{\partial p}{\partial \lambda} d q}{\oint \frac{\partial p}{\partial E} d q} \tag{10.37}
\end{equation*}
$$

Since the left-hand part of Eq. (37), and the derivative $d \lambda / d t$ do not depend on $q$, we may move them into the integrals over $q$ as constants, and rewrite that relation as

$$
\begin{equation*}
\oint\left(\frac{\partial p}{\partial E} \frac{\overline{d E}}{d t}+\frac{\partial p}{\partial \lambda} \frac{d \lambda}{d t}\right) d q=0 \tag{10.38}
\end{equation*}
$$

Now let us consider the following integral over the same phase-plane contour,

$$
\begin{equation*}
J \equiv \frac{1}{2 \pi} \oint p d q \tag{10.39}
\end{equation*}
$$

called the action variable. Just to understand its physical sense, let us calculate $J$ for a harmonic oscillator (14). As we know very well from Chapter 4, for such oscillator, $q=A \cos \Psi, p=-m_{\mathrm{ef}} \omega_{0} A \sin \Psi$ (with $\Psi=\omega_{0} t+$ const), so that $J$ may be easily expressed either via oscillations' amplitude $A$, or their energy $E=H=m_{\text {ef }} \omega_{0}^{2} A^{2} / 2$ :

$$
\begin{equation*}
J=\frac{1}{2 \pi} \oint p d q=\frac{1}{2 \pi} \int_{\Psi=0}^{\Psi=2 \pi}\left(-m_{\mathrm{ef}} \omega_{0} A \sin \Psi\right) d(A \cos \Psi)=\frac{1}{2 \pi} \frac{m_{\mathrm{ef}} \omega_{0}}{2} A^{2}=\frac{E}{\omega_{0}} . \tag{10.40}
\end{equation*}
$$

Returning to a general system with adiabatically changed parameter $\lambda$, let us use the definition of $J$, Eq. (39), to calculate its time derivative, again taking into account that at each point $q$ of the trajectory, $p$ is a function of $E$ and $\lambda$ :
cumbersome) proofs of Eq. (42) are still being offered in literature - see, e.g., C. Wells and S. Siklos, Eur. J. Phys. 28, 105 (2007) and/or A. Lobo et al., Eur. J. Phys. 33, 1063 (2012).

$$
\begin{equation*}
\frac{d J}{d t}=\frac{1}{2 \pi} \oint \frac{d p}{d t} d q=\frac{1}{2 \pi} \oint\left(\frac{\partial p}{\partial E} \frac{d E}{d t}+\frac{\partial p}{\partial \lambda} \frac{d \lambda}{d t}\right) d q . \tag{10.41}
\end{equation*}
$$

Within the accuracy of our approximation, in which the contour integrals (38) and (41) are calculated along a closed trajectory, factor $d E / d t$ is indistinguishable from its time average, and these integrals coincide, so that result (38) is applicable to Eq. (41) as well. Hence, we have finally arrived at a very important result: at a slow parameter variation, $d J / d t=0$, i.e. the action variable remains constant:

$$
\begin{equation*}
J=\text { const } . \tag{10.42}
\end{equation*}
$$

This is the famous adiabatic invariance. ${ }^{12}$ In particular, according to Eq. (40), in a harmonic oscillator, energy of oscillation changes proportionately to the (slowly changed) eigenfrequency.

Before moving on, let me briefly note that the adiabatic invariance is not the only application of the action variable $J$. Since the initial choice of generalized coordinates and velocities (and hence the generalized momenta) in analytical mechanics is arbitrary (see Sec. 2.1), it is almost evident that $J$ may be taken for a new generalized momentum corresponding to a certain new generalized coordinate $\Theta,{ }^{13}$ and that pair $\{J, \Theta\}$ should satisfy the Hamilton equations (7), in particular,

$$
\begin{equation*}
\frac{d \Theta}{d t}=\frac{\partial H}{\partial J} . \tag{10.43}
\end{equation*}
$$

Following the commitment of Sec. 1 (made there for the "old" arguments $q_{j}, p_{j}$ ), before the differentiation in the right-hand part in Eq. (43), $H$ should be expressed as a function of $t$, $J$, and $\Theta$. For time-independent Hamiltonian systems, $H$ is uniquely defined by $J$ - see, e.g., Eq. (40). Hence the righthand part of Eq. (43) does not depend on either $t$ or $\Theta$, so that according to that equation, $\Theta$ (called the angle variable) is a linear function of time:

$$
\begin{equation*}
\Theta=\frac{\partial H}{\partial J} t+\text { const } . \tag{10.44}
\end{equation*}
$$

For a harmonic oscillator, according to Eq. (40), derivative $\partial H / \partial J=\partial E / \partial J=\omega_{0}=2 \pi / T$, so that $\Theta$ $=\omega_{0} t+$ const. It may be shown that a more general form of this relation,

$$
\begin{equation*}
\frac{\partial H}{\partial J}=\frac{2 \pi}{\tau} \tag{10.45}
\end{equation*}
$$

is valid for an arbitrary system described by Eq. (10). Thus, Eq. (44) becomes

$$
\begin{equation*}
\Theta=2 \pi \frac{t}{T}+\text { const } \tag{10.46}
\end{equation*}
$$

[^153]To summarize, for a harmonic oscillator, the angle variable $\Theta$ is just the full phase $\Psi$ that we used so much in Ch. 4, while for an arbitrary (nonlinear) 1D oscillator, this is a convenient generalization of that notion. Due to this reason, variables $J$ and $\Theta$ present a convenient tool for discussion of certain fine points of dynamics strongly nonlinear oscillators - for whose discussion I, unfortunately, do not have time. ${ }^{14}$

### 10.3. The Hamilton principle

Now let me show that the Lagrangian equations of motion, that have been derived in Sec. 2.1 from the Newton laws, may be also obtained from the so-called Hamilton principle, namely the condition of a minimum (or rather an extremum) of the integral called action:

$$
\begin{equation*}
S \equiv \int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} L d t \tag{10.47}
\end{equation*}
$$

where $t_{\text {ini }}$ and $t_{\text {fin }}$ are, respectively, the initial and final moments of time, at which moments all generalized coordinates and velocities are considered fixed (not varied) - see Fig. 2.


Fig. 10.2. Deriving the Hamilton principle.

The proof of that statement is rather simple. Considering, similarly to Sec. 2.1, a possible virtual variation of the motion, described by infinitesimal deviations $\left\{\delta q_{j}(t), \delta \dot{q}_{j}(t)\right\}$ from the real motion, the necessary condition for $S$ to be minimal is

$$
\begin{equation*}
\delta S \equiv \int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \delta L d t=0 \tag{10.48}
\end{equation*}
$$

where $\delta S$ and $\delta L$ are the variations of the action and the Lagrange function, corresponding to the set $\left\{\delta q_{j}(t), \delta \dot{q}_{j}(t)\right\}$. As has been already discussed in Sec. 2.1, we can use the operation of variation just as the usual differentiation (but at fixed time, see Fig. 2.1), swapping these two operations if needed see Fig. 2.3 and its discussion. Thus, we may write

$$
\begin{equation*}
\delta L=\sum_{j}\left(\frac{\partial L}{\partial q_{j}} \delta q_{j}+\frac{\partial L}{\partial \dot{q}_{j}} \delta \dot{q}_{j}\right)=\sum_{j} \frac{\partial L}{\partial q_{j}} \delta q_{j}+\sum_{j} \frac{\partial L}{\partial \dot{q}_{j}} \frac{d}{d t} \delta q_{j} . \tag{10.49}
\end{equation*}
$$

[^154]After plugging the last expression into Eq. (48), we can integrate the second term by parts:

$$
\begin{align*}
\delta S & =\int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \sum_{j} \frac{\partial L}{\partial q_{j}} \delta q_{j} d t+\sum_{j}^{t_{\mathrm{fin}}} \int_{t_{\mathrm{ini}}} \frac{\partial L}{\partial \dot{q}_{j}} \frac{d}{d t} \delta q_{j} d t \\
& =\int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \sum_{j} \frac{\partial L}{\partial q_{j}} \delta q_{j} d t+\sum_{j}\left[\frac{\partial L}{\partial \dot{q}_{j}} \delta q_{j}\right]_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}}-\sum_{j} \int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \delta q_{j} d\left(\frac{\partial L}{\partial \dot{q}_{j}}\right)=0 . \tag{10.50}
\end{align*}
$$

Since the generalized coordinates in the initial and final points are considered fixed (not affected by the variation), all $\delta q_{j}\left(t_{\text {ini }}\right)=\delta q_{j}\left(t_{\text {fin }}\right)=0$, the second term in the right-hand part of Eq. (50) vanishes. Multiplying and dividing the last term of that part by $d t$, we finally get

$$
\begin{equation*}
\delta S=\int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \sum_{j} \frac{\partial L}{\partial q_{j}} \delta q_{j} d t-\sum_{j} \int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \delta q_{j} \frac{d}{d t}\left(\frac{\partial L}{\partial \dot{q}_{j}}\right) d t=-\int_{t_{\mathrm{ini}}}^{t_{\mathrm{fin}}} \sum_{j}\left[\frac{d}{d t}\left(\frac{\partial L}{\partial \dot{q}_{j}}\right)-\frac{\partial L}{\partial q_{j}}\right] \delta q_{j} d t=0 . \tag{10.51}
\end{equation*}
$$

This relation should hold for an arbitrary set of functions $\delta q_{j}(t)$, and for any time interval, so that it is only possible if the expressions in square brackets equal zero for all $j$, giving us the set of Lagrange equations (2.19). So, the Hamilton principle indeed gives the Lagrange equations of motion.

It is very useful to make the notion of action $S$, defined by Eq. (47), more transparent by calculating it for the simple case of a single particle moving in a potential field that conserves its energy $E=T+U$. In this case the Lagrangian function $L=T-U$ may be presented as

$$
\begin{equation*}
L=T-U=2 T-(T+U)=2 T-E=m v^{2}-E, \tag{10.52}
\end{equation*}
$$

with $E=$ const, so that

$$
\begin{equation*}
S=\int L d t=\int m v^{2} d t-E t+\text { const. } \tag{10.53}
\end{equation*}
$$

Presenting the expression under the remaining integral as $m \mathbf{v} \cdot \mathbf{v} d t=\mathbf{p} \cdot(d \mathbf{r} / d t) d t=\mathbf{p} \cdot d \mathbf{r}$, we finally get

$$
\begin{equation*}
S=\int \mathbf{p} \cdot d \mathbf{r}-E t+\text { const }=S_{0}-E t+\text { const } \tag{10.54}
\end{equation*}
$$

where the time-independent integral

$$
\begin{equation*}
S_{0} \equiv \int \mathbf{p} \cdot d \mathbf{r} \tag{10.55}
\end{equation*}
$$

is frequently called the abbreviated action. ${ }^{15}$
This expression may be used to establish one more connection between the classical and quantum mechanics, now in its Schrödinger picture. Indeed, in the quasiclassical (WKB) approximation of that picture ${ }^{16}$ a particle of fixed energy is described by a De Broglie wave

$$
\begin{equation*}
\Psi(\mathbf{r}, t) \propto \exp \left\{i\left(\int \mathbf{k} \cdot d \mathbf{r}-\omega t+\mathrm{const}\right)\right\}, \tag{10.56}
\end{equation*}
$$

[^155]where wavevector $\mathbf{k}$ is proportional to the particle's momentum, while frequency $\omega$, to its energy:
\[

$$
\begin{equation*}
\mathbf{k}=\frac{\mathbf{p}}{\hbar}, \quad \omega=\frac{E}{\hbar} . \tag{10.57}
\end{equation*}
$$

\]

Plugging these expressions into Eq. (56) and comparing the result with Eq. (54), we see that the WKB wavefunction may be presented as

$$
\begin{equation*}
\Psi \propto \exp \{i S / \hbar\} . \tag{10.58}
\end{equation*}
$$

Hence the Hamilton's principle (48) means that the total phase of the quasiclassical wavefunction should be minimal along particle's real trajectory. But this is exactly the so-called eikonal minimum principle well known from the optics (though valid for any other waves as well), where it serves to define the ray paths in the geometric optics limit - similar to the WKB approximation condition. Thus, the ratio $S / \hbar$ may be considered just as the eikonal, i.e. the total phase accumulation, of the de Broigle waves. ${ }^{17}$

Now, comparing Eq. (55) with Eq. (39), we see that the action variable $J$ is just the change of the abbreviated action $S_{0}$ along a single phase-plane contour (divided by $2 \pi$ ). This means that in the WKB approximation, $J$ is the number of de Broglie waves along the classical trajectory of a particle, i.e. an integer value of the corresponding quantum number. If system's parameters are changed slowly, the quantum number has to stay integer, and hence $J$ cannot change, giving a quantum-mechanical interpretation of the adiabatic invariance. It is really fascinating that a fact of classical mechanics may be "derived" (or at least understood) more easily from the quantum mechanics' standpoint. ${ }^{18}$

### 10.4. The Hamilton-Jacobi equation

Action S, defined by Eq. (47), may be used for one more formulation of classical mechanics. For that, we need one more, different commitment: $S$ to be considered a function of the following independent arguments: the final time point $t_{\text {fin }}$ (which I will, for brevity, denote as $t$ in this section), and the set of generalized coordinates (but not of the generalized velocities!) at that point:

$$
\begin{equation*}
S \equiv \int_{t_{\mathrm{ini}}}^{t} L d t=S\left[t, q_{j}(t)\right] \tag{10.59}
\end{equation*}
$$

Let us calculate a variation of this (essentially, new!) function, resulting from an arbitrary combination of variations of final values $q_{j}(t)$ of the coordinates, while keeping $t$ fixed. Formally this may be done by repeating the variation calculations described by Eqs. (49)-(52), besides that now variations $\delta q_{j}$ at the finite point $(t)$ do not necessarily equal zero. As a result, we get

$$
\begin{equation*}
\delta S=\left.\sum_{j} \frac{\partial L}{\partial \dot{q}_{j}} \delta q_{j}\right|_{t}-\int_{t_{\mathrm{ini}}}^{t} d t \sum_{j}\left[\frac{d}{d t}\left(\frac{\partial L}{\partial \dot{q}_{j}}\right)-\frac{\partial L}{\partial q_{j}}\right] \delta q_{j} . \tag{10.60}
\end{equation*}
$$

[^156]For the motion along the real trajectory, i.e. satisfying the Lagrange equations of motion, the second term of this expression equals zero. Hence Eq. (60) shows that, for (any) fixed time $t$,

$$
\begin{equation*}
\frac{\partial S}{\partial q_{j}}=\frac{\partial L}{\partial \dot{q}_{j}} \tag{10.61}
\end{equation*}
$$

But the last derivative is nothing else than the generalized momentum $p_{j}-$ see Eq. (2.31), so that

$$
\begin{equation*}
\frac{\partial S}{\partial q_{j}}=p_{j} \tag{10.62}
\end{equation*}
$$

(As a reminder, both parts of this relation refer to the final moment $t$ of the trajectory.) As a result, the full derivative of action $S\left[t, q_{j}(t)\right]$ over time takes the form

$$
\begin{equation*}
\frac{d S}{d t}=\frac{\partial S}{\partial t}+\sum_{j} \frac{\partial S}{\partial q_{j}} \dot{q}_{j}=\frac{\partial S}{\partial t}+\sum_{j} p_{j} \dot{q}_{j} \tag{10.63}
\end{equation*}
$$

Now, by the very definition (59), the full derivative $d S / d t$ is nothing more that the Lagrange function $L$, so that Eq. (63) yields

$$
\begin{equation*}
\frac{\partial S}{\partial t}=L-\sum_{j} p_{j} \dot{q}_{j} \tag{10.64}
\end{equation*}
$$

However, according to the definition (2) of the Hamiltonian function $H$, the right-hand part of Eq. (63) is just $(-H)$, so that we get an extremely simply-looking Hamilton-Jacobi equation

$$
\begin{equation*}
\frac{\partial S}{\partial t}=-H \tag{10.65}
\end{equation*}
$$

This simplicity is, however, rather deceiving, because in order to use this equation for the calculation of function $S\left(t, q_{j}\right)$ for any particular problem, the Hamiltonian function has to be first expressed as a function of time $t$, generalized coordinates $q_{j}$, and the generalized momenta $p_{j}$ (which may be, according to Eq. (62), presented just as derivatives $\partial S / \partial q_{j}$ ). Let us see how does this procedure work for the simplest case of a 1D system with the Hamiltonian function given by Eq. (10). In this case, the only generalized momentum is $p=\partial S / \partial q$, so that

$$
\begin{equation*}
H=\frac{p^{2}}{2 m_{\mathrm{ef}}}+U_{\mathrm{ef}}(q, t)=\frac{1}{2 m_{\mathrm{ef}}}\left(\frac{\partial S}{\partial q}\right)^{2}+U_{\mathrm{ef}}(q, t), \tag{10.66}
\end{equation*}
$$

and the Hamilton-Jacobi equation (65) is reduced to a partial differential equation,

$$
\begin{equation*}
\frac{\partial S}{\partial t}+\frac{1}{2 m_{\mathrm{ef}}}\left(\frac{\partial S}{\partial q}\right)^{2}+U_{\mathrm{ef}}(q, t)=0 \tag{10.67}
\end{equation*}
$$

Its solution may be readily found in the particular case of time-independent potential energy $U_{\text {ef }}$ $=U_{\text {ef }}(q)$. In this case, Eq. (67) is evidently satisfied by a variable-separated solution

$$
\begin{equation*}
S(t, q)=S_{0}(q)+\text { const } \times t \tag{10.68}
\end{equation*}
$$

Plugging this solution into Eq. (67), we see that since the sum of two last terms in the left-hand part of that equation presents the full mechanical energy $E$, the constant in Eq. (68) is nothing but ( $-E$ ). Thus for function $S_{0}$ we get an ordinary differential equation

$$
\begin{equation*}
-E+\frac{1}{2 m_{\mathrm{ef}}}\left(\frac{d S_{0}}{d q}\right)^{2}+U_{\mathrm{ef}}(q)=0 \tag{10.69}
\end{equation*}
$$

Integrating it, we get

$$
\begin{equation*}
S_{0}=\int\left\{2 m_{\mathrm{ef}}\left[E-U_{\mathrm{ef}}(q)\right]\right\}^{1 / 2} d q+\text { const }, \tag{10.70}
\end{equation*}
$$

so that, finally, the action is equal to

$$
\begin{equation*}
S=\int\left\{2 m_{\mathrm{ef}}\left[E-U_{\mathrm{ef}}(q)\right]\right\}^{1 / 2} d q-E t+\text { const. } \tag{10.71}
\end{equation*}
$$

For the case of 1D motion of a single 1D particle, i.e. for $q=x, m_{\text {ef }}=m, U_{\text {ef }}(q)=U(x)$, this solution is just the 1D case of the more general Eqs. (54)-(55), which were obtained by a much more simple way. (In particular, $S_{0}$ is just the abbreviated action.)

This particular case illustrates that the Hamilton-Jacobi equation is not the most efficient way for solution of most practical problems. However, it may be rather useful for studies of certain mathematical aspects of dynamics. ${ }^{19}$ Moreover, in the 1940s this approach was extended to a completely different field - the optimal control theory, in which the role of action $S$ is played by the so-called cost function a certain functional of a dynamic system, that should be minimized by an optical choice of a control signal - a function of time that affects system's dynamics. From the point of view of this mathematical theory, Eq. (65) is a particular case of a more general Hamilton-Jacobi-Bellman equation. ${ }^{20}$

### 10.5. Exercise problems

10.1. Derive the Hamilton equations of motion for our testbed problem (a bead on a ring rotating about its vertical diameter - see Fig. 2.1, partly reproduced on the right). Check that the equations are equivalent to those derived from the Lagrangian formalism.

10.2. Perform the same tasks as in Problem 10.1 for the system already considered in Problem 2.3, a fixed-length pendulum hanging from a horizontal support whose motion law $x_{0}(t)$ is fixed - see Fig. on the right. (No vertical plane constraint.)


[^157]10.3. Perform the same tasks as in Problems 1 and 2, for the system already considered in Problem 2.5 - a block of mass $m$ that can slide, without friction, along the inclined surface of a heavy wedge (mass $m^{\prime}$ ). The wedge is free to move, also without friction, along a horizontal surface - see Fig. on the right. (Both motions are within the vertical plane containing the steepest slope line.)

10.4. Find and solve equations of motion of a particle with the following Hamiltonian function:
$$
H=\frac{1}{2 m}(\mathbf{p}+a \mathbf{r})^{2},
$$
where $a$ is a constant scalar.
10.5. Let $L$ be the Lagrange function, and $H$ the Hamilton function, of the same system. What three of the following four statements,
(i) $\frac{d L}{d t}=0$,
(ii) $\frac{\partial L}{\partial t}=0$,
(iii) $\frac{d H}{d t}=0$,
(iv) $\frac{\partial H}{\partial t}=0$,
are equivalent? Give an example when those three equalities hold, but the forth one does not.
10.6. Calculate the Poisson brackets of the Cartesian components of the angular momentum $\mathbf{L}$ of a particle moving in a central force field and its Hamiltonian function $H$, and discuss the most important implication of the result.
10.7. After small oscillations had been initiated in a simple pendulum (Fig. on the right), the thread is being pulled up slowly, so that the pendulum length $l$ is being reduced. Neglecting dissipation,
(i) prove by a direct calculation that the oscillation energy is indeed changing proportionately to the oscillation frequency, as it follows from the constancy of the corresponding adiabatic invariant (40), and

(ii) find the $l$-dependence of amplitudes of the angular and linear deviations from the equilibrium.
10.8. The mass $m$ of a small body that performs 1D oscillations in potential $U(x)=a x^{2 n}$, with $n>$ 0 , is being changed slowly. Calculate the oscillation energy $E$ as a function of $m$.
10.9. A stiff ball is bouncing vertically from the floor of an elevator whose upward acceleration changes very slowly. Neglecting energy dissipation, calculate how much does the bounce height $h$ change during acceleration's increase from 0 to $g$.


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Essential Graduate Physics
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# Part EM: Classical Electrodynamics 

Last corrections: 2019/09/05

A revised version of this material is now published by the IOP under the title "Classical Electrodynamics: Lecture notes" (Essential Advanced Physics - Volume 3, ISBN 978-0-7503-1405-3), with the model solutions of the exercise problems published under the title
"Classical Electrodynamics: Problems with solutions"
(Essential Advanced Physics - Volume 4, ISBN 978-0-7503-1408-4)

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## Chapter 1. Electric Charge Interaction

This brief chapter describes the basics of electrostatics, the study of interactions between static (or slowly moving) electric charges. Much of this material should be known to the reader from his or her undergraduate studies; because of that, the explanations will be very succinct. ${ }^{1}$

### 1.1. The Coulomb law

A serious discussion of the Coulomb law ${ }^{2}$ requires a common agreement on the meaning of the following notions: ${ }^{3}$

- electric charges $q_{k}$, as revealed, most explicitly, by experimental observation of electrostatic interaction between the charged particles;
- electric charge conservation, meaning that the algebraic sum of $q_{k}$ of all particles inside any closed volume is conserved, unless the charged particles cross the volume's border; and
- a point charge, meaning the charge of an ultimately small ("point") particle whose position in space may be completely described (in a given reference frame) by its radius-vector $\mathbf{r}=\mathbf{n}_{1} r_{1}+\mathbf{n}_{2} r_{2}+$ $\mathbf{n}_{3} r_{3}$, where $\mathbf{n}_{j}$ (with $j=1,2,3$ ) are unit vectors directed along 3 mutually perpendicular axes, and $r_{j}$ are the corresponding Cartesian components of $\mathbf{r}$.

I will assume that these notions are well known to the reader - though my strong advice is to give some thought to their vital importance. Using them, the Coulomb law for the electrostatic interaction of two point charges in otherwise free space may be formulated as follows:

Coulomb
law for
2 point charges

$$
\begin{equation*}
\mathbf{F}_{k k^{\prime}}=\kappa q_{k} q_{k^{\prime}} \frac{\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}}{\left|\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right|^{3}} \tag{1.1}
\end{equation*}
$$

where $\mathbf{F}_{k k}$, denotes the force exerted on charge number $k$ by charge number $k$ '. This law is certainly very familiar to the reader, but several remarks may still be due:
(i) Flipping indices $k$ and $k$, we see that Eq. (1) $)^{4}$ complies with the $3^{\text {rd }}$ Newton law: the reciprocal force is equal in magnitude but opposite in direction: $\mathbf{F}_{k^{\prime} k}=-\mathbf{F}_{k k^{\prime}}$.
(ii) According to Eq. (1), the magnitude of the force, $F_{k k^{\prime}}$, is inversely proportional to the square of the distance between the two charges - the well-known undergraduate-level formulation of the Coulomb law.

[^158](iii) Since vector $\left(\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right)$ is directed from point $\mathbf{r}_{k}$, toward point $\mathbf{r}_{k}$ (Fig. 1), Eq. (1) implies that charges of the same sign (i.e. with $q_{k} q_{k^{\prime}}>0$ ) repulse, while those with opposite signs ( $q_{k} q_{k}<0$ ) attract each other.


Fig. 1.1. Direction of the Coulomb forces (for $q_{k} q_{k}{ }^{\prime}>0$ ).
(iv) Constant $\kappa$ in Eq. (1) depends on the system of units we use. In the Gaussian units, $\kappa$ is set to 1 , for the price of introducing a special unit of charge (the statcoulomb) that would fit the experimental data for Eq. (1), for forces $\mathbf{F}_{k k}$, measured in Gaussian units (dynes). On the other hand, in the International System ("SI") of units, the charge unit is one coulomb (abbreviated C), ${ }^{5}$ close to $3 \times 10^{9}$ statcoulombs, and $\kappa$ is different from unity: ${ }^{6}$

$$
\begin{equation*}
\kappa_{\mathrm{SI}}=\frac{1}{4 \pi \varepsilon_{0}} \equiv 10^{-7} \mathrm{c}^{2} \tag{1.2}
\end{equation*}
$$

Electric force constant

Unfortunately, the continuing struggle between zealot proponents of these two systems bears all ugly features of a religious war, with a similarly slim chances for any side to win it in any foreseeable future. In my humble view, each of these systems has its advantages and handicaps (to be noted on several occasions below), and every educated physicist should have no problem with using any of them. Following insisting recommendations of international scientific unions, I will mostly use SI units, but for readers' convenience, duplicate the most important formulas in the Gaussian units.

Besides Eq. (1), another key experimental law of electrostatics is the linear superposition principle: the electrostatic forces exerted on some point charge (say, $q_{k}$ ) by other charges do not affect each other and add up as vectors to form the net force:

$$
\begin{equation*}
\mathbf{F}_{k}=\sum_{k^{\prime} \neq k} \mathbf{F}_{k k^{\prime}}, \tag{1.3}
\end{equation*}
$$

where the summation is extended over all charges but $q_{k}$, and the partial force $\mathbf{F}_{k k}$, is described by Eq. (1). ${ }^{7}$ The fact that the sum is restricted to $k^{\prime} \neq k$ means that a point charge does not interact with itself.

[^159]This fact may look trivial from Eq. (1), whose right-hand part diverges at $\mathbf{r}_{k} \rightarrow \mathbf{r}_{k^{\prime}}$, but becomes less evident (though still true) in quantum mechanics where the charge of even an elementary particle is effectively spread around some volume, together with particle's wavefunction. ${ }^{8}$

Now we may combine Eqs. (1) and (3) to get the following expression for the net force $\mathbf{F}$ acting on some charge $q$ located at point $\mathbf{r}$ :

$$
\begin{equation*}
\mathbf{F}=q \frac{1}{4 \pi \varepsilon_{0}} \sum_{\mathbf{r}_{k} \neq \neq \mathbf{r}} q_{k^{\prime}} \frac{\mathbf{r}-\mathbf{r}_{k^{\prime}}}{\left|\mathbf{r}-\mathbf{r}_{k^{\prime}}\right|^{3}} . \tag{1.4}
\end{equation*}
$$

This equation implies that it makes sense to introduce the notion of the electric field at point $\mathbf{r}$, as an entity independent of the probe charge $q$, characterized by vector

$$
\begin{equation*}
\mathbf{E}(\mathbf{r}) \equiv \frac{\mathbf{F}}{q} \tag{1.5}
\end{equation*}
$$

formally called the electric field strength - but much more frequently, just the "electric field". In these terms, Eq. (4) becomes
Coulomb law for system of point charges

$$
\begin{equation*}
\mathbf{E}(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \sum_{\mathbf{r}_{k}^{\prime} \neq \mathbf{r}} q_{k^{\prime}} \frac{\mathbf{r}-\mathbf{r}_{k^{\prime}}}{\left|\mathbf{r}-\mathbf{r}_{k^{\prime}}\right|^{3}} \tag{1.6}
\end{equation*}
$$

This concept is so appealing that Eq. (5) is used well beyond the boundaries of free-space electrostatics. Moreover, the notion of field becomes virtually unavoidable for description of time-dependent phenomena (such as electromagnetic waves), where the electromagnetic field shows up as a specific form of matter, with zero rest mass, and hence different from the usual "material" particles.

Many problems involve many point charges $q_{k}, q_{k^{\prime \prime}}, \ldots$, located so closely that it is possible to approximate them with a continuous charge distribution. Indeed, for a group of charges within a very small volume $d^{3} r^{\prime}$, with the linear size satisfying strong condition $d r \ll{\mathbf{r}_{k}}-\mathbf{r}_{k^{\prime}} \mid$, the geometrical factor in Eq. (6) is essentially the same. As a result, all these charges may be treated as a single charge $d Q\left(\mathbf{r}^{\prime}\right)$. Since this charge is proportional to $d^{3} r^{\prime}$, we can define the local (3D) charge density $\rho\left(\mathbf{r}^{\prime}\right)$ by relation ${ }^{9}$

$$
\begin{equation*}
\rho\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime} \equiv d Q\left(\mathbf{r}^{\prime}\right) \equiv \sum_{r_{k^{\prime}} \in d^{3} r^{\prime}} q_{k^{\prime}}, \tag{1.7}
\end{equation*}
$$

and rewrite Eq. (6) as

$$
\begin{equation*}
\mathbf{E}(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \sum_{d^{3} r^{\prime}} d Q\left(\mathbf{r}^{\prime}\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}}=\frac{1}{4 \pi \varepsilon_{0}} \sum_{d^{3} r^{\prime}} \rho\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime} \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}}, \tag{1.8}
\end{equation*}
$$

[^160]i.e. as the integral (over the whole volume containing all essential charges): ${ }^{10}$
\[

$$
\begin{equation*}
\mathbf{E}(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int \rho\left(\mathbf{r}^{\prime}\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} d^{3} r^{\prime} \tag{1.9}
\end{equation*}
$$

\]

Coulomb law for continuous charge distribution

It is very convenient that Eq. (9) may be used even in the case of discrete point charges, employing the notion of Dirac's $\delta$-function, ${ }^{11}$ which is a mathematical approximation for a very sharp function equal to zero everywhere but one point, and still having a finite (unit) integral. Indeed, in this formalism, a set of point charges $q_{k^{\prime}}$ located in points $\mathbf{r}_{k^{\prime}}$ may be presented by the pseudo-continuous distribution with density

$$
\begin{equation*}
\rho\left(\mathbf{r}^{\prime}\right)=\sum_{k^{\prime}} q_{k^{\prime}} \delta\left(\mathbf{r}^{\prime}-\mathbf{r}_{k^{\prime}}\right) . \tag{1.10}
\end{equation*}
$$

Plugging this expression into Eq. (9), we come back to the discrete version (6) of the Coulomb law.

### 1.2. The Gauss law

Due to the extension to point ("discrete") charges, it may seem that Eqs. (5) and (9) is all we need for solving any problem of electrostatics. In practice, this is not quite true, first of all because the direct use of Eq. (9) frequently leads to complex calculations. Indeed, let us consider a very simple example: the electric field produced by a spherically-symmetric charge distribution with density $\rho\left(r^{\prime}\right)$. We may immediately use the problem symmetry to argue that the electric field should be also spherically-symmetric, with only one component in spherical coordinates: $\mathbf{E}(\mathbf{r})=E(r) \mathbf{n}_{r}$ where $\mathbf{n}_{r} \equiv \mathbf{r} / r$ is the unit vector in the direction of the field observation point $\mathbf{r}$ (Fig. 2).


Fig. 1.2. One of the simplest problems of electrostatics: electric field produced by a spherically-symmetric charge distribution.

Taking this direction as the polar axis of a spherical coordinate system, we can use the evident independence of the elementary radial field $d E$, created by the elementary charge $\rho\left(r^{\prime}\right) d^{3} r^{\prime}=\rho\left(r^{\prime}\right) r^{\prime 2} \sin \theta$ $d r^{\prime} d \theta^{\prime} d \varphi^{\prime}$, of the azimuth angle $\varphi^{\prime}$, and reduce integral (9) to

$$
\begin{equation*}
E=\frac{1}{4 \pi \varepsilon_{0}} 2 \pi \int_{0}^{\pi} \sin \theta^{\prime} d \theta^{\prime} \int_{0}^{\infty} r^{\prime 2} d r^{\prime} \frac{\rho\left(r^{\prime}\right)}{\left(r^{\prime \prime}\right)^{2}} \cos \theta \tag{1.11}
\end{equation*}
$$

[^161]where $\theta$ and $r "$ are the geometrical parameters marked in Fig. 2. Since they all may be readily expressed via $r^{\prime}$ and $\theta^{\prime}$ using auxiliary parameters $a$ and $h$,
\[

$$
\begin{equation*}
\cos \theta=\frac{r-a}{r^{\prime \prime}}, \quad\left(r^{\prime \prime}\right)^{2}=h^{2}+\left(r-r^{\prime} \cos \theta\right)^{2}, \quad a=r^{\prime} \cos \theta^{\prime}, \quad h=r^{\prime} \sin \theta, \tag{1.12}
\end{equation*}
$$

\]

integral (11) may be eventually reduced to an explicit integral over $r^{\prime}$ and $\theta$. and worked out analytically, but that would require some effort.

For more complex problem, integral (8) may be much more complex, defying an analytical solution. One could argue that with the present-day abundance of computers and numerical algorithm libraries, one can always resort to numerical integration. This argument may be enhanced by the fact that numerical integration is based on the replacement of the integral by a sum, and summation is much more robust to (unavoidable) discretization and rounding errors than the finite-difference schemes typical for the numerical solution of differential equations.

These arguments, however, are only partly justified, since in many cases the numerical approach runs into a problem sometimes called the curse of dimensionality, in which the last word refers to the number of input parameters of the problem to be solved, i.e. the dimensionality of its parameter space. Let us discuss this issue, because it is common for most fields of physics and, more generally, any quantitative science. ${ }^{12}$

If the number of the parameters of a problem is small, the results of its numerical solution may be of the same (and in some sense higher) value than the analytical ones. For example, if a problem has no parameters, and its result is just one number (say, $\pi^{2} / 4$ ), this "analytical" answer hardly carries more information than its numerical form $2.4674011 \ldots$ Now, if a problem has one input parameter (say, a), the result of an analytical approach in most cases may be presented as an analytical function $f(a)$. If the function is really simple, called elementary, with many properties well known (say, $f(a)=\sin a$ ), this function gives us virtually everything we want to know. However, if the function is complicated, you would need to tabulate it numerically for a set of values of parameter $a$ and possibly present the result as a plot. The same results (and the same plot) can be calculated numerically, without using analytics at all. This plot may certainly be very valuable, but since the analytical form has a potential of giving you more information (say, the values of $f(a)$ outside the plot range, or the asymptotic behavior of the function), it is hard to say that the numerics completely beat the analytics here.

Now let us assume that you have more input parameters. For two parameters (say, $a$ and $b$ ), instead of one curve you would need a family of such curves for several (sometimes many) values of $b$. Still, the plots sometimes may fit one page convenient for viewing, so it is still not too bad. Now, if you have three parameters, the full representation of the results may require many pages (maybe a book) full of curves, for four parameters we may speak about several bookshelves, for five parameters something like a library, etc. For large number of parameters, typical for many scientific problems, the number of points in the parameters space grows exponentially, even the volume of calculations necessary for the generation of this data may become impracticable, despite the dirt-cheap CPU time we have now.

Thus, despite the current proliferation of numerical methods in physics, analytical results have an ever-lasting value, and we should try to get them whenever we can. For our current problem of finding electric field generated by a fixed set of electric charges, large help comes from the Gauss law.

[^162]Let us consider a single point charge $q$ inside a smooth, closed surface $A$ (Fig. 3), and calculate product $E_{n} d^{2} r$, where $d^{2} r$ is an infinitesimal element of the surface (which may be well approximated with a plane of that area), and $E_{n}$ is the component of the electric field in that point, normal to that plane.

(b)

Fig. 1.3. Deriving the Gauss law: a point charge $q$ is (a) inside volume $V$ and (b) outside of that volume.

This component may be calculated as $E \cos \theta$, where $\theta$ is the angle between vector $\mathbf{E}$ and the unit vector $\mathbf{n}$ normal to the surface. (Equivalently, $E_{n}$ may be presented as the scalar product E.n.) Now let us notice that the product $\cos \theta d^{2} r$ is nothing more than the area $d^{2} r$ of the projection of $d^{2} r$ onto the plane perpendicular to vector $\mathbf{r}$ connecting charge $q$ with this point of the surface (Fig. 3), because the angle between the planes $d^{2} r^{\prime}$ and $d^{2} r$ is also equal to $\theta$. Using the Coulomb law for $\mathbf{E}$, we get

$$
\begin{equation*}
E_{n} d^{2} r=E \cos \theta d^{2} r=\frac{1}{4 \pi \varepsilon_{0}} \frac{q}{r^{2}} d^{2} r^{\prime} \tag{1.13}
\end{equation*}
$$

But the ratio $d^{2} r^{\prime} / r^{2}$ is nothing more than the elementary solid angle $d \Omega$ under which the areas $d^{2} r^{\prime}$ and $d^{2} r$ are seen from the charge point, so that $E_{n} d^{2} r$ may be presented as just a product of $d \Omega$ by a constant $\left(q / 4 \pi \varepsilon_{0}\right)$. Summing these products over the whole surface, we get

$$
\begin{equation*}
\oint_{S} E_{n} d^{2} r=\frac{q}{4 \pi \varepsilon_{0}} \oint_{S} d \Omega=\frac{q}{\varepsilon_{0}}, \tag{1.14}
\end{equation*}
$$

since the full solid angle equals $4 \pi$. (The integral in the left-hand part of this relation is called the flux of electric field through surface $S$.)

Equation (14) expresses the Gauss law for one point charge. However, it is only valid if the charge is located inside the volume limited by the surface. In order to find the flux created by a charge outside of the volume, we still can use Eq. (13), but to proceed we have to be careful with the signs of the elementary contributions $E_{n} d A$. Let us use the common convention to direct the unit vector $\mathbf{n}$ out of the closed volume we are considering (the so-called outer normal), so that the elementary product $E_{n} d^{2} r$ $=(\mathbf{E} \cdot \mathbf{n}) d^{2} r$ and hence $d \Omega=E_{n} d^{2} r^{\prime} / r^{2}$ is positive if vector $\mathbf{E}$ is pointing out of the volume (like in the example shown in Fig. 3a and the upper-right area in Fig. 3b), and negative in the opposite case (for example, in the lower-left area in Fig. 3b). As the latter figure shows, if the charge is located outside of the volume, for each positive contribution $d \Omega$ there is always equal and opposite contribution to the
integral. As a result, at the integration over the solid angle the positive and negative contributions cancel exactly, so that

$$
\begin{equation*}
\oint_{S} E_{n} d^{2} r=0 . \tag{1.15}
\end{equation*}
$$

The real power of the Gauss law is revealed by its generalization to the case of many charges within volume $V$. Since the calculation of flux is a linear operation, the linear superposition principle (3) means that the flux created by several charges is equal to the (algebraic) sum of individual fluxes from each charge, for which either Eq. (14) or Eq. (15) are valid, depending on the charge position (in or out of the volume). As the result, for the total flux we get:

$$
\begin{equation*}
\oint_{S} E_{n} d^{2} r=\frac{Q_{V}}{\varepsilon_{0}} \equiv \frac{1}{\varepsilon_{0}} \sum_{\mathbf{r}_{j} \in V} q_{j}=\frac{1}{\varepsilon_{0}} \int_{V} \rho\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime} \tag{1.16}
\end{equation*}
$$

where $Q_{V}$ is the net charge inside volume $V$. This is the full version of the Gauss law.
In order to appreciate the problem-solving power of the law, let us return to the problem presented in Fig. 2, i.e. a spherical charge distribution. Due to its symmetry, which had already been discussed above, if we apply Eq. (16) to a sphere of radius $r$, the electric field should be perpendicular to the sphere at each its point (i.e., $E_{n}=E$ ), and its magnitude the same at all points: $E_{n}=E=E(r)$. As a result, the flux calculation is elementary:

$$
\begin{equation*}
\oint E_{n} d^{2} r=4 \pi r^{2} E(r) . \tag{1.17}
\end{equation*}
$$

Now, applying the Gauss law (16), we get:

$$
\begin{equation*}
4 \pi r^{2} E(r)=\frac{1}{\varepsilon_{0}} \int_{r^{\prime}<r} \rho\left(r^{\prime}\right) d^{3} r^{\prime}=\frac{4 \pi}{\varepsilon_{0}} \int_{0}^{r} r^{\prime 2} \rho\left(r^{\prime}\right) d r^{\prime} \tag{1.18}
\end{equation*}
$$

so that, finally,

$$
\begin{equation*}
E(r)=\frac{1}{r^{2} \varepsilon_{0}} \int_{0}^{r} r^{\prime 2} \rho\left(r^{\prime}\right) d r^{\prime}=\frac{1}{4 \pi \varepsilon_{0}} \frac{Q(r)}{r^{2}} \tag{1.19}
\end{equation*}
$$

where $Q(r)$ is the full charge inside the sphere of radius $r$ :

$$
\begin{equation*}
Q(r) \equiv 4 \pi \int_{0}^{r} \rho\left(r^{\prime}\right) r^{\prime 2} d r^{\prime} \tag{1.20}
\end{equation*}
$$

In particular, this formula shows that the field outside of a sphere of a finite radius $R$ is exactly the same as if all its charge $Q=Q(R)$ was concentrated in the sphere's center. (Note that this important result is only valid for any spherically-symmetric charge distribution.) For the field inside the sphere, finding electric field still requires an explicit integration (20), but this 1D integral is much simpler than the 2D integral (11), and in some important cases may be readily worked out analytically. For example, if charge $Q$ is uniformly distributed inside a sphere of radius $R$,

$$
\begin{equation*}
\rho\left(r^{\prime}\right)=\rho=\frac{Q}{V}=\frac{Q}{(4 \pi / 3) R^{3}}, \tag{1.21}
\end{equation*}
$$

the integration is elementary:

$$
\begin{equation*}
E(r)=\frac{\rho}{r^{2} \varepsilon_{0}} \int_{0}^{r} r^{\prime 2} d r^{\prime}=\frac{\rho r}{3 \varepsilon_{0}}=\frac{1}{4 \pi \varepsilon_{0}} \frac{Q r}{R^{3}} . \tag{1.22}
\end{equation*}
$$

We see that in this case the field is growing linearly from the center to the sphere's surface, and only at $r$ $>R$ starts to decrease in agreement with Eq. (19) with constant $Q(r)=Q$. Another important observation is that the results for $r \leq R$ and $r \geq R$ give the same value $\left(Q / 4 \pi \varepsilon_{0} R^{2}\right)$ at the charged sphere's surface, $r=$ $R$, so that the electric field is continuous.

In order to underline the importance of the last fact, let us consider one more elementary but very important example of the Gauss law's application. Let a thin plane sheet (Fig. 4) be charged uniformly, with an areal density $\sigma=$ const (see Footnote 9 above).


Fig. 1.4. Electric field of a charged plane.

In this case, it is fruitful to use the Gauss volume in the form of a planar "pillbox" of thickness $2 z$ (where $z$ is the Cartesian coordinate perpendicular to charged plane) and certain area $A-$ see Fig. 4. Due to the symmetry of the problem, it is evident that the electric field should be: (i) directed along axis $z$, (ii) constant on each of the upper and bottom sides of the pillbox, (iii) equal and opposite on these sides, and (iv) parallel to the side surfaces of the box. As a result, the full electric field flux through the pillbox surface is just $2 A E(\mathrm{z})$, so that the Gauss law (16) yields

$$
\begin{equation*}
2 A E(\mathrm{z})=\frac{1}{\varepsilon_{0}} Q_{A}=\frac{1}{\varepsilon_{0}} \sigma A \tag{1.23}
\end{equation*}
$$

and we get a very simple but important formula

$$
\begin{equation*}
E(z)=\frac{\sigma}{2 \varepsilon_{0}}=\text { const. } \tag{1.24}
\end{equation*}
$$

Notice that, somewhat counter-intuitively, the field magnitude does not depend on the distance from the charged plane. From the point of view of the Coulomb law (5), this result may be explained as follows, the farther the observation point from the plane, the weaker the effect of each elementary charge, $d Q=\sigma d^{2} r$, but the more such elementary charges give contributions to the vertical component of vector $\mathbf{E}$.

Note also that though the magnitude $E \equiv|\mathbf{E}|$ of the electric field is constant, its vertical component $E_{z}$ changes sign at $z=0$ (Fig. 4), experiencing a discontinuity (jump) equal to $\Delta E_{z}=\sigma / \varepsilon_{0}$. This jump disappears if the surface is not charged ( $\sigma=0$ ). This statement remains true in a more general case of finite volume (but not surface!) charge density $\rho$. Returning for a minute to our charged
sphere problem, very close to its surface it may be considered planar, so that the electric field should indeed be continuous, as it is.

Admittedly, the integral form (16) of the Gauss law is immediately useful only for highly symmetrical geometries, like as in the two problems discussed above. However, it may be recast into an alternative, differential form whose field of useful applications is much wider. This form may be obtained from Eq. (16) using the divergence theorem that, according to the vector algebra, is valid for any space-differentiable vector, in particular $\mathbf{E}$, and for any volume $V$ limited by closed surface $S:{ }^{13}$

$$
\begin{equation*}
\oint_{S} E_{n} d^{2} r=\int_{V}(\nabla \cdot \mathbf{E}) d^{3} r, \tag{1.25}
\end{equation*}
$$

where $\nabla$ is the del (or "nabla") operator of spatial differentiation. ${ }^{14}$ Combining Eq. (25) with the Gauss law (16), we get

$$
\begin{equation*}
\int_{V}\left(\nabla \cdot \mathbf{E}-\frac{\rho}{\varepsilon_{0}}\right) d^{3} r=0 \tag{1.26}
\end{equation*}
$$

For a given distribution of electric charge (and hence of the electric field), this equation should be valid for any choice of volume $V$. This can hold only if the function under the integral vanishes at each point, i.e. if ${ }^{15}$

Inhomogeneous Maxwell equation for $E$

$$
\begin{equation*}
\nabla \cdot \mathbf{E}=\frac{\rho}{\varepsilon_{0}} \tag{1.27}
\end{equation*}
$$

Note that in a sharp contrast with the integral form (16), Eq. (26) is local: it relates the electric field divergence to the charge density at the same point. This equation, being the differential form of the Gauss law, is frequently called (the free-space version of) one of Maxwell equations. Another, homogeneous Maxwell equation's "embryo" may be obtained by noticing that curl of point charge's

Homogeneous Maxwell equation
for E field, and hence that of any system of charges, equals zero: ${ }^{16}$

$$
\begin{equation*}
\nabla \times \mathbf{E}=0 \tag{1.28}
\end{equation*}
$$

(We will arrive at two other Maxwell equations, for the magnetic field, in Chapter 5, and then generalize all the equations to their full, time-dependent form by the end of Chapter 6. However, Eq. (27) would stay the same.)

Just to get a better gut feeling of Eq. (27), let us apply it to the same example of a uniformly charged sphere (Fig. 2). The vector algebra tells us that the divergence of a spherically symmetric vector function $\mathbf{E}(\mathbf{r})=E(r) \mathbf{n}_{r}$ may be simply expressed in spherical coordinates: ${ }^{17}$

[^163]\[

$$
\begin{equation*}
\nabla \cdot \mathbf{E}=\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} E\right) . \tag{1.29}
\end{equation*}
$$

\]

As a result, Eq. (27) yields a linear, ordinary differential equation for the function $E(r)$ :

$$
\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} E\right)= \begin{cases}\rho / \varepsilon_{0}, & \text { for } r \leq R  \tag{1.30a}\\ 0, & \text { for } r \geq R\end{cases}
$$

that may be readily integrated on each of the segments:

$$
E(r)=\frac{1}{\varepsilon_{0}} \frac{1}{r^{2}} \times \begin{cases}\rho \int r^{2} d r=\rho r^{3} / 3+C_{1}, & \text { for } r \leq R  \tag{1.30b}\\ C_{2}, & \text { for } r \geq R\end{cases}
$$

In order to determine the integration constant $C_{1}$, we can use boundary condition $E(0)=0$. (It follows from problem's spherical symmetry: in the center of the sphere, electric field has to vanish, because otherwise, where would it be directed?) Constant $C_{2}$ may be found from the continuity condition $E(R-$ $0)=E(R+0)$, which has already been discussed above. As a result, we arrive at our previous results (19) and (22).

We can see that in this particular, highly symmetric case, using the differential form of the Gauss law is more complex than its integral form. (For our second example, shown in Fig. 4, it would be even less natural.) However, Eq. (27) and its generalizations are more convenient for asymmetric charge distributions, and invaluable in the cases where the charge distribution $\rho(\mathbf{r})$ is not known a priori and has to be found in a self-consistent way. (We will start discussing such cases in the next chapter.)

### 1.3. Scalar potential and electric field energy

One more help for solving electrostatics (and more complex) problems may be obtained from the notion of the electrostatic potential, which is just the electrostatic potential energy $U$ of a probe particle, normalized by its charge:

$$
\begin{equation*}
\phi \equiv \frac{U}{q} . \tag{1.31}
\end{equation*}
$$

## Electrostatic potential

As we know from classical mechanics, ${ }^{18}$ the notion of $U$ (and hence $\phi$ ) make sense only for the case of potential forces, for example those depending just on particle's position. Equations (6) and (8) show that, in the static situations, the electric field clearly falls into this category. For such a field, the potential energy may be defined as a scalar function $U(\mathbf{r})$ that allows the force to be calculated as its gradient (with the opposite sign):

$$
\begin{equation*}
\mathbf{F}=-\nabla U . \tag{1.32}
\end{equation*}
$$

Dividing both sides of this equation by the charge of the probe particle, and using Eqs. (5) and (31), we get ${ }^{19}$

[^164]Electrostatic field as a gradient

$$
\begin{equation*}
\mathbf{E}=-\nabla \phi \tag{1.33}
\end{equation*}
$$

In order to calculate the scalar potential, let us start from the simplest case of a single point charge $q$ placed at the origin. For it, the Coulomb law (5) takes a simple form

$$
\begin{equation*}
\mathbf{E}=\frac{1}{4 \pi \varepsilon_{0}} q \frac{\mathbf{r}}{r^{3}}=\frac{1}{4 \pi \varepsilon_{0}} q \frac{\mathbf{n}_{r}}{r^{2}} . \tag{1.34}
\end{equation*}
$$

It is straightforward to check that the last fraction in the right-hand part of this equation is equal to $\nabla(1 / r) .{ }^{20}$ Hence, according to the definition (33), for this particular case

Potential of a point charge

$$
\begin{equation*}
\phi=\frac{1}{4 \pi \varepsilon_{0}} \frac{q}{r} . \tag{1.35}
\end{equation*}
$$

(In the Gaussian units, this result is spectacularly simple: $\phi=q / r$.) Note that we could add an arbitrary constant to this potential (and indeed to any other distribution of $\phi$ discussed below) without changing the force, but it is convenient to define the potential energy to approach zero at infinity.

Before going any further, let us demonstrate how useful the notions of $U$ and $\phi$ are, on a very simple example. Let two similar charges $q$ be launched from afar, with an initial velocity $v_{0} \ll c$ each, straight toward each other (i.e. with the zero impact parameter) - see Fig. 5. Since, according to the Coulomb law, the charges repel each other with increasing force, they will stop at some minimum distance $r_{\text {min }}$ from each other, and than fly back.


Fig. 1.5. Simple problem of electric particle motion.
We could of course find $r_{\text {min }}$ directly from the Coulomb law. However, for that we would need to write the $2^{\text {nd }}$ Newton law for each particle (actually, due to the problem symmetry, they would be similar), then integrate them over time once to find the particle velocity $v$ as a function of distance, and then recover $r_{\min }$ from the requirement $v=0$. The notion of potential allows this problem to be solved in one line. Indeed, in the field of potential forces the system's total energy $E=T+U=T+q \phi$ is conserved. In our non-relativistic case, the kinetic energy $T$ is just $m v^{2} / 2$. Hence, equating the total energy of two particles in the points $r=\infty$ and $r=r_{\text {min }}$, and using Eq. (35) for $\phi$, we get

$$
\begin{equation*}
2 \frac{m v_{0}^{2}}{2}+0=0+\frac{1}{4 \pi \varepsilon_{0}} \frac{q^{2}}{r_{\min }} \tag{1.36}
\end{equation*}
$$

immediately giving us the final answer: $r_{\min }=q^{2} / 4 \pi \varepsilon_{0} m v_{0}{ }^{2}$.
Now let us calculate $\phi$ for an arbitrary configuration of charges. For a single charge in an arbitrary position (say, $\mathbf{r}_{k^{\prime}}$ ), $r$ in Eq. (35) should be evidently replaced for $\left|\mathbf{r}-\mathbf{r}_{k^{\prime}}\right|$. Now, the linear

[^165]superposition principle (3) allows for an easy generalization of this formula to the case of an arbitrary set of discrete charges,
\[

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \sum_{\mathbf{r}_{k^{\prime}} \neq \mathbf{r}} \frac{q_{k^{\prime}}}{\left|\mathbf{r}-\mathbf{r}_{k^{\prime}}\right|} \tag{1.37}
\end{equation*}
$$

\]

Finally, using the same arguments as in Sec. 1, we can use this result to argue that in the case of an arbitrary continuous charge distribution

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int \frac{\rho\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} \tag{1.38}
\end{equation*}
$$

Potential of a charge distribution

Again, the notion of Dirac's delta-function allows to use the last equation for discrete charges as well, so that Eq. (38) may be considered as the general expression for the electrostatic potential.

For most practical calculations, using this expression and then applying Eq. (33) to the result, is preferable to using Eq. (9), because $\phi$ is a scalar, while $\mathbf{E}$ is a 3 D vector - mathematically equivalent to 3 scalars. Still, this approach may lead to technical problems similar to those discussed in Sec. 2. For example, applying it to the spherically-symmetric distribution of charge (Fig. 2), we get integral

$$
\begin{equation*}
\phi=\frac{1}{4 \pi \varepsilon_{0}} 2 \pi \int_{0}^{\pi} \sin \theta^{\prime} d \theta^{\prime} \int_{0}^{\infty} r^{\prime 2} d r^{\prime} \frac{\rho\left(r^{\prime}\right)}{r^{\prime \prime}} \cos \theta, \tag{1.39}
\end{equation*}
$$

which is not much simpler than Eq. (11).
The situation may be much improved by re-casting Eq. (38) into a differential form. For that, it is sufficient to plug the definition of $\phi$, Eq. (33), into Eq. (27):

$$
\begin{equation*}
\nabla \cdot(-\nabla \phi)=\frac{\rho}{\varepsilon_{0}} \tag{1.40}
\end{equation*}
$$

The left-hand part of this equation is nothing more than the Laplace operator of $\phi$ (with the minus sign), so that we get the famous Poisson equation ${ }^{21}$ for the electrostatic potential:

$$
\begin{equation*}
\nabla^{2} \phi=-\frac{\rho}{\varepsilon_{0}} \tag{1.41}
\end{equation*}
$$

Poisson equation for $\phi$
(In the Gaussian units, the Poisson equation looks like $\nabla^{2} \phi=-4 \pi \rho$.) This differential equation is so convenient for applications that even its particular case for $\rho=0$,

$$
\begin{equation*}
\nabla^{2} \phi=0 \tag{1.42}
\end{equation*}
$$

has earned a special name - the Laplace equation. ${ }^{22}$
In order to get a feeling of the Poisson equation as a problem solving tool, let us return to the spherically-symmetric charge distribution (Fig. 2) with a constant charge density $\rho$. Using the

[^166]symmetry, we can present the potential as $\phi(\mathbf{r})=\phi(r)$, and hence use the following simple expression for its Laplace operator: ${ }^{23}$
\[

$$
\begin{equation*}
\nabla^{2} \phi=\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \phi}{d r}\right) \tag{1.43}
\end{equation*}
$$

\]

so that for the points inside the charged sphere $(r \leq R)$ the Poisson equation yields

$$
\begin{equation*}
\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \phi}{d r}\right)=-\frac{\rho}{\varepsilon_{0}}, \quad \text { i.e. } \frac{d}{d r}\left(r^{2} \frac{d \phi}{d r}\right)=-\frac{\rho}{\varepsilon_{0}} r^{2} \tag{1.44}
\end{equation*}
$$

Integrating the last form of the equation over $r$ once, with the natural boundary condition $d \phi /\left.d r\right|_{r=0}=0$ (because of the condition $E(0)=0$, which has been discussed above), we get

$$
\begin{equation*}
\frac{d \phi}{d r}(r)=-\frac{\rho}{r^{2} \varepsilon_{0}} \int_{0}^{r} r^{\prime 2} d r^{\prime}=-\frac{\rho r}{3 \varepsilon_{0}}=-\frac{1}{4 \pi \varepsilon_{0}} \frac{Q r}{R^{3}} . \tag{1.45}
\end{equation*}
$$

Since this derivative is nothing more than $-E(r)$, in this formula we can readily recognize our previous result (22). Now we may like to carry out the second integration to calculate the potential itself:

$$
\begin{equation*}
\phi(r)=-\frac{Q}{4 \pi \varepsilon_{0} R^{3}} \int_{0}^{r} r^{\prime} d r^{\prime}+c_{1}=-\frac{Q r^{2}}{8 \pi \varepsilon_{0} R^{3}}+c_{1} . \tag{1.46}
\end{equation*}
$$

Before making any judgment on the integration constant $c_{1}$, let us solve the Poisson equation (in this case, just the Laplace equation) for the range outside the sphere $(r>R)$ :

$$
\begin{equation*}
\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \phi}{d r}\right)=0 \tag{1.47}
\end{equation*}
$$

Its first integral,

$$
\begin{equation*}
\frac{d \phi}{d r}(r)=\frac{c_{2}}{r^{2}} \tag{1.48}
\end{equation*}
$$

also gives the electric field (with the minus sign). Now using Eq. (1.45) and requiring the field to be continuous at $r=R$, we get

$$
\begin{equation*}
\frac{c_{2}}{R^{2}}=-\frac{Q}{4 \pi \varepsilon_{0} R^{2}}, \text { i.e. } \frac{d \phi}{d r}(r)=-\frac{Q}{4 \pi \varepsilon_{0} r^{2}} \tag{1.49}
\end{equation*}
$$

in an evident agreement with Eq. (19). Integrating this result again,

$$
\begin{equation*}
\phi(r)=-\frac{Q}{4 \pi \varepsilon_{0}} \int \frac{d r}{r^{2}}=\frac{Q}{4 \pi \varepsilon_{0} r}+c_{3}, \quad \text { for } r>R \tag{1.50}
\end{equation*}
$$

we can select $c_{3}=0$, so that $\phi(\infty)=0$, in accordance with the usual (though not compulsory) convention. Now we can finally determine constant $c_{1}$ in Eq. (46) by requiring that this equation and Eq. (50) give the same value of $\phi$ at the boundary $r=R$. (According to Eq. (33), if the potential had a jump, the electric field at that point would be infinite.) The final answer may be presented as

[^167]\[

$$
\begin{equation*}
\phi(r)=\frac{Q}{4 \pi \varepsilon_{0} R}\left[\frac{R^{2}-r^{2}}{2 R^{2}}+1\right], \quad \text { for } r \leq R . \tag{1.51}
\end{equation*}
$$

\]

We see that using the Poisson equation to find the electrostatic potential distribution for highly symmetric problems may be more cumbersome than directly finding the electric field - say, from the Gauss law. However, we will repeatedly see below that if the electric charge distribution is not fixed in advance, using Eq. (41) may be the only practicable way to proceed.

Returning now to the general theory of electrostatic phenomena, let us calculate potential energy $U$ of an arbitrary system of electric charges $q_{k}$. Despite the apparently straightforward relation (31) between $U$ and $\phi$, the calculation is a little bit more complex than one might think. Indeed, let us rewrite Eqs. (32), (33) for a single charge in the integral form:

$$
\begin{equation*}
U(\mathbf{r})=-\int_{\mathbf{r}_{0}}^{\mathbf{r}} \mathbf{F}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime}, \quad \text { i.e. } \quad \phi(\mathbf{r})=-\int_{\mathbf{r}_{0}}^{\mathbf{r}} \mathbf{E}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime} \tag{1.52}
\end{equation*}
$$

where $\mathbf{r}_{0}$ is some reference point. These integrals reflect the fact that the potential energy is just the work necessary to move the charge from point $\mathbf{r}_{0}$ to point $\mathbf{r}$, and clearly depend on whether the charge motion affects force $\mathbf{F}$ (and hence electric field $\mathbf{E}$ ) or not. If it does not, i.e. if the field is produced by some external charges (such fields $\mathbf{E}_{\text {ext }}$ are also called external), everything is simple indeed: using the linearity of relations (31) and (32), for the total potential energy we may write

$$
\begin{equation*}
U_{\text {ext }}=\sum_{k} q_{k} \phi_{\text {ext }}\left(\mathbf{r}_{k}\right), \quad \text { where } \phi_{\text {ext }}(\mathbf{r}) \equiv-\int_{\mathbf{r}_{0}}^{\mathbf{r}} E_{\text {ext }}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime} . \tag{1.53}
\end{equation*}
$$

Repeating the argumentation that has led us to Eq. (9), we see that for a continuously distributed charge, this sum turns into an integral:

$$
\begin{equation*}
U_{\mathrm{ext}}=\int \rho(\mathbf{r}) \phi_{\mathrm{ext}}(\mathbf{r}) d^{3} r \tag{1.54}
\end{equation*}
$$

However, if the electric field is created by the charges whose energy we are calculating, the situation is somewhat different. To calculate $U$ for this case, let us use the fact its independence of the way the charge configuration has been created, considering the following process. First, let us move one charged particle (say, $q_{1}$ ) from infinity to an arbitrary point of space ( $\mathbf{r}_{1}$ ) in the absence of other charges. During the motion the particle does not experience any force (again, the charge does not interact with itself!), so that its potential energy is the same as at infinity (with the standard choice of the arbitrary constant, zero): $U_{1}=0$. Now let us fix the position of that charge, and move another charge $\left(q_{2}\right)$ from infinity to point $\mathbf{r}_{2}$ (with velocity $v \ll c$, in order to avoid any magnetic field effects, to be discussed in Chapter 5.) This particle, during its motion, does experience the Coulomb force exerted by fixed $q_{1}$, so that according to Eq. (31), its contribution to the final potential energy

$$
\begin{equation*}
U_{2}=q_{2} \phi_{1}\left(\mathbf{r}_{2}\right) . \tag{1.55}
\end{equation*}
$$

Since the first particle was not moving during this process, the total potential energy $U$ of the system is equal to just $U_{2}$. This is exactly the equality used for writing the right-hand part of Eq. (36). (Prescribing a similar energy to charge $q_{1}$ as well would constitute an error - a very popular one, and hence having a special name, double-counting.)

Now, fixing the first two charges in points $\mathbf{r}_{1}$ and $\mathbf{r}_{2}$, respectively, and bringing in the third charge from infinity, we increment the potential energy by

$$
\begin{equation*}
U_{3}=q_{3}\left[\phi_{1}\left(\mathbf{r}_{3}\right)+\phi_{2}\left(\mathbf{r}_{3}\right)\right] \tag{1.56}
\end{equation*}
$$

I believe that at this stage it is already clear how to generalize this result to the contribution from an arbitrary ( $k$-th) charge being moved in (Fig. 6):

$$
\begin{equation*}
U_{k}=q_{k}\left[\phi_{1}\left(\mathbf{r}_{k}\right)+\phi_{2}\left(\mathbf{r}_{k}\right)+\phi_{3}\left(\mathbf{r}_{k}\right)+\ldots+\phi_{k-1}\left(\mathbf{r}_{k}\right)\right]=q_{k} \sum_{k^{\prime}<k} \phi_{k^{\prime}}\left(\mathbf{r}_{k}\right) . \tag{1.57}
\end{equation*}
$$

(Notice condition $k^{\prime}<k$, which suppresses erroneous double-counting.)


Fig. 1.6. Deriving the potential energy of a system of electric charges.

Now, summing up all the increments, for the total electrostatic energy of the system we get:

$$
\begin{equation*}
U=\sum_{k} U_{k}=\sum_{\substack{k, k^{\prime} \\\left(k^{\prime} k\right)}} q_{k} \phi_{k^{\prime}}\left(\mathbf{r}_{k}\right) . \tag{1.58}
\end{equation*}
$$

This is our final result in its generic form; it is so important that is worthy of rewriting it in two other forms. First, for its generalization to the continuous charge distribution, we may use Eq. (35) to present Eq. (58) in a more symmetric form:

$$
\begin{equation*}
U=\frac{1}{4 \pi \varepsilon_{0}} \sum_{\substack{k, k^{\prime} \\\left(k^{\prime}<k\right)}} \frac{q_{k} q_{k^{\prime}}}{\left|\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right|} \tag{1.59}
\end{equation*}
$$

The expression under the sum is evidently symmetric with respect to the index swap, so that it may be rewritten in a fully symmetric form,

$$
\begin{equation*}
U=\frac{1}{4 \pi \varepsilon_{0}} \frac{1}{2} \sum_{\substack{k^{\prime}, k \\\left(k^{\prime} \neq k\right)}} \frac{q_{k} q_{k^{\prime}}}{\left|\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right|}, \tag{1.60}
\end{equation*}
$$

which is now easily generalized to the continuous case:

$$
\begin{equation*}
U=\frac{1}{4 \pi \varepsilon_{0}} \frac{1}{2} \int d^{3} r \int d^{3} r^{\prime} \frac{\rho(\mathbf{r}) \rho\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \tag{1.61}
\end{equation*}
$$

(As before, in this case the restriction expressed in the discrete charge case as $k \neq k$ ' is not important, because if the charge density is a continuous function, integral (61) does not diverge at point $\mathbf{r}=\mathbf{r}^{\prime}$.)

To present this result in one more form, let us notice that according to Eq. (38), the integral over $r$ ' in Eq. (61), divided by $4 \pi \varepsilon_{0}$, is just the full electrostatic potential at point $\mathbf{r}$, and hence

$$
\begin{equation*}
U=\frac{1}{2} \int \rho(\mathbf{r}) \phi(\mathbf{r}) d^{3} r . \tag{1.62}
\end{equation*}
$$

For the discrete charge case, this result becomes

$$
\begin{equation*}
U=\frac{1}{2} \sum_{k} q_{k} \phi\left(\mathbf{r}_{k}\right), \tag{1.63}
\end{equation*}
$$

but now it is important to remember that the "full" potential's value $\phi\left(\mathbf{r}_{k}\right)$ should exclude the (infinite) contribution of charge $k$ itself. Comparing the last two formulas with Eqs. (52) and (53), we see that the electrostatic energy of charge interaction, as expressed via the charge-potential product, is twice less than that of charge energy in a fixed ("external") field. This is evidently the result of the self-consistent build-up of the electric field as the charge system is being formed. ${ }^{24}$

Now comes an important conceptual question: can we locate this interaction energy in space? Expressions (60)-(63) seem to imply that contributions to $U$ come only from the regions where electric charges are located. However, one of the beautiful features of physics is that sometimes completely different interpretations of the same mathematical result are possible. In order to get an alternative view at our current result, let us write Eq. (62) for a volume $V$ so large that the electric field on the limiting surface $A$ is negligible, and plug into it the charge density expressed from the Poisson equation (41):

$$
\begin{equation*}
U=-\frac{\varepsilon_{0}}{2} \int_{V} \phi \nabla^{2} \phi d^{3} r . \tag{1.64}
\end{equation*}
$$

This expression may be integrated by parts as ${ }^{25}$

$$
\begin{equation*}
U=-\frac{\varepsilon_{0}}{2}\left[\oint_{A} \phi(\nabla \phi)_{n} d^{2} r-\int_{V}(\nabla \phi)^{2} d^{3} r\right] . \tag{1.65}
\end{equation*}
$$

According to our condition of negligible field $\mathbf{E}=-\nabla \phi$ on the surface, the first integral vanishes, and we get a very important formula

$$
\begin{equation*}
U=\frac{\varepsilon_{0}}{2} \int(\nabla \phi)^{2} d^{3} r=\frac{\varepsilon_{0}}{2} \int E^{2} d^{3} r . \tag{1.66}
\end{equation*}
$$

This result certainly invites an interpretation very much different than Eq. (62): it is natural to represent it in the following form:

$$
\begin{equation*}
U=\int u(\mathbf{r}) d^{3} r, \quad \text { with } u(\mathbf{r}) \equiv \frac{\varepsilon_{0}}{2} E^{2}(\mathbf{r}), \tag{1.67}
\end{equation*}
$$

Electric
field energy

[^168]and interpret $u(\mathbf{r})$ as the spatial density of the electric field energy, ${ }^{26}$ which is continuously distributed over all the space where the field exists - rather than just its part where the charges are located.

Let us have a look how these two alternative pictures work for our testbed problem, a uniformly charged sphere. If we start from Eq. (62), we may limit integration by the sphere volume ( $0 \leq r \leq R$ ) where $\rho \neq 0$. Using Eq. (51), and the spherical symmetry of the problem ( $d^{3} r=4 \pi r^{2} d r$ ), we get

$$
\begin{equation*}
U=\frac{1}{2} 4 \pi \int_{0}^{R} \rho \phi r^{2} d r=\frac{1}{2} 4 \pi \rho \frac{Q}{4 \pi \varepsilon_{0} R} \int_{0}^{R}\left[\frac{R^{2}-r^{2}}{2 R^{2}}+1\right] r^{2} d r=\frac{6}{5} \frac{1}{4 \pi \varepsilon_{0} R} \frac{Q^{2}}{2} . \tag{1.68}
\end{equation*}
$$

On the other hand, if we use Eq. (67), we need to integrate energy everywhere, i.e. both inside and outside of the sphere:

$$
\begin{equation*}
U=\frac{\varepsilon_{0}}{2} 4 \pi\left[\int_{0}^{R} E^{2} r^{2} d r+\int_{R}^{\infty} E^{2} r^{2} d r\right] \tag{1.69}
\end{equation*}
$$

Using Eqs. (19) and (22) for, respectively, the external and internal regions, we get

$$
\begin{equation*}
U=\frac{\varepsilon_{0}}{2} 4 \pi\left[\int_{0}^{R}\left(\frac{Q r}{4 \pi \varepsilon_{0}}\right)^{2} r^{2} d r+\int_{R}^{\infty}\left(\frac{Q}{4 \pi \varepsilon_{0} r^{2}}\right)^{2} r^{2} d r\right]=\left(\frac{1}{5}+1\right) \frac{1}{4 \pi \varepsilon_{0} R} \frac{Q^{2}}{2} . \tag{1.70}
\end{equation*}
$$

This is (fortunately :-) the same answer as given by Eq. (68), but to some extent it is more informative because it shows how exactly the electric field energy is distributed between the interior and exterior of the charged sphere. ${ }^{27}$

We see that, as we could expect, within the realm of electrostatics, Eqs. (62) and (67) are equivalent. However, when we examine electrodynamics in Chapter 6 and on, we will see that the latter equation is more general, and that it is more adequate to associate energy with the field itself rather than its sources - in our current case, electric charges.

### 1.4. Exercise problems

1.1. Calculate the electric field created by a thin, long, straight filament, electrically charged with a constant linear density $\lambda$, using two approaches:
(i) directly from the Coulomb law, and
(ii) using the Gauss law.
1.2. Two thin, straight parallel filaments, separated by distance $\rho$, carry equal and opposite uniformly distributed charges with linear density $\lambda$ - see Fig. on the right. Calculate the electrostatic force (per unit length) of the Coulomb


[^169]interaction between the wires. Compare the result with the Coulomb law for the force between the point charges, and interpret their difference.
1.3. A sphere of radius $R$, whose volume had been charged with a constant density $\rho$, is split with a very narrow, planar gap passing through its center. Find the Coulomb force between the resulting two hemispheres.
1.4. Calculate the distribution of the electrostatic potential created by a straight, thin filament of finite length $2 l$, charged with a constant linear density $\lambda$, and explore the result in the limits of very small and very large distances from the filament.
1.5. A thin plane sheet, perhaps of an irregular shape, carries an electric charge distributed over the sheet with a constant areal density $\sigma$.
(i) Express the electric field component normal to the plane, at a certain distance from it, via the solid angle $\Omega$ at which the sheet is visible from the observation point.
(ii) Use the result to calculate the field in the center of a cube, with one face charged with constant density $\sigma$.
1.6. Can one create electrostatic fields with the Cartesian components proportional to the following products of Cartesian coordinates $\{x, y, z\}$,
(i) $\{y z, x z, x y\}$,
(ii) $\{x y, x y, y z\}$,
in a finite region of space?
1.7. Distant sources have been used to create different electric fields on two sides of a wide and thin metallic membrane with a round hole of radius $R$ in it - see Fig. on the right. Besides the local perturbation created by the hole, the fields are uniform:
\[

\left.E\right|_{r \gg R}=\mathbf{n}_{z} \times $$
\begin{cases}E_{1}, & \text { at } z<0, \\ E_{2}, & \text { at } z>0 .\end{cases}
$$
\]

Prove that the system may serve as an electrostatic lens for charged particles flying along axis $z$, at distances $\rho \ll R$ from it, and calculate the focal distance $f$ of the lens. Spell out the
 conditions of validity of your result.
1.8. By direct calculation, find the average electric potential of the spherical surface of radius $R$, created by a point charge $q$ located at distance $r>R$ from the sphere's center. Use the result to prove the following general mean value theorem: the electric potential at any point is always equal to its average value on any spherical surface with the center at that point, and containing no electric charges inside it.
1.9. Calculate the electrostatic energy per unit area of the system of two thin, parallel planes with equal and opposite charges of a constant areal density $\sigma$, separated by distance $d$ - see Fig. on the right.

1.10. The system analyzed in the previous problem (two thin, parallel, oppositely charged planes) is now placed into an external, uniform, normal electric field $E_{\text {ext }}=\sigma / \varepsilon_{0}-$ see Fig. on the right. Find the forces (per unit area) acting on each plane, by two methods:
(i) directly from the electric field distribution, and
(ii) from the potential energy of the system.

1.11. A thin spherical shell of radius $R$, which had been charged with a constant areal density $\sigma$, is split into two equal halves by a very narrow, planar cut passing through sphere's center. Calculate the force of electrostatic repulsion between the resulting hemispheric shells.
1.12. Two similar thin, circular, coaxial disks of radius $R$, separated by distance $2 d$, are uniformly charged with equal and opposite areal densities $\pm \sigma$ - see Fig. on the right. Calculate and sketch the distribution of the electrostatic potential and the electric field of the disks along their common axis.

1.13. In a certain reference frame, the electrostatic potential created by some electric charge distribution, is

$$
\phi(\mathbf{r})=C\left(\frac{1}{r}+\frac{1}{2 r_{0}}\right) \exp \left\{-\frac{r}{r_{0}}\right\},
$$

where $C$ and $r_{0}$ are constants, and $r \equiv|\mathbf{r}|$ is the distance from the origin. Calculate the charge distribution in space.
1.14. A thin flat sheet, cut in a form of a rectangle of size $a \times b$, is electrically charged with a constant areal density $\sigma$. Without an explicit calculation of the spatial distribution $\phi(\mathbf{r})$ of the electrostatic potential induced by this charge, find the ratio of its values at the center and at the corners of the rectangle.

Hint: Consider partitioning the rectangle into several similar parts and using the linear superposition principle.
1.15. Explore the relation between the Laplace equation (42) and the condition of minimum of the electrostatic field energy (67).
1.16. Calculate the energy of electrostatic interaction of two spheres, of radii $R_{1}$ and $R_{2}$, each with a spherically-symmetric charge distribution, separated by distance $d>R_{1}+R_{2}$.
1.17. Prove the following reciprocity theorem of electrostatics: ${ }^{28}$ if two spatially-confined charge distributions $\rho_{1}(\mathbf{r})$ and $\rho_{2}(\mathbf{r})$ create respective distributions $\phi_{1}(\mathbf{r})$ and $\phi_{2}(\mathbf{r})$ of the electrostatic potential, then

$$
\int \rho_{1}(\mathbf{r}) \phi_{2}(\mathbf{r}) d^{3} r=\int \rho_{2}(\mathbf{r}) \phi_{1}(\mathbf{r}) d^{3} r
$$

Hint: Consider integral $\int \mathbf{E}_{1} \cdot \mathbf{E}_{2} d^{3} r$.

[^170]
## Chapter 2. Charges and Conductors

In this chapter I will start addressing the (very common) situations when the electric charge distribution in space is not known a priori, but rather should be calculated in a self-consistent way together with the electric field it creates. The simplest situations of this kind involve conductors, and lead to the so-called boundary problems in which partial differential equations are solved with appropriate boundary conditions. Such problems are also broadly used in other parts of electrodynamics (and indeed in other fields of physics as well), so that following tradition, I will use this chapter's material as a playground for a discussion of various methods of boundary problem solution, and the special functions most frequently encountered on this way.

### 2.1. Electric field screening

The basic principles of electrostatics outlined in Chapter 1 present the conceptually full solution for the problem of finding electric field (and hence Coulomb forces) induced by a charge distribution, for example, charge density $\rho(\mathbf{r})$. However, in most practical situation this function is not known but should be found self-consistently with the field. The conceptually simplest case of this type arises when certain point charges $q_{k}$ are placed near a surface of a good conductor, e.g., a metal: the electric field of these charges induces additional charges at conductor's surface, which also contribute to the field. Another important type of problems are those without space-positioned charges at all; here only the total charges of the involved conductors are fixed, but their spatial distribution inside each conductor has to be found. The full solution of such problems, of course, should satisfy Eq. (1.5) for the total field and total set of charges.

To approach the problems, I need to discuss, if only very briefly, ${ }^{1}$ the relevant physics of conductors. In the simplest macroscopic model, conductors are treated as materials having internal charged particles (e.g., electrons in metals) that are free to move under the effect of force - in particular, the force $\mathbf{F}=q \mathbf{E}$ exerted by electric field $\mathbf{E}$. In electrostatics (which specifically excludes the case dc current, to be discussed in Chapter 4 below), there should be no such motion, so that everywhere inside the conductor the electric field should vanish:

$$
\begin{equation*}
\mathbf{E}=0 \tag{2.1a}
\end{equation*}
$$ electrostatics

This is the electric field screening ${ }^{2}$ effect. According to Eq. (1.33), this condition may be rewritten in another, frequently more convenient form:

$$
\begin{equation*}
\phi=\text { const } ; \tag{2.1b}
\end{equation*}
$$

note, however, that if a problem includes several unconnected conductors, the constant in Eq. (1b) may be different for each of them.

[^171]Now let us examine what we can say about the electric field outside a conductor, within the same macroscopic model. At close proximity, any smooth surface (in our case that of a conductor) looks planar. Let us integrate Eq. (1.28) over a narrow ( $d \ll l$ ) rectangular loop $C$ encircling a part of such plane conductor's surface (see the dashed line in Fig. 1), and apply to the electric field the well-known vector algebra equality - the Stokes theorem ${ }^{3}$

$$
\begin{equation*}
\oint_{S}(\nabla \times \mathbf{E})_{n} d^{2} r=\oint_{C} \mathbf{E} \cdot d \mathbf{r}, \tag{2.2}
\end{equation*}
$$

where $S$ is the surface limited by contour $C$, in our case dominated by two straight lines of length $l$. This means that if $l$ is much smaller that the characteristic scale of field change, the right-hand part of Eq. (2) equals $\left[\left(E_{\tau}\right)_{\text {in }}-\left(E_{\tau}\right)_{\text {out }}\right] l$, where $E_{\tau}$ is field's component parallel to the surface. On the other hand, according to Eq. (1.28), the left-hand side of Eq. (2) equals zero. Hence, $E_{\tau}$ should be continuous at the surface, and in order to satisfy Eq. (1a) inside the conductor, immediately outside it, $E_{\tau}=0$ as well.


Fig. 2.1. Electric field near conductor's surface:
$E_{\tau}=0, E_{n}=\sigma / \varepsilon_{0}$.

Hence, the field just outside the conductor has be normal to its surface. In order to find this normal field, let us apply the Gauss law (1.16) to a plane pillbox of area $A$, similar to the one discussed in Sec. 1.2 - see Fig. 1.4. Due to Eq. (1), the total electric flux through the pillbox walls is now $\left(E_{n}\right)_{\text {out }} A$, so that for this surface field we get

$$
\begin{equation*}
\sigma=\varepsilon_{0}\left(E_{n}\right)_{\text {out }}=-\varepsilon_{0}(\nabla \phi)_{n} \equiv-\varepsilon_{0} \frac{\partial \phi}{\partial n} \tag{2.3}
\end{equation*}
$$

Surface charge density
where $\sigma$ is the areal density of conductor's surface charge. So, the normal component of the field is related to the surface charge density by the universal relation (3).

For the electrostatic potential the macroscopic model provides an even more simple result. Indeed, applying the latter of integrals (1.52) to a short path $d$ across the surface normal to it, we see that since $E_{n}$ is finite, the potential change $\Delta \phi$ vanishes as $d \rightarrow 0$. Hence Eq. (1b) is also valid for potential's value immediately outside conductor's surface.

Before starting to use the macroscopic model for solution of particular problems of electrostatics, let us briefly discuss its limitations. Since the argumentation leading to Eq. (3) is valid for any thickness $d$ of the Gauss pillbox, within the macroscopic model, the surface charge is located within an infinitely

[^172]thin surface layer. This is of course impossible physically: for one, this would require an infinite volume density $\rho$ of charge. In reality the charged layer (and hence the region of electric field's crossover from the finite value (3) to zero) has a nonvanishing thickness $\lambda$. At least three effects contribute to $\lambda$ :
(i) Atomic structure of matter. Within each atom, the electric field does exist and is highly nonuniform. Thus Eq. (1) is valid only for the spatial average of the field in a conductor, and cannot be taken seriously on the atomic scale $a_{0} \sim 10^{-10} \mathrm{~m} .{ }^{4}$
(ii) Thermal excitation. In conductor's bulk, the number of protons of atomic nuclei ( $n$ ) and electrons $\left(n_{e}\right)$ and per unit volume are balanced, so that the net charge density, $\rho=e\left(n-n_{e}\right)$, vanishes. ${ }^{5}$ However, if an external electric field penetrates a conductor, electrons can shift in or out of its affected part, depending on the field addition to their potential energy, $\Delta U=q_{e} \phi=-e \phi$. (Here the arbitrary constant in $\phi$ is chosen to give $\phi=0$ inside the conductor.) In classical statistics, this change is described by the Boltzmann distribution: ${ }^{6}$
\[

$$
\begin{equation*}
n_{e}(\mathbf{r})=n \exp \left\{-\frac{U(\mathbf{r})}{k_{\mathrm{B}} T}\right\}, \tag{2.4}
\end{equation*}
$$

\]

where $k_{\mathrm{B}} \approx 1.38 \times 10^{-23} \mathrm{~J} / \mathrm{K}$ is the Boltzmann constant, and $T$ is temperature in SI units (kelvins). As a result, the net charge density is

$$
\begin{equation*}
\rho(\mathbf{r})=e n\left(1-\exp \left\{\frac{e \phi(\mathbf{r})}{k_{\mathrm{B}} T}\right\}\right) . \tag{2.5}
\end{equation*}
$$

If the field did not move the atomic nuclei at all, we could plug the last formula directly into the Poisson equation (1.49). Actually, the penetrating electric field shifts the average charge of the nuclei as well. As will be discusses in the next chapter, this results in the reduction of the electric field by a media-specific dimensionless factor $\varepsilon_{r}$ (typically not too different from 1), called the dielectric constant. As a result, the Poisson equation takes the form, ${ }^{7}$

$$
\begin{equation*}
\frac{d^{2} \phi}{d z^{2}}=-\frac{\rho}{\varepsilon_{r} \varepsilon_{0}}=\frac{e n}{\varepsilon_{r} \varepsilon_{0}}\left(\exp \left\{\frac{e \phi}{k_{\mathrm{B}} T}\right\}-1\right), \tag{2.6}
\end{equation*}
$$

where we have taken advantage of the 1D geometry of the system to simplify the Laplace operator, with axis $z$ normal to the surface. Even with this simplification, Eq. (6) is a nonlinear differential equation allowing an analytical but rather bulky solution. Since our current goal is just to estimate of the field penetration depth $\lambda$, let us simplify the equation further by considering the low-field limit: $e|\phi| \sim e|E| \lambda$ $\ll k_{\mathrm{B}} T$. In this limit we can extend the exponent into the Taylor series, and limit ourselves to the two leading terms (of which the first one cancels with the unity). As a result, Eq. (6) becomes linear,

$$
\begin{equation*}
\frac{d^{2} \phi}{d z^{2}}=\frac{e n}{\varepsilon \varepsilon_{0}} \frac{e \phi}{k_{\mathrm{B}} T}, \quad \text { i.e. } \frac{d^{2} \phi}{d z^{2}}=\frac{1}{\lambda^{2}} \phi \tag{2.7}
\end{equation*}
$$

[^173]where constant $\lambda$ in this case is equal to the so-called Debye screening length $\lambda_{\mathrm{D}}$, defined by relation
\[

$$
\begin{equation*}
\lambda_{\mathrm{D}}^{2} \equiv \frac{\varepsilon_{r} \varepsilon_{0} k_{\mathrm{B}} T}{e^{2} n} . \tag{2.8}
\end{equation*}
$$

\]

Debye screening length

Equation (7) is easy to solve: it describes an exponential decrease of the electric potential, with the characteristic length $\lambda_{\mathrm{D}}: \phi \propto \exp \left\{-z / \lambda_{\mathrm{D}}\right\}$. Plugging in the fundamental constants $\varepsilon_{0}, e$, and $k_{\mathrm{B}}$, we get the following estimate: $\lambda_{\mathrm{D}}[\mathrm{m}] \approx 70\left(\varepsilon_{r} T[\mathrm{~K}] / h\left[\mathrm{~m}^{-3}\right]\right)^{1 / 2}$. According to this formula, in semiconductors at room temperature, the Debye length may be rather substantial. For example, in silicon ( $\varepsilon_{r} \approx 12$ ) doped to the charge carrier concentration $n=3 \times 10^{24} \mathrm{~m}^{-3}$ (the value typical for modern integrated circuits), ${ }^{8} \lambda_{\mathrm{D}} \approx 2$ nm , still well above the atomic size scale $a_{0}$. However, for typical good metals ( $n \sim 10^{28} \mathrm{~m}^{-3}, \varepsilon_{r} \sim 10$ ) the same formula gives an estimate $\lambda_{\mathrm{D}} \sim 4 \times 10^{-11} \mathrm{~m}$, less than $a_{0}$. In this case Eq. (8) should not be taken too literally, because it is based on the assumption of continuous charge distribution.
(iii) Quantum statistics. Actually, the last estimate is not valid for good metals (and highly doped semiconductors) for one more reason: their free electrons obey quantum (Fermi-Dirac) statistics rather that the Boltzmann distribution (4). ${ }^{9}$ As a result, at all realistic temperatures they form a degenerate quantum gas, occupying all available energy states below certain level $\varepsilon_{\mathrm{F}} \gg k_{\mathrm{B}} T$ called the Fermi energy. In these conditions, the screening of relatively low electric field ${ }^{10}$ may be described by replacing Eq. (5) with

$$
\begin{equation*}
\rho=e\left(n-n_{e}\right)=-e g\left(\varepsilon_{\mathrm{F}}\right)(-U)=-e^{2} g\left(\varepsilon_{\mathrm{F}}\right) \phi, \tag{2.9}
\end{equation*}
$$

where $g(\mathcal{\varepsilon})$ is the density of quantum states (per unit volume) at electron's energy $\varepsilon$. At the Fermi surface, the density is of the order of $n / \mathcal{E}_{\mathrm{F}} .{ }^{11}$ As a result, we again get the second of Eqs. (7), but with a different characteristic scale $\lambda$, defined by the following relation:

$$
\begin{equation*}
\lambda_{\mathrm{TF}}^{2} \equiv \frac{\varepsilon_{r} \varepsilon_{0}}{e^{2} g\left(\varepsilon_{\mathrm{F}}\right)} \sim \frac{\varepsilon_{r} \varepsilon_{0} \varepsilon_{\mathrm{F}}}{e^{2} n} \tag{2.10}
\end{equation*}
$$

and called the Thomas-Fermi screening length. Since for most good metals, $n$ is of the order of $10^{29} \mathrm{~m}^{-3}$, and $\varepsilon_{\mathrm{F}}$ is of the order of 10 eV , Eq. (10) typically gives $\lambda_{\mathrm{TF}}$ close to a few $a_{0}$, and makes the ThomasFermi screening theory valid at least semi-quantitatively.

To summarize, the electric field penetration into good conductors is limited to a depth $\lambda$ ranging from fractions of a nanometer to a few nanometers, so that for problems with the characteristic size much larger than that scale, the macroscopic boundary conditions (1) give a very good accuracy, and we will use them in the rest of this chapter. However, the reader should remember that in some situations

[^174]involving semiconductors, as well as at nanoscale experiments with metals, the electric field penetration effect should be taken into account.

### 2.2. Capacitance

Let us start with systems consisting of charged conductors alone. Our goal here is calculating the distributions of electric field $\mathbf{E}$ and potential $\phi$ in space, and the distribution of the surface charge density $\sigma$ over the conductor surfaces. However, before doing that for particular situations, let us see if there are any integral measures of these distributions, that should be our primary focus.

The simplest case is of course a single conductor in the otherwise free space. According to Eq. (1), all its volume should have a constant electrostatic potential $\phi$, evidently providing one convenient global measure of the situation. Another integral measure is evidently provided by the total charge

$$
\begin{equation*}
Q \equiv \int_{V} \rho d^{3} r=\oint_{S} \sigma d^{2} r \tag{2.11}
\end{equation*}
$$

where the latter integral is extended over the whole surface $S$ of the conductor. In the general case, what we can tell about the relation between $Q$ and $\phi$ ? At $Q=0$, there is no electric field in the system, and it is natural (though not necessary) to select the arbitrary constant in the electrostatic potential to have $\phi=0$. Then, if the conductor is charged with a finite $Q$, according to the Coulomb law, the electric field in any point of space is proportional to $Q$. Hence the electrostatic potential everywhere, including its value $\phi$ on the conductor, is also proportional to $Q$ :

$$
\begin{equation*}
\phi=p Q . \tag{2.12}
\end{equation*}
$$

The proportionality coefficient $p$, that depends on the conductor size and shape but not on $Q$, is called the reciprocal capacitance (or, not too often, "electrical elastance"). Usually, Eq. (12) is rewritten in a different form,

Selfcapacitance

$$
\begin{equation*}
Q=C \phi, \quad C \equiv \frac{1}{p} \tag{2.13}
\end{equation*}
$$

where $C$ is called self-capacitance. (Frequently, $C$ is called just capacitance, but we will soon see that for more complex situations the latter term may be too ambiguous.)

Before going to calculation of $C$, let us have a look at the electrostatic energy of a single conductor. In order to calculate it, of the several equations discussed in Chapter 1, Eq. (1.63) is most convenient, because all elementary charges $q_{k}$ are now parts of the conductor surface charge, and hence sit at the same potential $\phi$. As a result, the equation becomes very simple:

$$
\begin{equation*}
U=\frac{1}{2} \phi \sum_{k} q_{k}=\frac{1}{2} \phi Q . \tag{2.14}
\end{equation*}
$$

Moreover, using the linear relation (13), the same result may be re-written in two more forms:

> Electro-
> static energy

$$
U=\frac{Q^{2}}{2 C}=\frac{C}{2} \phi^{2}
$$

We will discuss several ways to calculate $C$ in the next sections, and right now will have a quick look at just the simplest example for which we have calculated everything necessary in the previous
chapter: a conducting sphere of radius $R$. Indeed, we already know the electric field distribution: according to Eq. (1), $E=0$ inside the sphere, while Eq. (1.19), with $Q(r)=Q$, describes the field distribution outside it. Moreover, since the latter formula is exactly the same as for the point charge placed in the sphere's center, the potential distribution in space can be obtained from Eq. (1.35) by replacing $q$ with sphere's full charge $Q$. Hence, on the surface of the sphere (and, according to Eq. (2), through its interior),

$$
\begin{equation*}
\phi=\frac{1}{4 \pi \varepsilon_{0}} \frac{Q}{R} . \tag{2.16}
\end{equation*}
$$

Comparing this result with the definition (13), for the self-capacitance we obtain ${ }^{12}$

$$
\begin{equation*}
C=4 \pi \varepsilon_{0} R=2 \pi \varepsilon_{0} D, \quad D \equiv 2 R . \tag{2.17}
\end{equation*}
$$

This formula, which should be well familiar to the reader, is convenient to get some feeling of how large the SI unit of capacitance ( 1 farad, abbreviated as F) is: the self-capacitance of Earth ( $R_{\mathrm{E}} \approx$ $6.34 \times 10^{6} \mathrm{~m}$ ) is below 1 mF ! Another important note is that while Eq. (17) is not exactly valid for a conductor of arbitrary shape, it implies an important estimate

$$
\begin{equation*}
C \sim 2 \pi \varepsilon_{0} a \tag{2.18}
\end{equation*}
$$

where $a$ is the scale of the linear size of any conductor. ${ }^{13}$
Now proceeding to a system of two conductors, we immediately see why we should be careful with the capacitance definition: one constant $C$ is insufficient to describe such system. Indeed, here we have two, generally different conductor potentials, $\phi_{1}$ and $\phi_{2}$, that may depend on both conductor charges, $Q_{1}$ and $Q_{2}$. Using the same arguments as for the one-conductor case, we may conclude that the dependence is always linear:

$$
\begin{align*}
& \phi_{1}=p_{11} Q_{1}+p_{12} Q_{2}  \tag{2.19}\\
& \phi_{2}=p_{21} Q_{1}+p_{22} Q_{2}
\end{align*}
$$

but still has to be described not with one but with four coefficients $p_{j j^{\prime}}\left(j, j^{\prime}=1,2\right)$ forming the so-called reciprocal capacitance matrix

$$
\left(\begin{array}{ll}
p_{11} & p_{12}  \tag{2.20}\\
p_{21} & p_{22}
\end{array}\right)
$$

Plugging relation (19) into Eq. (1.63), we see that the full electrostatic energy of the system may be expressed by a quadratic form:

[^175]\[

$$
\begin{equation*}
U=\frac{p_{11}}{2} Q_{1}^{2}+\frac{p_{12}+p_{21}}{2} Q_{1} Q_{2}+\frac{p_{22}}{2} Q_{2}^{2} \tag{2.21}
\end{equation*}
$$

\]

It is evident that the middle term in the right-hand part of this equation describes the electrostatic coupling of the conductors. (Without it, the energy would be just a sum of two independent electrostatic energies of conductors 1 and 2.) This is why systems with $\left|p_{12}\right|,\left|p_{21}\right| \ll p_{11}, p_{22}$ are called weakly coupled, and may be analyzed using approximate methods - see, e.g., Fig. 3 and its discussion below.

Before proceeding further, let us use the Lagrangian formalism of analytical mechanics ${ }^{14}$ to argue that the off-diagonal elements of matrix $p_{j j}$, are always equal:

$$
\begin{equation*}
p_{12}=p_{21} . \tag{2.22}
\end{equation*}
$$

Indeed, charges $Q_{1,2}$ may be taken for generalized coordinates $q_{j}(j=1,2)$ of the system; then the corresponding generalized forces may be found as

$$
\begin{equation*}
\boldsymbol{7}_{j}=-\frac{\partial U}{\partial q_{j}}=-\frac{\partial U}{\partial Q_{j}} \tag{2.23}
\end{equation*}
$$

Applying this equation to Eq. (21), we see that, for example

$$
\begin{equation*}
7_{1}=-\left(p_{11} Q_{1}+\frac{p_{12}+p_{21}}{2} Q_{2}\right) \tag{2.24}
\end{equation*}
$$

Now we may argue that dynamics of charge $Q_{j}$ should only depend on the electrostatic potential $\phi_{j}$ this charge "sees". This means, in particular, that $\phi_{1}$ should be a unique function of $\not \mathcal{I}_{1}$. Comparing Eq. (24) with the first of Eqs. (19), we see that for this to be true, Eq. (22) should indeed be valid.

Equations (19) and (21) show that for the general case of arbitrary charges $Q_{1}$ and $Q_{2}$, the system properties cannot be reduced to just one coefficient ("capacitance"). Let us consider three particular cases when such a reduction is possible.
(i) The system as the whole is electrically neutral: $Q_{1}=-Q_{2} \equiv Q$. In this case the most important function of $Q$ is the difference of conductor potentials, called voltage: ${ }^{15}$

Voltage

$$
\begin{equation*}
V \equiv \phi_{1}-\phi_{2} \tag{2.25}
\end{equation*}
$$

For that function, the subtraction of two Eqs. (19) gives

$$
\begin{equation*}
V=\frac{Q}{C_{m}}, \quad \text { with } C_{m} \equiv \frac{1}{\left(p_{11}+p_{22}\right)-\left(p_{12}+p_{21}\right)}, \tag{2.26}
\end{equation*}
$$

where coefficient $C_{m}$ is called the mutual capacitance between the conductors - or, again, just "capacitance". The same coefficient describes the electrostatic energy of the system. Indeed, plugging Eq. (25) into Eq. (21), we see that both forms of Eq. (15) are reproduced if $\phi$ is replaced with $V, Q_{1}$ with $Q$, and $C$ with $C_{m}$ :

[^176]\[

$$
\begin{equation*}
U=\frac{Q^{2}}{2 C_{m}}=\frac{C_{m}}{2} V^{2} \tag{2.27}
\end{equation*}
$$

\]

The best known system for which the mutual capacitance $C_{m}$ may be readily calculated is the plane (or "parallel-plate") capacitor, a system of two conductors separated with a narrow, plane gap (Fig. 2). Indeed, since the surface charges, that contribute to the opposite charges $\pm Q$ of the conductors in this system, attract each other, in the limit $d \ll a$ they sit entirely on the sides of the narrow gap.


Fig. 2.2. Plane capacitor.

Let us apply the Gauss law to a pillbox volume (shown by dashed line in Fig. 2) whose area is a small part of the gap (but nevertheless much larger than $d^{2}$ ), with one of the plane lids inside a conductor, and another one inside the gap. The result immediately shows that the electric field within the gap is $E=\sigma / \varepsilon_{0}$, i.e. is independent of the pillbox thickness. Integrating this field across thickness $d$ of the gap, we get $V=E d=\sigma d / \varepsilon_{0}$, so that $\sigma=\varepsilon_{0} V / d$. But this voltage should not depend on the selection of the point of the gap area. As a result, $\sigma$ should be also constant over all the gap area $A$, and hence $Q=$ $\sigma A=\varepsilon_{0} V / d$. Thus we may write $V=Q / C_{m}$, with

$$
\begin{equation*}
C_{m}=\frac{\varepsilon_{0}}{d} A \tag{2.28}
\end{equation*}
$$

[^177]Let me offer a few comments on this well-known formula. First, it is valid even if the gap is not quite planar, for example if it gently curves on a scale much larger than $d$. Second, Eq. (28) is only valid if $A \sim a^{2}$ is much larger than $d^{2}$, because its derivation ignores the electric field deviations from uniformity ${ }^{16}$ at distances $\sim d$ near the gap edges. Finally, the same condition $\left(A \gg d^{2}\right)$ assures that $C_{m}$ is much larger than the self-capacitance of each of the conductors - see Eq. (18). The opportunities given by this fact for electronic engineering and experimental physics practice are rather astonishing. For example, a very realistic $3-\mathrm{nm}$ layer of high-quality aluminum oxide (which may provide a nearly perfect electric insulation between two thin conducting films) with area of $0.1 \mathrm{~m}^{2}$ (which is a typical area of silicon wafers used in semiconductor industry) provides $C_{m} \sim 1 \mathrm{mF},{ }^{17}$ larger than the selfcapacitance of the whole planet Earth!

In the case shown in Fig. 2, the electrostatic coupling of the two conductors is evidently strong. As an opposite example of a weakly coupled system, let us consider two conducting spheres of the same radius $R$, separated by a much larger distance $d$ (Fig. 3).

[^178]

Fig. 2.3. A system of two well separated, similar conducting spheres.

In this case the diagonal components of matrix $p_{i j}$, may be approximately found from Eq. (16), i.e. by neglecting the coupling altogether:

$$
\begin{equation*}
p_{11}=p_{22} \approx \frac{1}{4 \pi \varepsilon_{0} R} . \tag{2.29}
\end{equation*}
$$

Now, if we had just one sphere (say, number 1), the electric potential at distance $d$ from its center would be given by Eq. (16): $\phi=Q_{1} / 4 \pi \varepsilon_{0} d$. Now if we move into this point a small ( $R \ll d$ ) sphere without its own charge, we may expect that its potential should not be too far from this result, so that $\phi_{2} \approx Q_{1} / 4 \pi \varepsilon_{0} d$. Comparing this expression with Eq. (19) (taken for $Q_{2}=0$ ), we get

$$
\begin{equation*}
p_{12}=p_{21} \approx \frac{1}{4 \pi \varepsilon_{0} d} \ll p_{11}, p_{22} \tag{2.30}
\end{equation*}
$$

From here and Eq. (26), the mutual capacitance

$$
\begin{equation*}
C_{m} \approx \frac{1}{p_{11}+p_{22}} \approx 2 \pi \varepsilon_{0} R . \tag{2.31}
\end{equation*}
$$

We see that (somewhat counter-intuitively), in this case $C_{m}$ does not depend substantially on the distance between the spheres, i.e. does not describe their electrostatic coupling. The off-diagonal coefficients of the reciprocal capacitance matrix (20) play this role much better - see Eq. (30).
(ii) Now let us consider the case when only one conductor of the two is charged, for example $Q_{1}$ $\equiv Q$, while $Q_{2}=0$. Then Eqs. (19) yield

$$
\begin{equation*}
\phi_{1}=p_{11} Q_{1} . \tag{2.32}
\end{equation*}
$$

Now, if we follow Eq. (13) and define $C_{j} \equiv 1 / p_{j j}$ as the partial capacitance of conductor number $j$, we see that it differs from the mutual capacitance $C_{m}$ - cf. Eq. (26). For example, in the case shown in Fig. $3, C_{1}=C_{2} \approx 4 \pi \varepsilon_{0} R \approx 2 C_{m}$.
(iii) Finally, let us consider a popular case when one of the conductors is charged by a certain charge (say, $Q_{1}=Q$ ), but the potential of another one is sustained constant, say $\phi_{2}=0 .{ }^{18}$ (This condition is especially easy to implement if the second conductor is much larger that the first one. Indeed, as the estimate (18) shows, in this case it would take much larger charge $Q_{2}$ to make potential $\phi_{2}$ comparable with $\phi_{1}$.) In this case the second of equations (19) yields $Q_{2}=-\left(p_{21} / p_{22}\right) Q_{1}$. Plugging this relation into the first of those equations, we get

[^179]\[

$$
\begin{equation*}
\phi_{1}=\left(p_{11}-\frac{p_{12} p_{21}}{p_{22}}\right) Q_{1} \tag{2.33}
\end{equation*}
$$

\]

Thus, if we treat the reciprocal of the expression in parentheses,

$$
\begin{equation*}
C_{1}^{\mathrm{ef}} \equiv\left(p_{11}-\frac{p_{12} p_{21}}{p_{22}}\right)^{-1} \tag{2.34}
\end{equation*}
$$

as the effective capacitance of the first conductor, it is generally different both from $C_{m}$ and (unless the conductors are far apart and their electrostatic coupling is negligible) from $C_{1}=1 / p_{11}$.

To summarize this section, the potential (and hence the actual capacitance) of a conductor in a two-conductor system may be very much dependent on what exactly is being done with the second conductor when the first one is charged. This is also true for multi-conductor systems (for whose description, Eqs. (19) and (21) may be readily generalized); moreover, in that case even the mutual capacitance between two selected conductors may depend on the electrostatics conditions of other components of the system.

### 2.3. The simplest boundary problems

In the general case when the electric field distribution in the free space between the conductors cannot be readily found from the Gauss law or by any other special methods, the best approach is to try to solve the differential Laplace equation (1.42), with boundary conditions (1b):

$$
\begin{equation*}
\nabla^{2} \phi=0,\left.\quad \phi\right|_{S_{k}}=\phi_{k} \tag{2.35}
\end{equation*}
$$

where $S_{k}$ is the surface of the $k$-th conductor of the system. After such boundary problem has been solved, i.e. the spatial distribution $\phi(\mathbf{r})$ has been found in all points outside the conductor, it is straightforward to use Eq. (3) to find the surface charge density, and finally the total charge

$$
\begin{equation*}
Q_{k}=\oint_{S_{k}} \sigma d^{2} r \tag{2.36}
\end{equation*}
$$

of each conductor, and hence any component of the reciprocal capacitance matrix $p_{i j}$. As an illustration, let us implement this program for three very simple problems.
(i) Plane capacitor (Fig. 2). In this case, the easiest way to solve the Laplace equation is to use linear (Cartesian) coordinates with one coordinate axis, say $z$, normal to the conductor surfaces (Fig. 4).


Fig. 2.4. Plane capacitor's geometry used for the solution of the boundary problem (35).

In these coordinates, the Laplace operator is just the sum of three second derivatives. ${ }^{19}$ It is evident that due to problem's translational symmetry in the $\{x, y\}$ plane, deep inside the gap (i.e. at the lateral distance from the edges much larger than $d$ ) the electrostatic potential may only depend on the coordinate perpendicular to the gap surfaces: $\phi(\mathbf{r})=\phi(z)$. For such a function, derivatives over $x$ and $y$ vanish, and the boundary problem (35) is reduced to a very simple ordinary differential equation

$$
\begin{equation*}
\frac{d^{2} \phi}{d z^{2}}(z)=0 \tag{2.37}
\end{equation*}
$$

with boundary conditions

$$
\begin{equation*}
\phi(0)=0, \quad \phi(d)=V . \tag{2.38}
\end{equation*}
$$

(For the sake of notation simplicity, I have used the discretion of adding a constant to the potential to make one of the potentials vanish, and also definition (25) of voltage $V$.) The general solution of Eq. (37) is a linear function: $\phi(z)=c_{1} z+c_{2}$, whose constant coefficients $c_{1,2}$ may be found, in an elementary way, from the boundary conditions (38). The final solution is

$$
\begin{equation*}
\phi=V \frac{z}{d} . \tag{2.39}
\end{equation*}
$$

From here the only nonvanishing component of the electric field is

$$
\begin{equation*}
E_{z}=-\frac{d \phi}{d z}=-\frac{V}{d}, \tag{2.40}
\end{equation*}
$$

and the surface charge of the capacitor plates

$$
\begin{equation*}
\sigma=\varepsilon_{0} E_{n}=\mp \varepsilon_{0} E_{z}= \pm \varepsilon_{0} \frac{V}{d}, \tag{2.41}
\end{equation*}
$$

where the upper and lower sign correspond to the upper and lower plate, respectively. Since $\sigma$ does not depend on coordinates $x$ and $y$, we can get the full charges $Q_{1}=-Q_{2} \equiv Q$ of the surfaces by its multiplication by the gap area $A$, giving us the again already known result (28) for the mutual capacitance $C_{m} \equiv Q / V$. I believe that this calculation, though very easy, may serve as a good introduction to the boundary problem solution philosophy.
(ii) Coaxial-cable capacitor. Coaxial cable is a system of two round cylindrical, coaxial conductors, with the cross-section shown in Fig. 5.


Fig. 2.5. Cross-section of a coaxial capacitor.

[^180]Evidently, in this case the cylindrical coordinates $\{\rho, \varphi, z\}$, with axis $z$ along the common axis of the cylinders, are most appropriate. Due to the axial symmetry of the problem, in these coordinates $\mathbf{E}(\mathbf{r})$ $=\mathbf{n}_{\rho} E(\rho), \phi(\mathbf{r})=\phi(\rho)$, so that in the general expression for the Laplace operator ${ }^{20}$ we can take $\partial / \partial \varphi=$ $\partial / \partial z=0$. As a result, only the first (radial) term of the operator survives, and the boundary problem (35) takes the form

$$
\begin{equation*}
\frac{1}{\rho} \frac{d}{d \rho}\left(\rho \frac{d \phi}{d \rho}\right)=0, \quad \phi(a)=V, \phi(b)=0 \tag{2.42}
\end{equation*}
$$

The sequential integration of this ordinary differential equation is elementary (and similar to that of the Poisson equation in spherical coordinates, performed in Sec. 1.3), giving

$$
\begin{equation*}
\frac{d \phi}{d \rho}=\frac{c_{1}}{\rho}, \quad \phi(\rho)=c_{1} \int_{a}^{\rho} \frac{d \rho^{\prime}}{\rho^{\prime}}+c_{2}=c_{1} \ln \frac{\rho}{a}+c_{2} \tag{2.43}
\end{equation*}
$$

Constants $c_{1,2}$ may be found using boundary conditions (42):

$$
\begin{equation*}
V=c_{2}, \quad 0=c_{1} \ln \frac{b}{a}+c_{2}, \tag{2.44}
\end{equation*}
$$

giving $c_{1}=-V / \ln (b / a)$, so that solution (43) takes the following form

$$
\begin{equation*}
\phi(\rho)=V\left(1-\frac{\ln (\rho / a)}{\ln (b / a)}\right) \tag{2.45}
\end{equation*}
$$

Next, for our axial symmetry the general expression for the gradient ${ }^{21}$ is reduced to the radial derivative, so that

$$
\begin{equation*}
E(\rho) \equiv-\frac{d \phi(\rho)}{d \rho}=\frac{V}{\rho \ln (b / a)} \tag{2.46}
\end{equation*}
$$

This expression, plugged into Eq. (2), allows us to find the density of conductors' surface charge. For example, for the inner electrode

$$
\begin{equation*}
\sigma_{a}=\varepsilon_{0} E_{a}=\frac{\varepsilon_{0} V}{a \ln (b / a)}, \tag{2.47}
\end{equation*}
$$

so that its full charge (per unit length of the system) is

$$
\begin{equation*}
\frac{Q}{L}=2 \pi a \sigma_{a}=\frac{2 \pi \varepsilon_{0} V}{\ln (b / a)} \tag{2.48}
\end{equation*}
$$

(It is straightforward to check that the charge of the outer electrode is equal and opposite.) Hence, by the definition of the mutual capacitance, its value per unit length is

$$
\begin{equation*}
\frac{C_{m}}{L} \equiv \frac{Q}{L V}=\frac{2 \pi \varepsilon_{0}}{\ln (b / a)} \tag{2.49}
\end{equation*}
$$

[^181]This expression shows that the total capacitance $C$ is proportional to the systems length $L$ (if $L$ $\gg a, b$ ), while being only logarithmically dependent on is the dimensions of its cross-section. Since log of a very large argument is an extremely slow function (sometimes called "quasi-constant"), if the external conductor is made large $(b \gg a)$ the capacitance diverges, but very weakly. Such a logarithmic divergence may be cut by any miniscule additional effect, for example by the finite length $L$ of the system. This allows one to get a crude but very useful estimate of self-capacitance of a single wire:

$$
\begin{equation*}
C \approx \frac{2 \pi \varepsilon_{0} L}{\ln (L / a)}, \quad \text { for } L \gg a \tag{2.50}
\end{equation*}
$$

On the other hand, if the gap between the conductors is narrow: $b=a+d$, with $d \ll a$, then $\ln (b / a)=$ $\ln (1+d / a)$ may be approximated as $d / a$, and Eq. (49) is reduced to $C_{m} \approx 2 \pi \varepsilon_{0} a L / d$, i.e. to Eq. (28) for the plane capacitor, with $A=2 \pi a L$.
(iii) Spherical capacitor. This is a system of two conductors, with the same central cross-section as the coaxial cable (Fig. 5), but now with the spherical rather than axial symmetry. This symmetry implies that we are better off using spherical coordinates, so that potential $\phi$ depends only on one of them, the distance $r$ from the common center of the conductors: $\phi(\mathbf{r})=\phi(r)$. As we already know from Sec. 1.3, in this case the general expression for the Laplace operator is reduced to its first (radial) term, so that the Laplace equation takes a simple form - see Eq. (1.47). Moreover, we have already found the general solution to this equation - see Eq. (1.50):

$$
\begin{equation*}
\phi(r)=\frac{c_{1}}{r}+c_{2}, \tag{2.51}
\end{equation*}
$$

Now acting exactly as above, i.e. determining constant $c_{1}$ from the boundary conditions $\phi(a)=V, \phi(b)=$ 0 , we get

$$
\begin{equation*}
V=c_{1}\left(\frac{1}{a}-\frac{1}{b}\right), \quad \text { so that } \quad \phi(r)=\frac{V}{r}\left(\frac{1}{a}-\frac{1}{b}\right)^{-1}+c_{2} . \tag{2.52}
\end{equation*}
$$

Next, we can use the spherical symmetry to find electric field, $\mathbf{E}(\mathbf{r})=\mathbf{n}_{r} E(r)$, with

$$
\begin{equation*}
E(r)=-\frac{d \phi}{d r}=\frac{V}{r^{2}}\left(\frac{1}{a}-\frac{1}{b}\right)^{-1} \tag{2.53}
\end{equation*}
$$

and hence its values on conductors' surfaces, and then the surface charge density $\sigma$ from Eq. (2). For example, for the inner conductor's surface,

$$
\begin{equation*}
\sigma_{a}=\varepsilon_{0} E(a)=\varepsilon_{0} \frac{V}{a^{2}}\left(\frac{1}{a}-\frac{1}{b}\right)^{-1}, \tag{2.54}
\end{equation*}
$$

so that, finally, for the full charge of that conductor we get

$$
\begin{equation*}
Q=4 \pi a^{2} \sigma=4 \pi \varepsilon_{0}\left(\frac{1}{a}-\frac{1}{b}\right)^{-1} V . \tag{2.55}
\end{equation*}
$$

(Again, the charge of the outer conductor is equal and opposite.) Now we can use the definition of the mutual capacitance to get the final result

$$
\begin{equation*}
C_{m} \equiv \frac{Q}{V}=4 \pi \varepsilon_{0}\left(\frac{1}{a}-\frac{1}{b}\right)^{-1}=4 \pi \varepsilon_{0} \frac{a b}{b-a} . \tag{2.56}
\end{equation*}
$$

For $b \gg a$, this result coincides with Eq. (17) for self-capacitance of the inner conductor. On the other hand, if the gap between two conductors is narrow, $d \equiv b-a \ll a$,

$$
\begin{equation*}
C_{m}=4 \pi \varepsilon_{0} \frac{a(a+d)}{d} \approx 4 \pi \varepsilon_{0} \frac{a^{2}}{d}, \tag{2.57}
\end{equation*}
$$

i.e. the capacitance approaches that of the planar capacitor of area $A=4 \pi a^{2}$ - as it should.

All this seems (and is) very straightforward, but let us contemplate what was the reason for such easy successes. We have managed to find such coordinate transformations, for example $\{x, y, z\} \rightarrow\{r$, $\theta, \varphi\}$ in the spherical case, that both the Laplace equation and the boundary conditions involve only one of the new coordinates (in this case, $r$ ). The necessary condition for the former fact is that the new coordinates (in this case, spherical ones) are orthogonal. This means that three vector components of differential $d \mathbf{r}$, due to small variations of the new coordinates (say, $d r, d \theta$, and $d \varphi$ ), are mutually perpendicular. If this were not so, the Laplace operator would not fall into the simple sum of three independent parts, and could not be reduced, at the proper symmetry of the problem, to just one of these components, making it readily integrable.

### 2.4. Other orthogonal coordinates

Since the cylindrical and spherical coordinates are only simplest examples of the orthogonal (or "orthogonal curvilinear") coordinates, this methodology may be extended to other coordinate systems of this type. As an example, let us have a look at the following problem: finding the self-capacitance of a thin, round conducting disk (and, as solution's by-products, the distributions of the electric field and surface charge) - see Fig. 6. The cylindrical or spherical coordinates would not give too much help here, because though they have the appropriate axial symmetry about axis $z$, they would make the boundary condition on the disk too complex (two coordinates, either $\rho$ and $z$, or $r$ and $\theta$ ).


Fig. 2.6. The thin conducting disk problem. (The crosssection of the system by the vertical plane $y=0$.)

The relief comes from noting that the disk, i.e. the area $z=0, r<R$, may be thought of as the limiting case of an axially-symmetric ellipsoid - the result of rotation of the usual ellipse about one of its axes - in our case, the vertical axis $z .{ }^{22}$ Analytically, such an ellipsoid may be described by the following equation:

[^182]\[

$$
\begin{equation*}
\frac{x^{2}+y^{2}}{a^{2}}+\frac{z^{2}}{b^{2}}=1 \tag{2.58}
\end{equation*}
$$

\]

where $a$ and $b$ are the so-called major semi-axes whose ratio determines the ellipse eccentricity (the degree of squeezing). For our problem, we will only need oblate ellipsoids with $a \geq b$; according to Eq. (58), they may be presented as surfaces of constant $\alpha$ in the system of degenerate ellipsoidal (or "spheroidal") coordinates $\{\alpha, \beta, \varphi\}$, which are related to the Cartesian coordinates as follows:

$$
\begin{align*}
& x=R \cosh \alpha \sin \beta \cos \varphi, \\
& y=R \cosh \alpha \sin \beta \sin \varphi,  \tag{2.59}\\
& z=R \sinh \alpha \cos \beta .
\end{align*}
$$

Such ellipsoidal coordinates are the evident generalization of the spherical coordinates, which correspond to the limit $\alpha \gg 1$ (i.e. $r \gg R$ ). In the opposite limit of small $\alpha$, the surface of constant $\alpha=$ 0 describes our thin disk of radius $R$. It is almost evident (and easy to prove) that coordinates (59) are also orthogonal, so that the Laplace operator may be expressed as a sum of three independent terms:

$$
\nabla^{2}=\frac{1}{R^{2}\left(\cosh ^{2} \alpha-\sin ^{2} \beta\right)} \times\left[\begin{array}{l}
\frac{1}{\cosh \alpha} \frac{\partial}{\partial \alpha}\left(\cosh \alpha \frac{\partial}{\partial \alpha}\right)  \tag{2.60}\\
+\frac{1}{\sin \beta} \frac{\partial}{\partial \beta}\left(\sin \beta \frac{\partial}{\partial \beta}\right)+\left(\frac{1}{\sin ^{2} \beta}-\frac{1}{\cosh ^{2} \alpha}\right) \frac{\partial^{2}}{\partial \varphi^{2}}
\end{array}\right]
$$

Though this expression may look a bit intimidating, let us notice that in our current problem, the boundary conditions depend only on coordinate $\alpha$ : ${ }^{23}$

$$
\begin{equation*}
\left.\phi\right|_{\alpha=0}=V,\left.\quad \phi\right|_{\alpha=\infty}=0 . \tag{2.61}
\end{equation*}
$$

Hence there is every reason to believe that the electrostatic potential in all space is the function of $\alpha$ alone. (In other words, all ellipsoids $\alpha=$ const are the equipotential surfaces.) Indeed, acting on such function $\phi(\alpha)$ by the Laplace operator (60), we see that the two last terms in the square brackets vanish, and the Laplace equation (35) is reduced to a simple ordinary differential equation

$$
\begin{equation*}
\frac{d}{d \alpha}\left[\cosh \alpha \frac{d \phi}{d \alpha}\right]=0 \tag{2.62}
\end{equation*}
$$

Integrating it twice, just as we did in the previous problems, we get

$$
\begin{equation*}
\phi(\alpha)=c_{1} \int \frac{d \alpha}{\cosh \alpha} \tag{2.63}
\end{equation*}
$$

This integral may be readily taken, for example, using the substitution $\xi \equiv \sinh \alpha$ (with $d \xi \equiv \cosh \alpha d \alpha$, $\cosh ^{2} \alpha=1+\sinh ^{2} \alpha=1+\xi^{2}$ ):

$$
\begin{equation*}
\phi(\alpha)=c_{1} \int_{0}^{\sinh \alpha} \frac{d \xi}{1+\xi^{2}}+c_{2}=c_{1} \tan ^{-1}(\sinh \alpha)+c_{2} \tag{2.64}
\end{equation*}
$$

[^183]The integration constants $c_{1,2}$ are again simply found from boundary conditions, in this case Eqs. (61), and we arrive at the final expression for the electrostatic potential:

$$
\begin{equation*}
\phi(\alpha)=V\left[1-\frac{2}{\pi} \tan ^{-1}(\sinh \alpha)\right] . \tag{2.65}
\end{equation*}
$$

This solution satisfies both the Laplace equation and the boundary conditions. Mathematicians tell us that the solution of any boundary problem of the type (35) is unique, so we do not need to look any further.

Now we may use Eq. (3) to find the surface density of electric charge, but in the case of thin disk, it is more natural to add up such densities on its top and bottom surfaces at the same distance $r=$ $\left(x^{2}+y^{2}\right)^{1 / 2}$ from the disk center (which are evidently equal, due to the problem symmetry about plane $z=$ $0): \sigma=\left.2 \varepsilon_{0} E_{n}\right|_{z=+0}$. According to Eq. (65), the electric field on the surface is

$$
\begin{equation*}
E_{n \mid \alpha=+0}=-\left.\frac{\partial \phi}{\partial z}\right|_{z=+0}=-\left.\frac{\partial \phi(\alpha)}{\partial(R \sinh \alpha \cos \beta)}\right|_{\alpha=+0}=\frac{2}{\pi} V \frac{1}{R \cos \beta}=\frac{2}{\pi} V \frac{1}{\left(R^{2}-r^{2}\right)^{1 / 2}} \tag{2.66}
\end{equation*}
$$

and we see that the charge is distributed along the disk very nonuniformly:

$$
\begin{equation*}
\sigma=\frac{4}{\pi} \varepsilon_{0} V \frac{1}{\left(R^{2}-r^{2}\right)^{1 / 2}}, \tag{2.67}
\end{equation*}
$$

with a singularity at the disk edge. Below we will see that such singularities are very typical for sharp edges of conductors. ${ }^{24}$ Fortunately, in our current case the divergence is integrable, giving a finite disk charge:

$$
\begin{equation*}
Q=\int_{\substack{\text { disk } \\ \text { surface }}} \sigma d^{2} r=\int_{0}^{R} \sigma(r) 2 \pi r d r=\frac{4}{\pi} \varepsilon_{0} V 2 \pi \int_{0}^{R} \frac{r d r}{\left(R^{2}-r^{2}\right)^{1 / 2}}=4 \varepsilon_{0} V R \int_{0}^{1} \frac{d \xi}{\sqrt{1-\xi}}=8 \varepsilon_{0} R V \tag{2.68}
\end{equation*}
$$

Thus, for disk's self-capacitance we get a very simple result,

$$
\begin{equation*}
C=8 \varepsilon_{0} R=\frac{2}{\pi} 4 \pi \varepsilon_{0} R, \tag{2.69}
\end{equation*}
$$

a factor of $2 / \pi \approx 0.64$ lower than that for the conducting sphere of the same equal radius, but still complying with the general estimate (18).

Can we always find a "good" system of orthogonal coordinates? Unfortunately, the answer is no, even for highly symmetric geometries. This is why the practical value of this approach is limited, and other methods of boundary problem solution are clearly needed. Before moving to them, however, let us note that in the case of 2D problems (i.e. cylindrical geometries), the orthogonal coordinate method gets help from the following conformal mapping approach.

Let us consider the pair of Cartesian coordinates $\{x, y\}$ of the cross-section plane as a complex variable $\boldsymbol{z}=x+i y,{ }^{25}$ where $i$ is the imaginary unity $\left(i^{2}=-1\right)$, and let $\boldsymbol{u}(z)=u+i v$ be an analytic complex

[^184]function of $\boldsymbol{z} .{ }^{26}$ For our current purposes, the most important property of an analytic function is that its real and imaginary parts obey the following Cauchy-Riemann relations: ${ }^{27}$
\[

$$
\begin{equation*}
\frac{\partial u}{\partial x}=\frac{\partial v}{\partial y}, \quad \frac{\partial v}{\partial x}=-\frac{\partial u}{\partial y} \tag{2.70}
\end{equation*}
$$

\]

For example, for the function

$$
\begin{equation*}
\boldsymbol{u}=z^{2}=(x+i y)^{2}=\left(x^{2}-y^{2}\right)+2 i x y \tag{2.71}
\end{equation*}
$$

whose real and imaginary parts are

$$
\begin{equation*}
u \equiv \operatorname{Re} \boldsymbol{u}=x^{2}-y^{2}, \quad v \equiv \operatorname{Im} \boldsymbol{u}=2 x y \tag{2.72}
\end{equation*}
$$

we immediately see that $\partial u / \partial x=2 x=\partial v / \partial y$, and $\partial v / \partial x=2 y=-\partial u / \partial y$, in accordance with Eq. (70).
Let us differentiate the first of Eqs. (70) over $x$ again, then change the order of differentiation, and after that use the latter of those equations:

$$
\begin{equation*}
\frac{\partial^{2} u}{\partial x^{2}}=\frac{\partial}{\partial x} \frac{\partial u}{\partial x}=\frac{\partial}{\partial x} \frac{\partial v}{\partial y}=\frac{\partial}{\partial y} \frac{\partial v}{\partial x}=-\frac{\partial}{\partial y} \frac{\partial u}{\partial y}=-\frac{\partial^{2} u}{\partial y^{2}} \tag{2.73}
\end{equation*}
$$

and similarly for $v$. This means that the sum of second-order partial derivatives of each of real functions $u(x, y)$ and $v(x, y)$ is zero, i.e. that both functions obey the 2 D Laplace equation. This mathematical fact opens a nice way of solving problems of electrostatics for (relatively simple) 2D geometries. Imagine that for a particular boundary problem we have found a function $u(z)$ for which either $u(x, y)$ or $v(x, y)$ is constant on all electrode surfaces. Then all lines of constant $u$ (or $v$ ) present equipotential surfaces, i.e. the problem of the potential distribution has been essentially solved.

As a simple example, consider a practically important problem: the quadrupole electrostatic lens- a system of four cylindrical ${ }^{28}$ electrodes with hyperbolic cross-sections, whose boundaries obey the following relations:

$$
x^{2}-y^{2}=\left\{\begin{array}{l}
+a^{2}, \quad \text { for the left and right electrodes, }  \tag{2.74}\\
-a^{2},
\end{array} \text { for the top and bottom electrodes }, ~ \$\right.
$$

voltage-biased as shown in Fig. 7a. Comparing these relations with Eqs. (72), we see that each electrode surface corresponds to a constant value of $u= \pm a^{2}$. Moreover, potentials of both surfaces with $u=+a^{2}$ are equal to $+V / 2$, while those with $u=-a^{2}$ are equal to $-V / 2$. Hence we may conjecture that the electrostatic potential at each point is a function of $u$ alone; moreover, a simple linear function,

$$
\begin{equation*}
\phi=c_{1} u+c_{2}=c_{1}\left(x^{2}-y^{2}\right)+c_{2}, \tag{2.75}
\end{equation*}
$$

[^185]is a valid (and hence the unique) solution of our boundary problem. Indeed, it does satisfy the Laplace equation, while its constants $c_{1,2}$ may be selected in a way to satisfy all the boundary conditions shown in Fig. 7a:
\[

$$
\begin{equation*}
\phi=\frac{V}{2} \frac{x^{2}-y^{2}}{a^{2}} . \tag{2.76}
\end{equation*}
$$

\]

so that the boundary problem has been solved.


Fig. 2.7. (a) Quadrupole electrostatic lens geometry and (b) its analysis using conformal mapping.

According to Eq. (76), all equipotential surfaces are hyperbolic cylinders, similar to those of the electrode surfaces. What remains is to find the electric field at an arbitrary point inside the system:

$$
\begin{equation*}
E_{x}=-\frac{\partial \phi}{\partial x}=-V \frac{x}{a^{2}}, \quad E_{y}=-\frac{\partial \phi}{\partial y}=V \frac{y}{a^{2}} . \tag{2.77}
\end{equation*}
$$

These formulas show that if charged particles (e.g., electrons in an electron optics system) are launched to fly ballistically through the lens, along axis $z$, they experience a force pushing them toward the symmetry axis and proportional to particle's deviation from the axis (and thus equivalent in action to an optical lens with positive refraction power) in one direction, and a force pushing them out (negative refractive power) in the perpendicular direction. One can show that letting charged particles fly through several such lenses, with alternating voltage polarities, in series, enables beam focusing. ${ }^{29}$

Hence, we have reduced the 2D Laplace boundary problem to that of finding the proper analytic function $\boldsymbol{u}(z)$. This task may be also understood as that of finding a conformal map, i.e. a correspondence between components of any point pair, $\{x, y\}$ and $\{u, v\}$, residing, respectively, on the initial Cartesian plane $z$ and the plane $\boldsymbol{\mu}$ of the new variables. For example, Eq. (71) maps the real electrode configuration onto the plane capacitor with infinite area (Fig. 7b), and the simplicity of Eq. $(75)$ is due to the fact that for the latter system the equipotential surfaces are just parallel planes.

For more complex geometries, the suitable analytic function $\boldsymbol{\omega}(\boldsymbol{z})$ may be hard to find. However, for conductors with piece-linear cross-section boundaries, substantial help may be obtained from the following Schwarz-Christoffel integral

[^186]\[

$$
\begin{equation*}
\boldsymbol{u}(\boldsymbol{z})=\text { const } \times \int \frac{d \boldsymbol{z}}{\left(\boldsymbol{z}-x_{1}\right)^{k_{1}}\left(\boldsymbol{z}-x_{2}\right)^{k_{2}} \ldots\left(\boldsymbol{z}-x_{N-1}\right)^{k_{N-1}}} . \tag{2.78}
\end{equation*}
$$

\]

that provides the conformal mapping of the interior of an arbitrary $N$-sided polygon on plane $\boldsymbol{\mu}=u+i v$, and the upper-half $(y>0)$ of plane $\boldsymbol{z}=x+i y$. Here $x_{j}(j=1,2, N-1)$ are the points of axis $y=0$ (i.e., of the boundary of the mapped region on plane $z$ ) to which the corresponding polygon vertices are mapped, while $k_{j}$ are the exterior angles at the polygon vertices, measured in the units of $\pi$, with $-1 \leq k_{j} \leq+1-$ see Fig. $8 .{ }^{30}$ Of points $x_{j}$, two may be selected arbitrarily (because their effects may be compensated by the multiplicative constant in Eq. (78), and the constant of integration), while all the others have to be adjusted to provide the correct mapping.


Fig. 2.8. Schwartz-Christoffel mapping of polygon's interior on the upper half-plane.

In the general case, the complex integral (78) may be hard to tackle. However, in some important cases, in particular those with right angles ( $k_{j}= \pm 1 / 2$ ) and/or with some points $\boldsymbol{\omega}_{j}$ at infinity, the integrals may be readily worked out, giving explicit analytical expressions for the mapping functions $\boldsymbol{\omega}(\boldsymbol{z})$. For example, let us consider a semi-infinite strip, defined by restrictions $-1 \leq u \leq+1$ and $0 \leq v$, on plane $\boldsymbol{\omega}-$ see the left panel of Fig. 9.


Fig. 2.9. Semi-infinite strip mapped onto the upper half-plane.

[^187]The strip may be considered as a polygon, with one vertex at the infinitely distant vertical point $\boldsymbol{\omega}_{3}=0+i \infty$. Let us map it on the upper half of plane $\boldsymbol{z}$, shown on the right panel of Fig. 9, with vertex $\boldsymbol{\omega}_{1}=-1+i 0$ mapped onto point $x_{1}=-1, y_{1}=0$, and vertex $\boldsymbol{\omega}_{2}=+1+i 0$ mapped onto point $x_{2}=+1, y_{2}=$ 0 . Since in this case both external angles are equal to $+\pi / 2$, and hence $k_{1}=k_{2}=+1 / 2$, Eq. (78) is reduced to

$$
\begin{equation*}
\boldsymbol{u}(\boldsymbol{z})=\text { const } \times \int \frac{d \boldsymbol{z}}{(\boldsymbol{z}+1)^{1 / 2}(z-1)^{1 / 2}}=\operatorname{const} \times \int \frac{d \boldsymbol{z}}{\left(z^{2}-1\right)^{1 / 2}}=\operatorname{const} \times i \int \frac{d z}{\left(1-z^{2}\right)^{1 / 2}} . \tag{2.79}
\end{equation*}
$$

This complex integral may be taken, just as for real $\boldsymbol{z}$, by the substitution $\boldsymbol{z}=\sin \xi$, giving

$$
\begin{equation*}
w(\boldsymbol{z})=\text { const }^{\prime} \times \int^{\sin ^{-1} \boldsymbol{z}} d \xi=c_{1} \sin ^{-1} z+c_{2} \tag{2.80}
\end{equation*}
$$

Determining constants $c_{1,2}$ from the required mapping, i.e. from the equations $\boldsymbol{\mu}(-1+i 0)=-1+i 0$ and $\boldsymbol{u}(+1+i 0)=+1+i 0$ (see Fig. 9), we finally get

$$
\begin{equation*}
\boldsymbol{\omega}(\boldsymbol{z})=\frac{2}{\pi} \sin ^{-1} z, \quad \text { i.e. } \boldsymbol{z}=\sin \frac{\pi \boldsymbol{u}}{2} . \tag{2.81a}
\end{equation*}
$$

Using the well-known expression for the sine of a complex argument, ${ }^{31}$ we may rewrite this elegant result in either of the two following forms for the real and imaginary components of $z$ and $\boldsymbol{w}$ :

$$
\begin{gather*}
u=\frac{2}{\pi} \sin ^{-1} \frac{2 x}{\left[(x+1)^{2}+y^{2}\right]^{1 / 2}+\left[(x-1)^{2}+y^{2}\right]^{1 / 2}}, \quad v=\frac{2}{\pi} \cosh ^{-1} \frac{\left[(x+1)^{2}+y^{2}\right]^{1 / 2}+\left[(x-1)^{2}+y^{2}\right]^{1 / 2}}{2} \\
x=\sin \frac{\pi u}{2} \cosh \frac{\pi v}{2}, \quad y=\cos \frac{\pi u}{2} \sinh \frac{\pi v}{2} \tag{2.81b}
\end{gather*}
$$

It is amazing how perfectly does the last formula manage to keep $y \equiv 0$ at different borders of our $\boldsymbol{\omega}$ region (Fig. 9): at its side borders ( $u= \pm 1,0 \leq v<\infty$ ), this is performed by the first multiplier, while at the bottom border $(-1 \leq u \leq+1, v=0)$, the equality is insured by the second operand.

This mapping may be used to solve several electrostatics problems with the geometry shown in Fig. 9; probably the most surprising of them is the following one. A straight gap of width $2 t$ is cut in a thin conducting plane, and voltage $V$ is applied between the resulting half-planes - see the bold lines in Fig. 10. Selecting a Cartesian coordinate system with axis $z$ along the cut, axis $y$ perpendicular to the plane, and the origin in the middle of the cut, we can write the boundary conditions of this Laplace problem as

$$
\phi=\left\{\begin{array}{l}
+V / 2, \quad \text { at } x>t, y=0  \tag{2.82}\\
-V / 2,
\end{array} \quad \text { at } x<-t, y=0 . ~ \$\right.
$$

(Due to problem's symmetry, we may expect that in the middle of the gap, i.e. at $-t<x<+t$ and $y=0$, the electric field is parallel to the plane and hence $\partial \phi / \partial y=0$.) The comparison of Figs. 9 and 10 shows that if we normalize our coordinates to $t$, Eq. (81) provides the conformal mapping of our system on plane $z$ to the field in a plane capacitor on plane $\boldsymbol{\omega}$, with voltage $V$ between two planes $u= \pm 1$. Since we

[^188]already know that in that case $\phi=(V / 2) u$, we may immediately use the first of Eqs. (81b) to write the final solution of the problem (in the dimensional coordinates): ${ }^{32}$
\[

$$
\begin{equation*}
\phi=\frac{V}{2} u=\frac{V}{\pi} \sin ^{-1} \frac{2 x}{\left[(x+t)^{2}+y^{2}\right]^{1 / 2}+\left[(x-t)^{2}+y^{2}\right]^{1 / 2}} . \tag{2.83}
\end{equation*}
$$

\]



Fig. 2.10. Equipotential surfaces of the electric field between two thin conducting semi-planes (or rather their cross-sections by the perpendicular plane $z=$ const).

Thin lines in Fig. 10 show the corresponding equipotential surfaces; ${ }^{33}$ it is evident that the electric field concentrates at the gap edges, just as it did at the edge of the thin disk (Fig. 6). Let me leave the remaining calculation of the surface charge distribution and the mutual capacitance between the half-planes (per unit length) for reader's exercise.

### 2.5. Variable separation

The general approach of the methods discussed in the last two sections was to satisfy the Laplace equation by a function of a single variable that also satisfies the boundary conditions. Unfortunately, in many cases this cannot be done (at least, using practicably simple functions). In this case, a very powerful method, called variable separation, may work, frequently producing "semi-analytical" results in the form of series (infinite sums) of either elementary or well-studied special functions. The main idea of the method is to present the solution of the general boundary problem (35) as the sum of partial solutions,

$$
\begin{equation*}
\phi=\sum_{k} c_{k} \phi_{k}, \tag{2.84}
\end{equation*}
$$

where each function $\phi_{k}$ satisfies the Laplace equation, and then select the set of coefficients $c_{k}$ to satisfy the boundary conditions. More specifically, in the variable separation method the partial solutions $\phi_{k}$ are looked for in the form of a product of functions, each depending of just one spatial coordinate.

[^189](i) Cartesian coordinates. Let us discuss this approach on the classical example of a rectangular box with conducting walls (Fig. 11), with the same potential (that I will take for zero) at all the walls, but a different potential $V$ fixed at the top lid. Moreover, in order to demonstrate the power of the variable separation method, let us carry out all the calculations for a more general case when the top lead potential is an arbitrary 2D function $V(x, y) .{ }^{34}$


Fig. 2.11. Standard playground for the variable separation method discussion: a rectangular box with five conducting, grounded walls and a fixed potential distribution $V(x, y)$ on the top lid.

For this geometry, it is natural to use Cartesian coordinates $\{x, y, z\}$ and hence present each of the partial solutions in Eq. (84) as a product

$$
\begin{equation*}
\phi_{k}=X(x) Y(y) Z(z) . \tag{2.85}
\end{equation*}
$$

Plugging it into the Laplace equation expressed in the Cartesian coordinates,

$$
\begin{equation*}
\frac{\partial^{2} \phi_{k}}{\partial x^{2}}+\frac{\partial^{2} \phi_{k}}{\partial y^{2}}+\frac{\partial^{2} \phi_{k}}{\partial z^{2}}=0, \tag{2.86}
\end{equation*}
$$

and dividing the result by product $X Y Z$, we get

$$
\begin{equation*}
\frac{1}{X} \frac{d^{2} X}{d x^{2}}+\frac{1}{Y} \frac{d^{2} Y}{d y^{2}}+\frac{1}{Z} \frac{d^{2} Z}{d z^{2}}=0 \tag{2.87}
\end{equation*}
$$

Here comes the punch line of the variable separation method: since the first term of this sum may depend only on $x$, the second one only of $y$, etc., Eq. (87) may be satisfied everywhere in the volume only if each of these terms equals a constant. In a minute we will see that for our current problem (Fig. 11), these constant $x$ - and $y$-terms have to be negative; hence let us denote these variable separation constants as $\left(-\alpha^{2}\right)$ and $\left(-\beta^{2}\right)$, respectively. Now Eq. (87) shows that the constant $z$-term has to be positive; if we denote it as $\gamma^{2}$, we get the following relation:

$$
\begin{equation*}
\alpha^{2}+\beta^{2}=\gamma^{2} . \tag{2.88}
\end{equation*}
$$

Now the variables are separated in the sense that for functions $X(x), Y(y)$, and $Z(z)$ we have got separate ordinary differential equations,

[^190]\[

$$
\begin{equation*}
\frac{d^{2} X}{d x^{2}}+\alpha^{2} X=0, \quad \frac{d^{2} Y}{d y^{2}}+\beta^{2} Y=0, \quad \frac{d^{2} Z}{d z^{2}}-\gamma^{2} Z=0, \tag{2.89}
\end{equation*}
$$

\]

which are related only by Eq. (88) for their parameters. Let us start from the equation for function $X(x)$. Its general solution is the sum of functions $\sin \alpha x$ and $\cos \alpha x$, multiplied by arbitrary coefficients. Let us select these coefficients to satisfy our boundary conditions. First, since $\phi \propto X$ should vanish at the back vertical wall of the box (i.e., with the choice of coordinate origin shown in Fig. 11, at $x=0$ for any $y$ and $z$ ), the coefficient at $\cos \alpha x$ should be zero. The remaining coefficient (at $\sin \alpha x$ ) may be included into the general factor $c_{k}$ in Eq. (84), so that we may take $X$ in the form

$$
\begin{equation*}
X=\sin \alpha x . \tag{2.90}
\end{equation*}
$$

This solution satisfies the boundary condition at the opposite wall $(x=a)$ only if its argument $\alpha a$ is a multiple of $\pi$, i.e. if $\alpha$ is equal to any of the following numbers (commonly called eigenvalues): ${ }^{35}$

$$
\begin{equation*}
\alpha_{n}=\frac{\pi}{a} n, \quad n=1,2, \ldots \tag{2.91}
\end{equation*}
$$

(Terms with negative values of $n$ would not be linearly-independent from those with positive $n$, and may be dropped from the sum (84). Value $n=0$ is formally possible, but would give $X=0$, i.e. $\phi_{k}=0$, at any $x$, i.e. no contribution to sum (84), so it may be dropped as well.) Now we see that we indeed had to take $\alpha$ real, (i.e. $\alpha^{2}$ positive); otherwise, instead of the oscillating function (90) we would have a sum of two exponential functions, which cannot equal zero in two independent points of axis $x$.

Since the equation for function $Y(y)$ is similar to that for $X(x)$, and the boundary conditions on the walls perpendicular to axis $y(y=0$ and $y=b)$ are similar to those for $x$-walls, the absolutely similar reasoning gives

$$
\begin{equation*}
Y=\sin \beta y, \quad \beta_{m}=\frac{\pi}{b} m, \quad m=1,2, \ldots \tag{2.92}
\end{equation*}
$$

where the choice of integer $m$ is independent of that of integer $n$. Now we see that according to Eq. (88), the separation constant $\gamma$ depends on two indices, $n$ and $m$, so that the relation may be rewritten as

$$
\begin{equation*}
\gamma_{n m}=\left[\alpha_{n}^{2}+\beta_{m}^{2}\right]^{1 / 2}=\pi\left[\left(\frac{n}{a}\right)^{2}+\left(\frac{m}{b}\right)^{2}\right]^{1 / 2} . \tag{2.93}
\end{equation*}
$$

The corresponding solution of the differential equation for $Z$ may be presented as a sum of two exponents $\exp \left\{ \pm \gamma_{n m} z\right\}$, or alternatively as a linear combination of two hyperbolic functions, $\sinh \gamma_{n m} z$ and $\cosh \gamma_{n m} z$, with arbitrary coefficients. At our choice of coordinate origin, the latter option is preferable, because $\cosh \gamma_{n m} z$ cannot satisfy the zero boundary condition at the bottom lid of the box $(z=0)$. Hence we may take $Z$ in the form

$$
\begin{equation*}
Z=\sinh \gamma_{n m} z \tag{2.94}
\end{equation*}
$$

[^191]that automatically satisfies that condition.
Now it is the right time to combine Eqs. (84) and (85) for our case in a more explicit form, replacing symbol $k$ for the set of two integer indices $n$ and $m$ :
\[

$$
\begin{equation*}
\phi(x, y, z)=\sum_{n, m=1}^{\infty} c_{n m} \sin \frac{\pi n x}{a} \sin \frac{\pi m y}{b} \sinh \gamma_{n m} z, \tag{2.95}
\end{equation*}
$$

\]

where $\gamma_{n m}$ is given by Eq. (93). This solution satisfies our boundary conditions on all walls of the box, besides the top lid, for arbitrary coefficients $c_{n m}$. The only job left for us is to choose these coefficients from the top-lid requirement:

$$
\begin{equation*}
\phi(x, y, c)=V(x, y)=\sum_{n, m=1}^{\infty} c_{n m} \sin \frac{\pi n x}{a} \sin \frac{\pi m y}{b} \sinh \gamma_{n m} c . \tag{2.96}
\end{equation*}
$$

It seems like a bad luck to have just one equation for the infinite set of coefficients $c_{n m}$. However, the decisive help come from the fact that the functions of $x$ and $y$ that participate in Eq. (96), form full, orthogonal sets of 1D functions. The last term means that the integrals of the products of the functions with different integer indices over the region of interest equal zero. Indeed, direct integration gives

$$
\int_{0}^{a} \sin \frac{\pi n x}{a} \sin \frac{\pi n^{\prime} x}{a} d x= \begin{cases}a / 2, & \text { for } n=n^{\prime},  \tag{2.97}\\ 0, & \text { for } n \neq n^{\prime},\end{cases}
$$

and similarly for $y$ (with evident replacements $a \rightarrow b, n \rightarrow m$ ). Hence, the fruitful way to proceed is to multiply both sides of Eq. (96) by the product of the basis functions, with arbitrary indices $n$ ' and $m^{\prime}$, and integrate the result over $x$ and $y$ :

$$
\begin{equation*}
\int_{0}^{a} d x \int_{0}^{b} d y V(x, y) \sin \frac{\pi n^{\prime} x}{a} \sin \frac{\pi m^{\prime} y}{b}=\sum_{n, m=1}^{\infty} c_{n m} \sinh \gamma_{n m} c \int_{0}^{a} \sin \frac{\pi n x}{a} \sin \frac{\pi n^{\prime} x}{a} d x \times \int_{0}^{b} \sin \frac{\pi m y}{b} \sin \frac{\pi m^{\prime} y}{b} d y \tag{2.98}
\end{equation*}
$$

Due to Eq. (97), all terms in the right-hand part of the last equation, besides those with $n=n$ ' and $m=$ $m^{\prime}$, vanish, and (replacing $n$ ' with $n$, and $m^{\prime}$ with $m$ ) we finally get

$$
\begin{equation*}
c_{n m}=\frac{4}{a b \sinh \gamma_{n m}} \int_{0}^{a} d x \int_{0}^{b} d y V(x, y) \sin \frac{\pi n x}{a} \sin \frac{\pi m y}{b} . \tag{2.99}
\end{equation*}
$$

Relations (93), (95) and (99) present the complete solution of the posed boundary problem; we can see both good and bad news here. The first bit of bad news is that in the general case we still need to work out (formally, the infinite number of) integrals (99). In some cases, it is possible to do this analytically. For example, in our initial problem of constant potential on the top lid, $V(x, y)=\mathrm{const} \equiv V_{0}$, both 1D integrations are elementary; for example

$$
\int_{0}^{a} \sin \frac{\pi n x}{a} d x=\frac{2 a}{\pi n} \times\left\{\begin{array}{lc}
1, & \text { for } n \text { odd }  \tag{2.100}\\
0, & \text { for } n \text { even }
\end{array}\right.
$$

and similarly for the integral over $y$, so that

$$
c_{n m}=\frac{16 V_{0}}{\pi^{2} n m \sinh \gamma_{n m} c} \times\left\{\begin{array}{lr}
1, & \text { if both } n \text { and } m \text { are odd }  \tag{2.101}\\
0, & \text { otherwise }
\end{array}\right.
$$

The second bad news is that even at such a happy occasion, we still have to sum up the series (95), so that our result may only be called analytical with some reservations, because in most cases we need a computer to get the finial numbers or plots.

Now the first good news. Computers are very efficient for both operations (95) and (99), i.e. summation and integration. (As was discussed in Sec. 1.2, random errors are averaged out at these operations.) As an example, Fig. 12 shows the plots of the electrostatic potential in a cubic box ( $a=b=$ c), with an equipotential top lid ( $V=V_{0}=$ const), obtained by numerical summation of series (95), using the analytical expression (101). The remarkable feature of this calculation is the very fast convergence of the series; for the middle cross-section of the cubic box ( $\mathrm{z} / \mathrm{c}=0.5$ ), already the first term (with $n=m$ $=1$ ) gives accuracy about $6 \%$, while the sum of four leading terms (with $n, m=1,3$ ) reduces the error to just $0.2 \%$. (For a longer box, $c>a, b$, the convergence is even faster - see the discussion below.) Only close to the corners between the top lid and the side walls, where the potential changes very rapidly, several more terms are necessary to get a reasonable accuracy.


Fig. 2.12. Distribution of the electrostatic potential within a cubic box $(a=b=c)$ with constant voltage $V_{0}$ on the top lid (Fig. 11), calculated numerically from Eqs. (93), (95) and (101). The dashed line on the left panel shows the contribution of the main term (with $n=m=1$ ) to the full result.

The second good news is that our "semi-analytical" result allow its ultimate limits to be explored analytically. For example, Eq. (93) shows that for a very flat box ( $c \ll a, b$ ), $\gamma_{n, m} z \leq \gamma_{n, m} c \ll 1$ at least for the lowest terms of series (95), with $n, m \ll c / a, c / b$. In these terms, sinh functions in Eqs. (96) and (99) may be well approximated with their arguments, and their ratio by $z / c$. This means that if we limit the summation to these term, Eq. (95) gives a very simple result

$$
\begin{equation*}
\phi(x, y) \approx \frac{z}{c} V(x, y) \tag{2.102}
\end{equation*}
$$

which means that each segment of the flat box behaves just as a plane capacitor. Only near the vertical walls (or near possible locations where $V(x, y)$ is changed sharply), the higher terms in the series (95) are important, producing deviations from Eq. (102). In the opposite limit ( $a, b \ll c$ ), Eq. (93) shows that, in contrast, $\gamma_{n, m} c \gg 1$ for all $n$ and $m$. Moreover, the ratio $\sinh \gamma_{n, m} z / \sinh \gamma_{n, m} c$ drops sharply if either $n$ or $m$ is increased, if $z$ is not too close to $c$. Hence in this case a very good approximation may be obtained by keeping just the leading term, with $n=m=1$, in Eq. (95), so that the problem of summation disappears. (We saw above that this approximation works reasonably well even for a cubic box.) In particular, for the constant potential of the upper lid, we can use Eq. (101) and the exponential asymptotic for both sinh functions, to get a very simple formula:

$$
\begin{equation*}
\phi=\frac{16}{\pi^{2}} \sin \frac{\pi x}{a} \sin \frac{\pi y}{b} \exp \left\{-\pi \frac{\left(a^{2}+b^{2}\right)^{1 / 2}}{a b}(c-z)\right\} \tag{2.103}
\end{equation*}
$$

The same variable separation method may be used to solve more general problems as well. For example, if all walls of the box shown in Fig. 11 have an arbitrary potential distribution, one can use the linear superposition principle to argue that the electrostatic potential distribution inside the box as the sum of 6 partial solutions of the type of Eq. (95), each with one wall biased by the corresponding voltage, and all other grounded ( $\phi=0$ ).

To summarize, the results given by the variable separation method are closer to what we could call a genuinely analytical solution than to purely numerical solutions - see Sec. 6 below. Now, let us explore the issues that arise when this method is applied in other orthogonal coordinate systems.
(ii) Polar coordinates. If a system of conductors is cylindrical, the potential distribution is independent of the coordinate $z$ along the cylinder axis: $\partial \phi / \partial \mathrm{z}=0$, and the Laplace equation becomes two-dimensional. If conductor's cross-section is rectangular, the variable separation method works best in Cartesian coordinates $\{x, y\}$, and is just a particular case of the 3D solution discussed above. However, if the cross-section is circular, much more compact results may be obtained by using polar coordinates $\{\rho, \varphi\}$. As we already know from the last section, these 2D coordinates are orthogonal, so that the two-dimensional Laplace operator is a simple sum. ${ }^{36}$ Requiring, just as we have done above, each component of sum (84) to satisfy the Laplace equation, we get

$$
\begin{equation*}
\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial \phi_{k}}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2} \phi_{k}}{\partial \varphi^{2}}=0 \tag{2.104}
\end{equation*}
$$

In a full analogy with Eq. (75), let us present each particular solution as a product: $\left.\phi_{k}=\mathbb{X} \rho\right) \mathbb{C} \varphi$ ). Plugging this expression into Eq. (104) and then dividing all its parts by $R \mathcal{F} / \rho^{2}$, we get

$$
\begin{equation*}
\frac{\rho}{R} \frac{d}{d \rho}\left(\rho \frac{d R}{d \rho}\right)+\frac{1}{\neq} \frac{d^{2} \neq}{d \varphi^{2}}=0 . \tag{2.105}
\end{equation*}
$$

Following the same reasoning as for the Cartesian coordinates, we get two separated ordinary differential equations

[^192]\[

$$
\begin{align*}
\rho \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right) & =v^{2} R,  \tag{2.106}\\
\frac{d^{2} \neq}{d \varphi^{2}}+v^{2} \neq & =0 \tag{2.107}
\end{align*}
$$
\]

where $v^{2}$ is the variable separation constant.
Let us start their analysis from Eq. (106), plugging into it a probe solution $\mathbb{R}=c \rho^{\alpha}$, where $c$ and $\alpha$ are some constants. Elementary differentiation shows that if $\alpha \neq 0$, the equation is indeed satisfied for any $c$, with just one requirement on constant $\alpha$, namely $\alpha^{2}=v^{2}$. This means that the following linear superposition

$$
\begin{equation*}
R=a_{v} \rho^{+v}+b_{v} \rho^{-v}, \quad \text { for } v \neq 0, \tag{2.108}
\end{equation*}
$$

with constant coefficients $a_{v}$ and $b_{v}$, is also a solution to Eq. (106). Moreover, the general theory of linear ordinary differential equations tells us that the solution of a second-order equation like Eq. (106) may only depend on just two constant factors that scale two linearly-independent functions. Hence, for all values $v^{2} \neq 0$, Eq. (108) presents the general solution of that equation. The case when $v=0$, in which functions $\rho^{+v}$ and $\rho^{-v}$ are just constants and hence are not linearly-independent, is special, but in this case the integration of Eq. (106) is straightforward, ${ }^{37}$ giving

$$
\begin{equation*}
尺=a_{0}+b_{0} \ln \rho, \quad \text { for } v=0 \tag{2.109}
\end{equation*}
$$

In order to specify the separation constant, we should use Eq. (107), whose general solution is

$$
\neq \begin{cases}c_{v} \cos v \varphi+s_{v} \sin v \varphi, & \text { for } v \neq 0,  \tag{2.110}\\ c_{0}+s_{0} \varphi, & \text { for } v=0 .\end{cases}
$$

There are two possible cases here. In many boundary problems solvable in cylindrical coordinates, the free space region, in which the Laplace equation is valid, extends continuously around the origin point $\rho$ $=0$. In this region, the potential has to be continuous and uniquely defined, so that $\nexists$ has to be a $2 \pi$ periodic function of angle $\varphi$. For that, one needs $v(\varphi+2 \pi)$ to be equal to $v(\varphi+2 \pi n)$, with $n$ an integer, immediately giving us a discrete spectrum of possible values of the variable separation constant:

$$
\begin{equation*}
v=n=0, \pm 1, \pm 2, \ldots \tag{2.111}
\end{equation*}
$$

In this case both functions $\mathbb{R}$ and $\neq 7$ may be labeled with the integer index $n$. Taking into account that the terms with negative values of $n$ may be summed up with those with positive $n$, and that $s_{0}$ should equal zero (otherwise the $2 \pi$-periodicity of function 7 would be violated), we see that the general solution to the 2D Laplace equation may be presented as

Variable separation in polar coordinates

$$
\begin{equation*}
\phi(\rho, \varphi)=a_{0}+b_{0} \ln \rho+\sum_{n=1}^{\infty}\left(a_{n} \rho^{n}+\frac{b_{n}}{\rho^{n}}\right)\left(c_{n} \cos n \varphi+s_{n} \sin n \varphi\right) . \tag{2.112}
\end{equation*}
$$

Let us see how all this machinery works on the classical problem of a round cylindrical conductor placed into an electric field that is uniform and perpendicular to cylinder's axis at large
${ }^{37}$ Actually, we have already done it in Sec. 3 - see Eq. (43).
distances - see Fig. 13a. ${ }^{38}$ First of all, let us explore the effect of system's symmetries on coefficients in Eq. (112). Selecting the coordinate system as shown in Fig. 13a, and taking the cylinder's potential for zero, we immediately have $a_{0}=0$. Moreover, due to the mirror symmetry about plane $[x, z]$, the solution has to be an even function of angle $\varphi$, and hence all coefficients $s_{n}$ should also equal zero. Also, at large distances $(\rho \gg R)$ from the cylinder axis its effect on the electric field should vanish, and the potential should approach that of the uniform field $\mathbf{E}=E_{0} \mathbf{n}_{x}$ :

$$
\begin{equation*}
\phi \rightarrow-E_{0} x=-E_{0} \rho \cos \varphi, \quad \text { for } \rho \rightarrow \infty . \tag{2.113}
\end{equation*}
$$

This is only possible if in Eq. (112), $b_{0}=0$, and also all coefficients $a_{n}$ with $n \neq 1$ vanish, while product $a_{1} c_{1}$ should be equal to $\left(-E_{0}\right)$. Thus the solution is reduced to the following form

$$
\begin{equation*}
\phi(\rho, \varphi)=-E_{0} \rho \cos \varphi+\sum_{n=1}^{\infty} \frac{B_{n}}{\rho^{n}} \cos n \varphi, \tag{2.114}
\end{equation*}
$$

in which coefficients $B_{n} \equiv b_{n} c_{n}$ should be found from the boundary condition on the cylinder's surface, i.e. at $\rho=R$ :

$$
\begin{equation*}
\phi(R, \varphi)=0 . \tag{2.115}
\end{equation*}
$$



Fig. 2.13. Conducting cylinder inserted into an initially uniform electric field perpendicular to is axis: (a) the problem's geometry, and (b) the equipotential surfaces given by Eq. (117).

This requirement yields the following equation,

$$
\begin{equation*}
\left(\frac{B_{1}}{R}-E_{0} R\right) \cos \varphi+\sum_{n=2}^{\infty} \frac{B_{n}}{R^{n}} \cos n \varphi=0, \tag{2.116}
\end{equation*}
$$

[^193]which should be satisfied for all $\varphi$. But since functions $\cos n \varphi$ are orthogonal, this equality is only possible if all $B_{n}$ for $n \geq 2$ are equal zero, while $B_{1}=E_{0} R^{2}$. Hence our final answer (which is of course only valid outside of the cylinder, i.e. for $\rho \geq R$ ), is
\[

$$
\begin{equation*}
\phi(\rho, \varphi)=-E_{0}\left(\rho-\frac{R^{2}}{\rho}\right) \cos \varphi=-E_{0}\left(1-\frac{R^{2}}{x^{2}+y^{2}}\right) x . \tag{2.117}
\end{equation*}
$$

\]

This result (Fig. 13b) shows a smooth transition between the uniform field (113) far from the cylinder, to the equipotential surface of the cylinder (with $\phi=0$ ). Such smoothening is very typical for Laplace equation solutions. Indeed, as we know from Chapter 1, these solutions corresponds to the lowest potential energy (1.67), and hence the lowest values of potential gradient modulus, possible at the given boundary conditions.

To complete the problem, let us calculate the distribution of the surface charge density over the cylinder's cross-section, using Eq. (3):

$$
\begin{equation*}
\sigma=\left.\varepsilon_{0} E_{n}\right|_{\text {surface }}=-\left.\varepsilon_{0} \frac{\partial \phi}{\partial \rho}\right|_{\rho=R}=\left.\varepsilon_{0} E_{0} \cos \varphi \frac{\partial}{\partial \rho}\left(\rho-\frac{R^{2}}{\rho}\right)\right|_{\rho_{=R}}=2 \varepsilon_{0} E_{0} \cos \varphi . \tag{2.118}
\end{equation*}
$$

This very simple formula shows that at the field direction shown in Fig. 13a ( $E_{0}>0$ ), the surface charge is positive on the right side of the cylinder and negative on its left side, thus creating a field directed from the right to the left, that compensates the external field inside the conductor, where the net field is zero. Note also that the net electric charge of the cylinder is zero, in the correspondence with the problem symmetry. Another useful by-product of calculation (118) is that the surface electric field equals $2 E_{0} \cos \varphi$, and hence its largest magnitude is twice the field far from the cylinder. Such electric field concentration is very typical for all convex conducting surfaces.

The last observation gets additional confirmation for the second possible topology, when Eq. (110) is used to describe problems with no angular periodicity. A typical example is a cylindrical conductor with a cross-section that features a corner limited by straight lines (Fig. 14). Indeed, at we may argue that at $\rho<R$ (where $R$ is the scale of radial extension of the straight sides of the corner), the Laplace equation may be satisfied by a sum of partial solutions $\mathbb{Z}(\rho)$ 民 $\varphi$ ) if the angular components of the products satisfy the boundary conditions on the corner sides. Taking (just for the simplicity of notation) the conductor's potential to be zero, and one of the corner's sides as axis $x(\varphi=0)$, these boundary conditions are

$$
\begin{equation*}
7(0)=7(\beta)=0, \tag{2.119}
\end{equation*}
$$

where angle $\beta$ may be anywhere between 0 and $2 \pi$ (Fig. 14).


Fig. 2.14. Cylindrical conductor cross-sections with (a) a corner and (b) a wedge.

Comparing this condition with Eq. (110), we see that it requires $c_{v}$ to vanish, and $v$ to take one of the values of the following discrete spectrum:

$$
\begin{equation*}
v_{m}=(\pi / \beta) m, \tag{2.120}
\end{equation*}
$$

with positive integer $m$. Hence the full solution of the Laplace equation takes the form

$$
\begin{equation*}
\phi=\sum_{m=1}^{\infty} a_{m} \rho^{\pi m / \beta} \sin \frac{\pi m \varphi}{\beta}, \quad \text { for } \rho<R, \tag{2.121}
\end{equation*}
$$

where constants $s_{\nu}$ have been incorporated into $a_{m}$. The set of constants $a_{m}$ cannot be simply determined, because it depends on the exact shape of the conductor outside the corner, and the externally applied electric field. However, whatever the set is, in the limit $\rho \rightarrow 0$, solution (121) is almost ${ }^{39}$ always dominated by the term with lowest $v$ (corresponding to $m=1$ ),

$$
\begin{equation*}
\phi \rightarrow a_{1} \rho^{\pi / \beta} \sin \frac{\pi}{\beta} \varphi \tag{2.122}
\end{equation*}
$$

because the higher terms go to zero faster. This potential distribution corresponds to the surface charge density

$$
\begin{equation*}
\sigma=\left.\varepsilon_{0} E_{n}\right|_{\text {surface }}=-\left.\varepsilon_{0} \frac{\partial \phi}{\partial(\rho \varphi)}\right|_{\rho=\text { const, } \varphi \rightarrow+0}=-\varepsilon_{0} \frac{\pi a_{1}}{\beta} \rho^{(\pi / \beta-1)} . \tag{2.123}
\end{equation*}
$$

(It is similar on the opposite face of the angle.)
Equation (123) shows that if we are dealing with a usual, concave corner ( $\beta<\pi$, see Fig. 14a), the charge density (and the surface electric field) tends to zero. On the other case, at a "convex corner" with $\beta>\pi$ (actually, a wedge - see Fig. 14b), both charge and field concentrate, formally diverging at $\rho$ $\rightarrow 0$. (So, do not sit on a roof's ridge during a thunderstorm; rather hide in a ditch!) We already saw qualitatively similar effects at our analyses of the thin round disk and split plane in the past section.
(iii) Cylindrical coordinates. Now, let us discuss whether it is possible to generalize our approach to problems whose geometry is still axially-symmetric, but with a substantial dependence of the potential on the axial coordinate $(\partial \phi / \partial \mathrm{z} \neq 0)$. The classical example of such a problem is shown in Fig. 15. Here the side wall and the bottom lid of a round cylinder are kept at fixed potential (say, $\phi=0$ ), but the potential $V$ fixed at the top lid is different. This problem is qualitatively similar to the rectangular box problem solved above (Fig. 11), and we will also try to solve it for the case of arbitrary voltage distribution over the top lid: $V=V(\rho, \varphi)$.


Fig. 2.15. Round cylinder with conducting walls.

[^194]Following the main idea of the variable separation method，let us require that each partial function $\phi_{k}$ in Eq．（84）satisfies the Laplace equation，now in full cylindrical coordinates $\{\rho, \varphi, z\}: 40$

$$
\begin{equation*}
\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial \phi_{k}}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2} \phi_{k}}{\partial \varphi^{2}}+\frac{\partial^{2} \phi_{k}}{\partial z^{2}}=0 \tag{2.124}
\end{equation*}
$$

Plugging in $\phi_{k}$ in the form $\mathbb{R}(\rho) \mathcal{Z}(\varphi) \mathcal{Z}(z)$ into Eq．（124）and dividing both parts by product $\mathbb{R} \mathcal{Z}$ ，we get

$$
\begin{equation*}
\frac{1}{\rho 尺} \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right)+\frac{1}{\rho^{2} \neq} \frac{d^{2} \neq}{d \varphi^{2}}+\frac{1}{Z} \frac{d^{2} \mathcal{Z}}{d z^{2}}=0 . \tag{2.125}
\end{equation*}
$$

Since the first two terms of Eq．（125）can only depend on polar variables $\rho$ and $\varphi$ ，while the third term， only on $z$ ，at least that term should be a constant．Denoting it（just like in the rectangular box problem） by $\gamma^{2}$ ，we get，instead of Eq．（125），a set of two equations：

$$
\begin{gather*}
\frac{d^{2} \mathcal{z}}{d z^{2}}=\gamma^{2} \boldsymbol{z},  \tag{2.126}\\
\frac{1}{\rho 尺} \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right)+\gamma^{2}+\frac{1}{\rho^{2} \neq \frac{d^{2} \neq}{d \varphi^{2}}=0 .} \tag{2.127}
\end{gather*}
$$

Now，multiplying all the terms of Eq．（127）by $\rho^{2}$ ，we see that the last term，$\left(d^{2} \neq / d \varphi^{2}\right) / \mathcal{7}$ ，may depend only on $\varphi$ ，and thus should be constant．Calling that constant $\nu^{2}$（as in Sec．（ii）above），we separate Eq． （127）into an angular equation，

$$
\begin{equation*}
\frac{d^{2} \neq}{d \varphi^{2}}+v^{2} \neq 0, \tag{2.128}
\end{equation*}
$$

and a radial equation：

$$
\begin{equation*}
\frac{d^{2} R}{d \rho^{2}}+\frac{1}{\rho} \frac{d R}{d \rho}+\left(\gamma^{2}-\frac{v^{2}}{\rho^{2}}\right) R=0 . \tag{2.129}
\end{equation*}
$$

We see that the ordinary differential equations for functions $\mathcal{Z}(z)$ and $\mathcal{X}(\varphi)$（and hence their solutions）are identical to those discussed earlier in this section．However，Eq．（129）for the radial function $R(\rho)$（called the Bessel equation）is more complex than in the 2D case，and depends on two independent constant parameters，$\gamma$ and $\nu$ ．The latter challenge may be readily overcome if we notice that any change of $\gamma$ may be reduced to re－scaling the radial coordinate $\rho$ ．Indeed，introducing a dimensionless variable $\xi \equiv \gamma \rho,{ }^{41} \mathrm{Eq}$ ．（129）may be reduced to an equation with just one parameter，$v$ ．

$$
\begin{equation*}
\frac{d^{2} R}{d \xi^{2}}+\frac{1}{\xi} \frac{d R}{d \xi}+\left(1-\frac{v^{2}}{\xi^{2}}\right) 尺=0 \tag{2.130}
\end{equation*}
$$

[^195]Moreover, we already know that for angle-periodic problems the spectrum of eigenvalues of Eq. (128) is discrete $v=n$.

Unfortunately, even in this case, Eq. (130) cannot be satisfied by a single "elementary" function, and is the canonical form of an equation defining the Bessel function of the first kind, of order $v$, commonly denoted as $J_{\cup}(\xi)$. Let me review in brief the Bessel function properties most relevant for the boundary problems of physics - and some other problems discussed in these notes. ${ }^{42}$

First of all, the Bessel function of a negative integer order is very simply related to that with the positive order:

$$
\begin{equation*}
J_{-n}(\xi)=(-1)^{n} J_{n}(\xi) \tag{2.131}
\end{equation*}
$$

enabling us to limit our discussion to the functions with $n \geq 0$. Figure 16 shows four functions with a few lowest positive $n$.


Fig. 2.16. Several first-kind Bessel functions $J_{n}(\xi)$ of integer order. Dashed lines show the envelope of asymptotes (135).

As its argument is increased, each function is initially close to a power law: $J_{0}(\xi) \approx 1, J_{1}(\xi) \approx$ $\xi / 2=\xi / 2, J_{2}(\xi) \approx \xi^{2} / 8$, etc. This behavior follows from the Taylor series

$$
\begin{equation*}
J_{n}(\xi)=\left(\frac{\xi}{2}\right)^{n} \sum_{k=0}^{\infty} \frac{(-1)^{k}}{k!(n+k)!}\left(\frac{\xi}{2}\right)^{2 k} \tag{2.132}
\end{equation*}
$$

which that is formally valid for any $\xi$, and may even serve as an alternative definition of function $J_{n}(\xi)$. However, this series is converging fast only at relatively small arguments, $\xi<n$, where its main term is

[^196]\[

$$
\begin{equation*}
\left.J_{n}(\xi)\right|_{\xi \rightarrow 0} \rightarrow \frac{1}{n!}\left(\frac{\xi}{2}\right)^{n} . \tag{2.133}
\end{equation*}
$$

\]

At $\xi \approx n+1.86 n^{1 / 3}$, the Bessel function reaches its maximum ${ }^{43}$

$$
\begin{equation*}
\max _{\xi}\left[J_{n}(\xi)\right] \approx \frac{0.675}{n^{1 / 3}}, \tag{2.134}
\end{equation*}
$$

and then starts to oscillate with a period that gradually approaches $2 \pi$, a phase shift that increases by $\pi / 2$ with each unit increment of $n$, and an amplitude that decreases as $\xi^{1 / 2}$. These features are described by the following asymptotic formula

$$
\begin{equation*}
J_{n}(\xi) \rightarrow\left(\frac{2}{\pi \xi}\right)^{1 / 2} \cos \left(\xi-\frac{\pi}{4}-\frac{n \pi}{2}\right), \quad \text { for } \xi / n \rightarrow \infty \tag{2.135}
\end{equation*}
$$

that starts to give reasonable results very soon above the function peaks - see Fig. 16. ${ }^{44}$
Now we are ready to return to our case study (Fig. 15). Let us select functions $\mathfrak{Z}(z)$ to satisfy the bottom-lid boundary condition $\mathcal{Z}(0)=0$, i.e. proportional to $\sinh \gamma z-\mathrm{cf}$. Eq. (95). Then

$$
\begin{equation*}
\phi=\sum_{n=0}^{\infty} \sum_{\gamma} J_{n}(\gamma \rho)\left(c_{n \gamma} \cos n \varphi+s_{n \gamma} \sin n \varphi\right) \sinh \gamma z . \tag{2.136}
\end{equation*}
$$

Next, we need to satisfy the zero boundary condition at the cylinder's side wall $(\rho=R)$. This may be ensured by taking

$$
\begin{equation*}
J_{n}(\gamma R)=0 . \tag{2.137}
\end{equation*}
$$

Since each function $J_{n}(x)$ has an infinite number of positive zeros (see Fig. 16), which may be numbered by an integer index $m=1,2, \ldots$, Eq. (137) may be satisfied with an infinite number of discrete values of the separation parameter $\gamma$.

$$
\begin{equation*}
\gamma_{n m}=\frac{\xi_{n m}}{R}, \tag{2.138}
\end{equation*}
$$

where $\xi_{n m}$ is the $m$-th zero of function $J_{n}(x)$ - see the top numbers in the cells of Table 1. (Very soon we will see what do we need the bottom numbers for.)

Hence, Eq. (136) may be presented in a more explicit form:

$$
\begin{equation*}
\phi(\rho, \varphi, z)=\sum_{n=0}^{\infty} \sum_{m=1}^{\infty} J_{n}\left(\xi_{n m} \frac{\rho}{R}\right)\left(c_{n m} \cos n \varphi+s_{n m} \sin n \varphi\right) \sinh \left(\xi_{n m} \frac{z}{R}\right) . \tag{2.139}
\end{equation*}
$$

[^197]Here coefficients $c_{n m}$ and $s_{n m}$ have to be selected to satisfy the only remaining boundary condition - that on the top lid:

$$
\begin{equation*}
V(\rho, \varphi)=\phi(\rho, \varphi, L)=\sum_{n=0}^{\infty} \sum_{m=1}^{\infty} J_{n}\left(\xi_{n m} \frac{\rho}{R}\right)\left(c_{n m} \cos n \varphi+s_{n m} \sin n \varphi\right) \sinh \left(\xi_{n m} \frac{L}{R}\right) . \tag{2.140}
\end{equation*}
$$

To use it, let us multiply both parts of Eq. (140) by $J_{n}\left(\xi_{n m} ’ \rho / R\right) \cos n^{\prime} \varphi$, integrate the result over the lid area, and use the following property of the Bessel functions:

$$
\begin{equation*}
\int_{0}^{1} J_{n}\left(\xi_{n m} s\right) J_{n}\left(\xi_{n m^{\prime}} s\right) s d s=\frac{1}{2}\left[J_{n+1}\left(\xi_{n m}\right)\right]^{2} \delta_{m m^{\prime}}, \tag{2.141}
\end{equation*}
$$

where $\delta_{m m}$, is the Kronecker symbol. ${ }^{45}$
Table 2.1. Approximate values of a few first zeros of a few lowest-order Bessel functions $J_{n}(\xi)$ (the top number in each cell), and the values of $d J_{n} / d \xi$ at those points (the bottom number in the cell).

|  | $m=1$ | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n=0$ | 2.40482 | 5.52008 | 8.65372 | 11.79215 | 14.93091 | 18.07106 |
|  | -0.51914 | +0.34026 | -0.27145 | +0.23245 | -0.20654 | +0.18773 |
| 1 | 3.83171 | 7.01559 | 10.17347 | 13.32369 | 16.47063 | 19.61586 |
|  | -0.40276 | +0.30012 | -0.24970 | +0.21836 | -0.19647 | +0.18006 |
| 2 | 5.13562 | 8.41724 | 11.61984 | 14.79595 | 17.95982 | 21.11700 |
|  | -0.33967 | +0.27138 | -0.23244 | +0.20654 | -0.18773 | +0.17326 |
| 3 | 6.38016 | 9.76102 | 13.01520 | 16.22347 | 19.40942 | 22.58273 |
|  | -0.29827 | +0.24942 | -0.21828 | +0.19644 | -0.18005 | +0.16718 |
| 4 | 7.58834 | 11.06471 | 14.37254 | 17.61597 | 20.82693 | 24.01902 |
|  | -0.26836 | +0.23188 | -0.20636 | +0.18766 | -0.17323 | +0.16168 |
| 5 | 8.77148 | 12.33860 | 15.70017 | 18.98013 | 22.21780 | 25.43034 |
|  | -0.24543 | +0.21743 | -0.19615 | +0.17993 | -0.16712 | +0.15669 |

Relation (141) expresses a very specific ("2D") orthogonality of Bessel functions with different indices $m$ - do not confuse them with the function's order $n$, please! ${ }^{46}$ Since it relates two Bessel functions with the same index $n$, it is natural to ask why its right-hand part contains the function with a different index $(n+1)$. Some clue may come from one more very important property of the Bessel functions, the so-called recurrence relations: ${ }^{47}$
${ }^{45}$ Let me hope the reader knows what it is; if not - see MA Eq. (13.1).
${ }^{46}$ The Bessel functions of the same argument but of different orders are also orthogonal, but in a different way:

$$
\int_{0}^{\infty} J_{n}(\xi) J_{n^{\prime}}(\xi) \frac{d \xi}{\xi}=\frac{1}{n+n^{\prime}} \delta_{n n^{\prime}}
$$

${ }^{47}$ These relations provide, in particular, a convenient way for fast numerical computation of all $J_{n}(\xi)$ after $J_{0}(\xi)$ has been computed. (The latter is usually done with an algorithm using Eq. (132) for smaller $\xi$ and an extension of Eq. (135) for larger $\xi$.) Note that most mathematical software packages, including all those listed in MA Sec. 16(iv), include ready subroutines for calculation of functions $J_{n}(\xi)$ and other special functions used in this lecture series. In this sense, the line separated these "special functions" from "elementary functions" is rather blurry.

$$
\begin{align*}
& J_{n-1}(\xi)+J_{n+1}(\xi)=\frac{2 n J_{n}(\xi)}{\xi}  \tag{2.142a}\\
& J_{n-1}(\xi)-J_{n+1}(\xi)=2 \frac{d J_{n}(\xi)}{d \xi} \tag{2.142b}
\end{align*}
$$

that in particular yield the following relation (convenient for working out some Bessel function integrals):

$$
\begin{equation*}
\frac{d}{d \xi}\left(\xi^{n} J_{n}(\xi)\right)=\xi^{n} J_{n-1}(\xi) \tag{2.143}
\end{equation*}
$$

For our current purposes, let us apply the recurrence relations at special points $\xi_{n m}$. At these points, $J_{n}$ vanishes, and the system of two equations (142) may be readily solved to get, in particular,

$$
\begin{equation*}
J_{n+1}\left(\xi_{n m}\right)=-\frac{d J_{n}}{d \xi}\left(\xi_{n m}\right) \tag{2.144}
\end{equation*}
$$

so that the square bracket in the right-hand part of Eq. (141) is just $\left(d J_{n} / d \xi\right)^{2}$ at $\xi=\xi_{n m}$. Thus the values of the Bessel function derivatives at the zero points (given by the lower numbers in the cells of Table 1) are as important for boundary problem solutions as the zeros themselves.

Since the angular functions $\cos n \varphi$ are also orthogonal - both to each other,

$$
\begin{equation*}
\int_{0}^{2 \pi} \cos (n \varphi) \cos \left(n^{\prime} \varphi\right) d \varphi=\pi \delta_{n n^{\prime}} \tag{2.145}
\end{equation*}
$$

and to all functions $\sin n \varphi$, the integration over the lid area kills all terms of both series in right-hand part of Eq. (140), besides just one term proportional to $c_{n^{\prime} m^{\prime}}$, and hence gives an explicit expression for that coefficient. The counterpart coefficients $s_{n^{\prime} m}$ may be found by repeating the same procedure with the replacement of $\cos n^{\prime} \varphi$ by $\sin n^{\prime} \varphi$. This evaluation (left for reader's exercise) completes the solution of our problem for an arbitrary lid potential $V(\rho, \varphi)$.

Still, before leaving the Bessel functions (for a while :-), we need to address two important issues. First, we have seen that in our cylinder problem (Fig. 15), the set of functions $J_{n}\left(\xi_{n m} \rho / R\right)$ with different indices $m$ (that characterize the degree of Bessel function's stretch along axis $\rho$ ) play the role similar to that of functions $\sin (\pi n x / a)$ in the rectangular box problem shown in Fig. 11. In this context, what is the analog of functions $\cos (\pi n x / a)$ - which may be important for some boundary problems? In a more formal language, are there any functions of the same argument $\xi \equiv \xi_{n m} \rho / R$, that would be linearly independent of the Bessel functions of the first kind, while satisfying the same differential equation (130)?

The answer is yes. For the definition of such functions, we first need to generalize our prior formulas for $J_{n}(\xi)$, and in particular Eq. (132), to the case of arbitrary order $v$. The generalization may be performed in the following way:

$$
\begin{equation*}
J_{v}(\xi)=\left(\frac{\xi}{2}\right)^{v} \sum_{k=0}^{\infty} \frac{(-1)^{k}}{k!\Gamma(v+k+1)}\left(\frac{\xi}{2}\right)^{2 k} \tag{2.146}
\end{equation*}
$$

where $\Gamma(s)$ is the so-called gamma function that may be defined, for almost any real $s$, as ${ }^{48}$

$$
\begin{equation*}
\Gamma(s) \equiv \int_{0}^{\infty} \xi^{s-1} e^{-\xi} d \xi \tag{2.147}
\end{equation*}
$$

The simplest, and the most important property of the gamma function is that for integer values of argument it gives the factorial of a number smaller by one:

$$
\begin{equation*}
\Gamma(n+1)=n!\equiv 1 \cdot 2 \cdot \ldots n \tag{2.148}
\end{equation*}
$$

so it is essentially a generalization of the notion of factorial to all real numbers.
The Bessel functions defined by Eq. (146) satisfy (after replacements $n \rightarrow v$ and $n!\rightarrow \Gamma(n+1)$ ), virtually all the relations we have discussed above, including the Bessel equation (130), the asymptotic formula (135), the orthogonality condition (141), and the recurrence relations (142). Moreover, it may be shown that $v \neq n$, functions $J_{V}(\xi)$ and $J_{-1}(\xi)$ are linearly independent and hence their linear combination may be used to present a general solution of the Bessel equation. Unfortunately, as Eq. (131) shows, for $v=n$ this is not true, and a solution independent of $J_{n}(\xi)$ has to be formed in a different way.

The most common way of overcoming this difficulty is first to define, for all $v \neq n$, function

$$
\begin{equation*}
Y_{v}(\xi) \equiv \frac{J_{v}(\xi) \cos v \pi-J_{-v}(\xi)}{\sin v \pi} \tag{2.149}
\end{equation*}
$$

called the Bessel function of second kind, or more often as the Weber functions, ${ }^{49}$ and then to follow the limit $v \rightarrow n$. At this, both the numerator and denominator of the right-hand part of Eq. (149) tend to zero, but their ratio tends to a finite value called $Y_{n}(x)$. It may be shown that these functions are still the solutions of the Bessel equation and are linearly independent of $J_{n}(x)$, though are related just as those functions if the sign of $n$ changes:

$$
\begin{equation*}
Y_{-n}(\xi)=(-1)^{n} Y_{n}(\xi) \tag{2.150}
\end{equation*}
$$

Figure 17 shows a few Weber functions of the lowest integer orders. The plots show that the asymptotic behavior is very much similar to that of $J_{n}(\xi)$,

$$
\begin{equation*}
Y_{n}(\xi) \rightarrow\left(\frac{2}{\pi \xi}\right)^{1 / 2} \sin \left(\xi-\frac{\pi}{4}-\frac{n \pi}{2}\right), \quad \text { for } \xi \rightarrow \infty \tag{2.151}
\end{equation*}
$$

but with the phase shift necessary to make these Bessel functions orthogonal to those of the fist order cf. Eq. (135). However, for small values of argument $\xi$, the Bessel functions of the second kind behave completely differently from those of the first kind:

$$
Y_{n}(\xi) \rightarrow \begin{cases}(2 / \pi)[\ln (\xi / 2)+\gamma], & \text { for } n=0,  \tag{2.152}\\ -\frac{(n-1)!}{\pi}\left(\frac{\xi}{2}\right)^{-n}, & \text { for } n \neq 0,\end{cases}
$$

[^198]where
\[

$$
\begin{equation*}
\gamma \equiv \lim _{n \rightarrow \infty}\left(1+\frac{1}{2}+\frac{1}{3}+\ldots+\frac{1}{n}-\ln n\right) \approx 0.577157 \ldots \tag{2.153}
\end{equation*}
$$

\]

is the so-called Euler constant. Relations (152) and Fig. 17 show that functions $Y_{n}(\xi)$ diverge at $\xi \rightarrow 0$ and hence cannot describe the behavior of any physical variable, in particular the electrostatic potential.


Fig. 2.17. A few Bessel functions of the second kind (a.k.a. the Neumann functions, a.k.a. the Weber functions).

One may wonder: if this is true, when do we need these functions in physics? This does not happen too often, but still does. Figure 18 shows an example of a boundary problem of electrostatics that requires both functions $J_{n}(\xi)$ and $Y_{n}(\xi)$.


Fig. 2.18. Simple boundary problem that cannot be solved using just one kind of Bessel functions.

Two round, coaxial conducting cylinders are kept at the same (say, zero) potential, but at least one of two horizontal lids has a different potential. The problem is almost completely similar to that discussed above (Fig. 15), but now we need to find the potential distribution in the free space between the cylinders, $R_{1}<\rho<R_{2}$. If we use the same variable separation as in the simpler counterpart problem,
we need the radial functions $\mathbb{R}(\rho)$ to satisfy two zero boundary conditions：at $\rho=R_{1}$ and $\rho=R_{2}$ ．With the Bessel functions of just first kind，$J_{n}(\gamma \rho)$ ，it is impossible to do，because the two boundaries would impose two independent（and generally incompatible）conditions，$J_{n}\left(\gamma R_{1}\right)=0$ ，and $J_{n}\left(\gamma R_{2}\right)=0$ ，for one ＂compression parameter＂$\gamma$ ．The existence of the Bessel functions of the second kind immediately saves the day，because if a solution is presented as a linear combination，${ }^{50}$

$$
\begin{equation*}
c_{J} J_{n}(\gamma \rho)+c_{Y} Y_{n}(\gamma \rho), \tag{2.154}
\end{equation*}
$$

two zero boundary conditions give two equations for $\gamma$ and ratio $c \equiv c_{Y} / c_{J}$ ．（Due to the oscillating character of both Bessel functions，these conditions would be typically satisfied by an infinite set of discrete pairs $\{\gamma, c\}$ ．）Note，however，that generally none of these pairs would correspond to zeros of either $J_{n}$ nor $Y_{n}$ ，so that having an analog of Table 1 for the latter function would not help much．Hence， even the simple problems of this kind（like the one shown in Fig．18）typically require numerical solutions of algebraic（transcendental）equations．

One more issue we need to address，before moving on to the spherical coordinates，are the so－ called modified Bessel functions：of the first kind，$I_{\downarrow}(\xi)$ ，and of the second kind，$K_{V}(\xi)$ ．They are two linearly－independent solutions of the modified Bessel equation，

$$
\begin{equation*}
\frac{d^{2} 尺}{d \xi^{2}}+\frac{1}{\xi} \frac{d 尺}{d \xi}-\left(1+\frac{v^{2}}{\xi^{2}}\right) 尺=0 \tag{2.155}
\end{equation*}
$$

Modified Bessel equation
that differs from Eq．（130）＂only＂by the sign of one of its terms．Figure 19 shows a simple problem that leads to this equation：a round conducting cylinder is sliced，perpendicular to its axis，to rings of equal height $h$ ，which are kept at equal but sign－alternating potentials．


Fig．2．19．Typical boundary problem whose solution may be conveniently described in terms of the modified Bessel functions．

If the gaps between the sections are narrow，$t \ll h$ ，we may use the variable separation method for the solution to this problem，but now we evidently need periodic（rather than exponential）solutions

[^199]along axis $z$, i.e. linear combinations of $\sin k z$ and $\cos k z$ with various real values of constant $k$. Separating the variables, we arrive at a differential equation similar to Eq. (129), but with the negative sign before the separation constant:
\[

$$
\begin{equation*}
\frac{d^{2} R}{d \rho^{2}}+\frac{1}{\rho} \frac{d R}{d \rho}-\left(k^{2}+\frac{v^{2}}{\rho^{2}}\right) R=0 . \tag{2.156}
\end{equation*}
$$

\]

Radial coordinate normalization, $\xi \equiv k \rho$, immediately leads us to Eq. (155), and hence (for $v=n$ ) to the modified Bessel functions $I_{n}(\xi)$ and $K_{n}(\xi)$.

Figure 20 shows the behavior of a few such functions, of a few lowest orders. One can see that at $\xi \rightarrow 0$ it is virtually similar to that of the "usual" Bessel functions - cf. Eqs. (132) and (152), with $K_{n}(\xi)$ multiplied (due to purely historical reasons) by an additional coefficient, $\pi / 2$ :

$$
I_{n}(\xi) \rightarrow \frac{1}{n!}\left(\frac{\xi}{2}\right)^{n}, \quad K_{n}(\xi) \rightarrow \begin{cases}-\left[\ln \left(\frac{\xi}{2}\right)+\gamma\right], & \text { for } n=0  \tag{2.157}\\ \frac{(n-1)!}{2}\left(\frac{\xi}{2}\right)^{-n}, & \text { for } n \neq 0\end{cases}
$$

However, the asymptotic behavior of the modified functions is very much different, with $I_{n}(x)$ exponentially growing and $K_{n}(\xi)$ exponentially dropping at $\xi \rightarrow \infty$ :

$$
\begin{equation*}
I_{n}(\xi) \rightarrow\left(\frac{1}{2 \pi \xi}\right)^{1 / 2} e^{\xi}, \quad K_{n}(\xi) \rightarrow\left(\frac{\pi}{2 \xi}\right)^{1 / 2} e^{-\xi} \tag{2.158}
\end{equation*}
$$




Fig. 2.20. Modified Bessel functions of the first kind (left panel) and the second kind (right panel).

To complete our brief survey of the Bessel functions, let me note that all the functions we have discussed so far may be considered as particular cases of Bessel functions of the complex argument, say $J_{n}(\boldsymbol{z})$ and $Y_{n}(\boldsymbol{z})$, or, alternatively, $H_{n}^{(1,2)}(\boldsymbol{z})=J_{n}(\boldsymbol{z}) \pm i Y_{n}(\boldsymbol{z}) .{ }^{51}$ The "usual" Bessel functions $J_{n}(\xi)$ and

[^200]$Y_{n}(\xi)$ may be considered as a set of values of these generalized functions on the real axis $(\boldsymbol{z}=\xi)$, while the modified functions as their particular case at $\boldsymbol{z}=i \xi$ :
\[

$$
\begin{equation*}
I_{\nu}(\xi)=i^{-v} J_{v}(i \xi), \quad K_{v}(\xi)=\frac{\pi}{2} i^{v+1} H_{v}^{(1)}(i \xi) \tag{2.159}
\end{equation*}
$$

\]

Moreover, this generalization of the Bessel functions to the whole complex plane $z$ enables the use of their values along other directions on that plane, for example under angles $\pi / 4 \pm \pi / 2$. As a result, one arrives at the so-called Kelvin functions

$$
\begin{align*}
& \operatorname{ber}_{v} \xi+i \operatorname{bei}_{\nu} \xi \equiv J_{v}\left(\xi e^{-i \pi / 4}\right) \\
& \operatorname{ker}_{v} \xi+i \operatorname{kei}_{v} \xi \equiv i \frac{\pi}{2} H_{v}^{(1)}\left(\xi e^{-i 3 \pi / 4}\right) \tag{2.160}
\end{align*}
$$

which are also useful for some important problems of mathematical physics and engineering. Unfortunately, we do not have time to discuss these problems in this course. ${ }^{52}$
(iv) Spherical coordinates are very important in physics, because of the (approximate) spherical symmetry of many objects - from electrons and nuclei and atoms to planets and stars. Let us again require each component $\phi_{k}$ of Eq. (84) to satisfy the Laplace equation. Using the well known expression for the Laplace operator in spherical coordinates, ${ }^{53}$ we get

$$
\begin{equation*}
\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial \phi_{k}}{\partial r}\right)+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial \phi_{k}}{\partial \theta}\right)+\frac{1}{r^{2} \sin ^{2} \theta} \frac{\partial^{2} \phi_{k}}{\partial \varphi^{2}}=0 \tag{2.161}
\end{equation*}
$$

Let us look for a solution of this equation in the following variable-separated form:

$$
\begin{equation*}
\phi_{k}=\frac{R(r)}{r} \mathcal{P}(\cos \theta) \mathcal{F}(\varphi), \tag{2.162}
\end{equation*}
$$

Separating equations one by one, just like this has been done in cylindrical coordinates, we get the following equations for the functions participating in this solution:

$$
\begin{gather*}
\frac{d^{2} 尺}{d r^{2}}-\frac{l(l+1)}{r^{2}} 尺=0,  \tag{2.163}\\
\frac{d}{d \xi}\left[\left(1-\xi^{2}\right) \frac{d \mathcal{P}}{d \xi}\right]+\left[l(l+1)-\frac{v^{2}}{1-\xi^{2}}\right] \mathcal{P}=0,  \tag{2.164}\\
\frac{d^{2} \ngtr}{d \varphi^{2}}+v^{2} \neq 0, \tag{2.165}
\end{gather*}
$$

where $\xi \equiv \cos \theta$ is a new variable in lieu of $\theta$ (so that $-1 \leq \xi \leq+1$ ), and $v^{2}$ and $l(l+1)$ are the separation constants. (The reason for selection of the latter one in this form will be clear in a minute.) One can see that, in contrast with the cylindrical coordinates, the equation for the radial functions is quite simple.

[^201]Indeed, let us look for its solution in the form $c r^{\alpha}$ - just as we have done with Eq. (106). Plugging this solution into Eq. (163), we immediately get the following condition on parameter $\alpha$ :

$$
\begin{equation*}
\alpha(\alpha-1)=l(l+1) . \tag{2.166}
\end{equation*}
$$

This quadratic equation has two roots, $\alpha=l+1$ and $\alpha=-l$, so that the general solution to Eq. (163) is

$$
\begin{equation*}
\mathrm{R}=a_{l} r^{l+1}+\frac{b_{l}}{r^{l}} . \tag{2.167}
\end{equation*}
$$

Equation (165) is also very simple, and is absolutely similar to the Eq. (107) we had for the cylindrical coordinates. However, Eq. (164) function $\mathcal{P}(\xi)$, where $\xi$ is the cosine of the polar angle $\theta$, is the so-called Legendre differential equation, whose solution cannot be expressed via what is usually called "elementary functions" - though, again, there is no generally accepted line between them and "special functions".

Let us start with axially-symmetric problems for which $\partial \phi / \partial \varphi=0$. This means $\pi \varphi)=$ const, and thus $v=0$, so that Eq. (164) is reduced to so-called Legendre's ordinary differential equation:

$$
\begin{equation*}
\frac{d}{d \xi}\left[\left(1-\xi^{2}\right) \frac{d \mathcal{P}}{d \xi}\right]+l(l+1) \mathcal{P}=0 \tag{2.168}
\end{equation*}
$$

One can readily check that the solutions of this equation for integer values of $l$ are specific (Legendre) polynomials ${ }^{54}$ that may be defined, for example, by the following Rodrigues' formula:

$$
\begin{equation*}
\mathcal{P}_{l}(\xi)=\frac{1}{2^{l} l!} \frac{d^{l}}{d \xi^{l}}\left(\xi^{2}-1\right)^{l}, \quad l=0,1,2, \ldots \tag{2.169}
\end{equation*}
$$

As follows from this formula, the first few Legendre polynomials are pretty simple:

$$
\begin{align*}
& P_{0}(\xi)=1 \\
& P_{1}(\xi)=\xi \\
& P_{2}(\xi)=\frac{1}{2}\left(3 \xi^{2}-1\right)  \tag{2.170}\\
& P_{3}(\xi)=\frac{1}{2}\left(5 \xi^{3}-3 \xi\right) \\
& P_{4}(\xi)=\frac{1}{8}\left(35 \xi^{4}-30 \xi^{2}+3\right), \ldots
\end{align*}
$$

though such explicit expressions become more and more bulky as $l$ is increased. As Fig. 21 shows, all these functions, that are defined on the $[-1,+1]$ segment, start at one point, $\mathcal{P}_{l}(+1)=+1$, and end up either at the same point or in the opposite point: $\mathcal{P}_{( }(-1)=(-1)^{l}$. On the way between these two end points, the $l$-th polynomial crosses the horizontal axis $l$ times. It is straightforward to use Eq. (169) for proving that these polynomials form a full, orthogonal set of functions, with the following normalization rule:

[^202]\[

$$
\begin{equation*}
\int_{-1}^{+1} \mathcal{P}_{l}(\xi) \mathcal{P}_{l^{\prime}}(\xi) d \xi=\frac{2}{2 l+1} \delta_{l l^{\prime}} \tag{2.171}
\end{equation*}
$$

\]

so that any function $f(\xi)$, defined on the segment $[-1,+1]$, may be presented as a unique series over the polynomials. ${ }^{55}$


Fig. 2.21. A few lowest Legendre polynomials $P_{l}(\xi)$.

Thus, taking into account the additional division by $r$ in Eq. (162), the general solution of any axially-symmetric Laplace problem may be presented as

$$
\begin{equation*}
\phi(r, \theta)=\sum_{l=0}^{\infty}\left(a_{l} r^{l}+\frac{b_{l}}{r^{l+1}}\right) \mathcal{P}_{l}(\cos \theta) . \tag{2.172}
\end{equation*}
$$

Please note a strong similarity between this solution and Eq. (112) for the 2D Laplace problem in polar coordinates. However, besides the difference in angular functions, there is also a difference (by one) in the power of the second radial function, and this difference immediately shows up in core problems.

Indeed, let us solve a problem similar to that shown in Fig. 13: find the electric field around a conducting sphere of radius $R$, placed into an initially uniform external field $\mathbf{E}_{0}$ (whose direction we will take for axis $z$ ) - see Fig. 22a. If we select $\left.\phi\right|_{z=0}=0$, then $a_{0}=b_{0}=0$. Now, just as has been argued for the cylindrical case, at $r \gg R$ the potential should approach that for the uniform field:

$$
\begin{equation*}
\phi \rightarrow-E_{0} z=-E_{0} r \cos \theta \tag{2.173}
\end{equation*}
$$

and this again means that in Eq. (172), only one of coefficients $a_{l}$ survives: $a_{l}=-E_{0} \delta_{l 1}$. Now, and from the boundary condition on the surface, $\phi(R, \theta)=0$, we get:

$$
\begin{equation*}
0=\left(-E_{0} R+\frac{b_{1}}{R^{2}}\right) \cos \theta+\sum_{l \geq 2} \frac{b_{l}}{R^{l+1}} \mathcal{P}_{l}(\cos \theta) . \tag{2.174}
\end{equation*}
$$

This expression may be viewed as the expansion of function $f(\xi) \equiv 0$ into a series of orthogonal functions $P_{l}(\xi)$. Since such expansions are unique, and Eq. (174) is satisfied if

[^203]\[

$$
\begin{equation*}
b_{l}=E_{0} R^{3} \delta_{l, 1}, \tag{2.175}
\end{equation*}
$$

\]

this is indeed the only possibility to satisfy the boundary condition, so that, finally,

$$
\begin{equation*}
\phi=-E_{0}\left(r-\frac{R^{3}}{r^{2}}\right) \cos \theta . \tag{2.176}
\end{equation*}
$$

(a)
(b)


Fig. 2.22. Conducting sphere in a uniform electric field: (a) problem' geometry, and (b) the equipotential surface pattern given by Eq. (176). The pattern is qualitatively similar but quantitatively different from that for the conducting cylinder in a perpendicular field -cf. Fig. 13.

This distribution, shown in Fig. 22b, is very much similar to Eq. (117) for the cylindrical case, but with a different power of radius in the second term. This leads to a quantitatively different distribution of the surface electric field:

$$
\begin{equation*}
E_{n}=-\left.\frac{\partial \phi}{\partial r}\right|_{r=R}=3 E_{0} \cos \theta \tag{2.177}
\end{equation*}
$$

so that its maximal value is a factor of 3 (rather than 2) larger than the external field.
Now let us discuss the Laplace equation solution in the general case (no axial symmetry), but only for most important systems in which the free space surrounds the origin from all sides. In this case the solutions to Eq. (165) have to be $2 \pi$-periodic, and hence $v=n=0, \pm 1, \pm 2, \ldots$ Mathematics says that the Legendre equation (164) with integer $v=n$ and a fixed integer $l$ has a solution only for a limited range of $n:{ }^{56}$

$$
\begin{equation*}
-l \leq n \leq+l . \tag{2.178}
\end{equation*}
$$

These solutions are called the associated Legendre functions. For $n \geq 0$, they may be defined via the Legendre polynomials using the following formula:

[^204]\[

$$
\begin{equation*}
\mathcal{P}_{l}^{n}(\xi)=(-1)^{n}\left(1-\xi^{2}\right)^{n / 2} \frac{d^{n}}{d \xi^{n}} \mathcal{P}_{l}(\xi) . \tag{2.179}
\end{equation*}
$$

\]

On the segment $\xi \in[-1,+1]$, each set of the associated Legendre functions with a fixed index $n$ and nonnegative $l$ form a full, orthogonal set, with the normalization relation,

$$
\begin{equation*}
\int_{-1}^{+1} P_{l}^{n}(\xi) P_{l^{\prime}}^{n}(\xi) d \xi=\frac{2}{2 l+1} \frac{(l+n)!}{(l-n)!} \delta_{l l^{\prime}} \tag{2.180}
\end{equation*}
$$

that is evidently a generalization of Eq. (171).
Since these relations may seem a bit intimidating, let me write down explicit expressions for a few $P_{l}^{n}(\cos \theta)$ with the lowest values of $l$ and $n \geq 0$ :

$$
\begin{align*}
& l=0: \quad P_{0}^{0}(\cos \theta)=1 ;  \tag{2.181}\\
& l=1:\left\{\begin{array}{l}
P_{1}^{0}(\cos \theta)=\cos \theta, \\
P_{1}^{1}(\cos \theta)=-\sin \theta
\end{array}\right.  \tag{2.182}\\
& l=2:\left\{\begin{array}{l}
P_{2}^{0}(\cos \theta)=\left(3 \cos ^{2} \theta-1\right) / 2, \\
P_{2}^{1}(\cos \theta)=-2 \sin \theta \cos \theta, \\
P_{2}^{2}(\cos \theta)=-3 \cos ^{2} \theta .
\end{array}\right. \tag{2.183}
\end{align*}
$$

The reader should agree there is not much intimidation is these functions - which are most important for applications.

Now the general solution (162) to the Laplace equation in the spherical coordinates may be spelled out as

$$
\begin{equation*}
\phi(r, \theta, \varphi)=\sum_{l=0}^{\infty}\left(a_{l} r^{l}+\frac{b_{l}}{r^{l+1}}\right) \sum_{n=0}^{l} \mathcal{P}_{l}^{n}(\cos \theta) \mathcal{\not}_{n}(\varphi), \quad \not_{n}(\varphi)=c_{n} \cos n \varphi+s_{n} \sin n \varphi \tag{2.184}
\end{equation*}
$$

Since the difference between angles $\theta$ and $\varphi$ is somewhat artificial, physicists prefer to think not about functions $P$ and $\mathcal{F}$ in separation, but directly about their products that participate in this solution. Figure 23 shows a few such angular functions ${ }^{57}$ by plotting their modulus along the radius, and using bi-color to show the function sign. While the lowest function $(l=0, n=0)$ is just a constant, two "dipole" functions $(l=1)$ differ from each other by their spatial orientation. Functions with higher $l($ say, $l=2)$ differ more substantially, with the following general trend: for each value of $l$, the function with $n=0$ is

[^205]Variable
separation in spherical coordinates (general case)
axially-symmetric ${ }^{58}$ and has $l$ zeros on its way from $\theta=0$ to $\theta=\pi$, while the functions with $n=l$ do not have zeros inside that interval, while oscillating most strongly as functions of $\varphi$.


As an exception, in order to save time, I will skip an example of application of the associated Legendre functions, because several such examples are given in the quantum mechanics part of these series. (Note that in this field, index $n$ is traditionally called $m$ - the magnetic quantum number.)

### 2.6. Charge images

So far, we have discussed various methods of solution of the Laplace boundary problem (35). Let us now move on to the discussion of its generalization, the Poisson equation (1.41), that we need when besides the conductors, we also have "free" charges with a known spatial distribution $\rho(\mathbf{r})$. (This will also allow us, better equipped, to revisit the Laplace problem again in the next section.)

Let us start with a somewhat limited, but sometimes very useful charge image (or "image charge") method. Consider a very simple problem: a single point charge near a conducting half-space see Fig. 24. Let us prove that its solution, above conductor's surface ( $z \geq 0$ ), may be presented as:

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}}\left(\frac{q}{r_{1}}-\frac{q}{r_{2}}\right)=\frac{q}{4 \pi \varepsilon_{0}}\left(\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}-\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime \prime}\right|}\right), \tag{2.185}
\end{equation*}
$$

[^206]or in a more explicit (coordinate) form:
\[

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{q}{4 \pi \varepsilon_{0}}\left(\frac{1}{\left[\rho^{2}+(z-d)^{2}\right]^{1 / 2}}-\frac{1}{\left[\rho^{2}+(z+d)^{2}\right]^{1 / 2}}\right) \tag{2.186}
\end{equation*}
$$

\]

where $\rho$ is the distance of the observation point from the vertical line on which the charge is located. Indeed, this solution evidently satisfies both the boundary condition of zero potential at the surface of the conductor $(z=0)$, and the Poisson equation (1.41), with the single $\delta$-functional source at point $\mathbf{r}^{\prime}=$ $\{0,0, d\}$ in its right-hand part, because its another singularity, at point $\mathbf{r}^{\prime \prime}=\{0,0,-d\}$, is outside the region of validity of this solution $(z \geq 0)$.


Fig. 2.24. The simplest problem readily solvable by the charge image method. Point colors in this section are used, here and in the balance of this section, to denote charges of the original (red) and opposite (blue) sign.

Physically, the solution may be interpreted as the sum of the fields of the actual charge $(+q)$ at point $\mathbf{r}$ ', and an equal but opposite charge $(-q)$ at the "mirror image" point $\mathbf{r}$ " (Fig. 24). This is the basic idea of the charge image method. Before moving to more complex problems, let us discuss the situation shown in Fig. 24 in a little bit more detail. First, we can use Eqs. (3) and (186) to calculate the surface charge density:

$$
\begin{equation*}
\sigma=-\left.\varepsilon_{0} \frac{\partial \phi}{\partial z}\right|_{z=0}=-\frac{q}{4 \pi} \frac{\partial}{\partial z}\left(\frac{1}{\left[\rho^{2}+(z-d)^{2}\right]^{1 / 2}}-\frac{1}{\left[\rho^{2}+(z+d)^{2}\right]^{1 / 2}}\right)_{z=0}=-\frac{q}{4 \pi} \frac{2 d}{\left(\rho^{2}+d^{2}\right)^{3 / 2}} . \tag{2.187}
\end{equation*}
$$

The total surface charge is

$$
\begin{equation*}
Q=\int_{A} \sigma d^{2} r=2 \pi \int_{0}^{\infty} \sigma(\rho) \rho d \rho=-\frac{q}{2} \int_{0}^{\infty} \frac{d}{\left(\rho^{2}+d^{2}\right)^{3 / 2}} 2 \rho d \rho \tag{2.188}
\end{equation*}
$$

This integral may be easily taken using the substitution $\xi \equiv \rho^{2} / d^{2}$ (giving $d \xi=2 \rho d \rho / d^{2}$ ):

$$
\begin{equation*}
Q=-\frac{q}{2} \int_{0}^{\infty} \frac{d \xi}{(\xi+1)^{3 / 2}}=-q \tag{2.189}
\end{equation*}
$$

This result is very natural, because the conductor "wants" to bring as much surface charge from its interior to the surface as necessary to fully compensate the initial charge $(+q)$ and hence to kill the
electric field at large distances as efficiently as possible, hence reducing the total electrostatic energy (1.67) to the lowest possible value.

For a deeper understanding of this polarization charge of the surface, let us take our calculations to the extreme - to $q$ equal to one elementary change $e$, and place a particle with this charge (for example, a proton) at a macroscopic distance - say 1 m - from conductor's surface. Then, according to Eq. (189), the total polarization charge of the surface equals to that of an electron, and according to Eq. (187), its spatial extent is of the order of $d^{2}=1 \mathrm{~m}^{2}$. This means that if we consider a much smaller part of the surface, $\Delta A \ll d^{2}$, its polarization charge magnitude $\Delta Q=\sigma \Delta A$ is much less than one electron! For example, Eq. (187) shows that the polarization charge of quite a macroscopic area $\Delta A=1 \mathrm{~cm}^{2}$ right under the initial charge $(\rho=0)$ is $e \Delta A / 2 \pi d^{2} \approx 1.6 \times 10^{-5} e$. Can this be true, or our theory is somehow limited to the charges much larger than $e$ ?

Surprisingly enough, the answer to this question has become clear (at least to some physicists :-) only as late as in the mid-1980s when several experiments demonstrated, and theorists accepted, some rather grudgingly that the usual polarization charge formulas are valid for elementary charges $q$ as well, i.e., such the polarization charge $\Delta Q$ of a macroscopic surface area can indeed be less than $e$. The underlying reason for this paradox is the nature of the polarization charge of the conductor surface: as should be clear from our discussion in Sec. 1, it is due not to new charged particles brought into the conductor (such charge would be in fact quantized in the units of $e$ ), but to a small shift of the free charges of a conductor by a very small distance from their equilibrium positions that they had in the absence of the external field induced by charge $q$. This shift is not quantized, at least on the scale relevant for our issue, and neither is $\Delta Q$. This understanding has opened a way toward the invention and experimental demonstration of several new devices including so-called single-electron transistors, ${ }^{59}$ which may be, in particular, used to measure polarization charges as small as $\sim 10^{-6} \mathrm{e}$.

To complete the discussion of our initial problem (Fig. 24), let us find the potential energy $U$ of the charge-to-surface interaction. For that we may use the value of the electrostatic potential (185) in the point of the charge itself ( $\mathbf{r}=\mathbf{r}$ '), of course ignoring the infinite potential created by the charge itself, so that the remaining potential is that of the image charge

$$
\begin{equation*}
\phi_{\text {image }}\left(\mathbf{r}^{\prime}\right)=-\frac{1}{4 \pi \varepsilon_{0}} \frac{q}{2 d} . \tag{2.190}
\end{equation*}
$$

Looking at the definition of the electrostatic potential, given by Eq. (1.31), it may be tempting to immediately write $U=q \phi_{\text {image }}=-\left(1 / 4 \pi \varepsilon_{0}\right)\left(q^{2} / 2 d\right)$ [WRONG!], but this would not be correct. The reason is that potential $\phi_{\text {image }}$ is not independent of $q$, but is actually induced by this charge. This is why the correct approach is to use Eq. (1.63), with just one term:

$$
\begin{equation*}
U=\frac{1}{2} q \phi_{\text {image }}=-\frac{1}{4 \pi \varepsilon_{0}} \frac{q^{2}}{4 d}, \tag{2.191}
\end{equation*}
$$

twice lower in magnitude than the wrong result cited above. In order to double-check this result, and also get a better feeling of the factor $1 / 2$ that distinguishes it from the wrong guess, we can recalculate

[^207]energy $U$ as the integral of the force exerted on the charge by the conductor (i.e., in our formalism, by the image charge):
\[

$$
\begin{equation*}
U=-\int_{\infty}^{d} F(z) d z=\frac{1}{4 \pi \varepsilon_{0}} \int_{\infty}^{d} \frac{q^{2}}{(2 z)^{2}} d z=-\frac{1}{4 \pi \varepsilon_{0}} \frac{q^{2}}{4 d} . \tag{2.192}
\end{equation*}
$$

\]

This calculation clearly accounts for the gradual build-up of force $F$, as the real charge is brought from afar (where we have opted for $U=0$ ) toward the surface.

This result, used for electrons, particles with charge $q=-e$, has several important applications. For example, let us plot energy $U$ for an electron near a metallic surface, as a function of $d$. For that, we may use Eq. (192) until our macroscopic approximation (2) becomes invalid, and $U$ transitions to some negative constant value ( $-\psi$ ) inside the conductor - see Fig. 25a.



Fig. 2.25. (a) Origin of the workfunction and (b) the field emission of electrons (schematically).

The positive constant $\psi$ is called workfunction, because it describes how much work should be done on an electron to remove it from the conductor. As was discussed in Sec. 1, in good metals the electric field screening happens at interatomic distances $a_{0} \approx 10^{-10} \mathrm{~m}$. Plugging $d=a$ and $q=-e$ into Eq. (191), we get $\approx 6 \times 10^{-19} \mathrm{~J} \approx 3.5 \mathrm{eV}$. This crude estimate is in a surprisingly good agreement with the experimental values of the workfunction, ranging between 4 and 5 eV for most metals. ${ }^{60}$

Next, let us consider the effect of an additional external electric field $\mathbf{E}_{0}$ applied perpendicular to a metallic surface, on this potential profile. Assuming the field to be uniform, we can add its potential $e E_{0} d$ at distance $d$ from the surface, to that created by the image charge. (As we know from Eq. (1.53), since field $\mathbf{E}_{0}$ is independent of the electron position, its recalculation to the potential energy does not require the coefficient $1 / 2$.) As the result, the potential energy of an electron near the surface becomes

$$
\begin{equation*}
U(d)=-e E_{0} d-\frac{1}{4 \pi \varepsilon_{0}} \frac{e^{2}}{4 d}, \quad \text { for } d>a_{0} \tag{2.193}
\end{equation*}
$$

with a similar crossover to $U=-\psi$ inside the conductor - see Fig. 25b. One can see that at the appropriate sign, and sufficient magnitude of the applied field, it lowers the potential barrier that prevented electron from leaving the conductor. At $E_{0} \sim \psi / a_{0}$ this suppression becomes so strong that electrons just below the Fermi surface start quantum-mechanical tunneling through the remaining thin

[^208]barrier. This is the field emission effect, which is used in vacuum electronics to provide efficient cathodes that do not require heating to high temperatures. ${ }^{61}$

Returning to the basic electrostatics, let us consider some other geometries where the method of images may be effectively applied. First, let us consider a right corner (Fig. 26a). Reflecting the initial charge in the vertical plane we get the image charge shown in the top left corner of the panel, that makes the boundary condition $\phi=$ const satisfied on the vertical surface of the corner. However, in order the same to be true on the horizontal surface, we have to reflect both the initial charge and the image charge in the horizontal plane, flipping their signs. The final configuration of 4 charges, shown in Fig. 26a, satisfies all the boundary conditions. The resulting potential distribution may be readily written as the evident generalization of Eq. (185). From there, the electric field and electric charge distributions, and the potential energy and forces acting on the charge may be calculated exactly as above.


Fig. 2.26. Charge images for ( $\mathrm{a}, \mathrm{b}$ ) internal corners with angles $\pi$ and $\pi / 2$, (c) plane capacitor, and (d) rectangular box, and (d) equipotential surfaces for the last system.

[^209]Next, consider a corner with angle $\pi / 4$ (Fig. 26b). Here we need to repeat the reflection operation not 2 but 4 times before we arrive at the final pattern of 8 positive and negative charges. (Any attempt to continue this process would lead to an overlap with the already existing charges.) This reasoning can be readily extended to any 2 D corner with angle $\beta=\pi / n$, with any integer $n$, that requires $2 n$ charges (including the initial one) to satisfy all the boundary conditions.

Some configurations require an infinite number of images that are, however, tractable. The most important of them is a system of two parallel conducting surfaces, i.e. a plane capacitor of infinite area (Fig. 26c). Here the repeated reflection leads to an infinite system of charges $\pm q$ at points

$$
\begin{equation*}
x_{j}^{ \pm}= \pm d+2 D j \tag{2.194}
\end{equation*}
$$

where $0<d<D$ is the position of the initial charge and $j$ an arbitrary integer. However, the resulting infinite sum for the potential of the real charge $q$, created by the field of its images,

$$
\begin{equation*}
\phi(d)=\frac{1}{4 \pi \varepsilon_{0}}\left[-\frac{q}{2 d}+\sum_{j \neq 0} \sum_{ \pm} \frac{ \pm q}{\left|d-x_{j}^{ \pm}\right|}\right]=-\frac{q}{4 \pi \varepsilon_{0}}\left[\frac{1}{2 d}+\frac{d^{2}}{D^{3}} \sum_{j=1}^{\infty} \frac{1}{j\left[j^{2}-(d / D)^{2}\right]}\right] \tag{2.195}
\end{equation*}
$$

is converging (in its last form) very fast. For example, the exact value, $\phi(D / 2)=-2 \ln 2\left(q / 4 \pi \varepsilon_{0} D\right)$, differs by less than $5 \%$ from the approximation using just the first term of the sum.

The same method may be applied to 2D (cylindrical) and 3D rectangular boxes that require, respectively, a 2D or 3D infinite lattices of images; for example in a 3D box with sides $a, b$, and $c$, charges $\pm q$ are located at points (Fig. 26d)

$$
\begin{equation*}
\mathbf{r}_{j k l}^{ \pm}= \pm \mathbf{r}^{\prime}+2 j a+2 k b+2 l c, \tag{2.196}
\end{equation*}
$$

where $\mathbf{r}$ ' is the location of the initial (real) charge, and $j, k$, and $l$ are arbitrary integers. Figure 26e shows the results of summation of the potentials of such charge set, including the real one, in a 2 D box (within the plane of the real charge). One can see that the equipotential surfaces, concentric near the charge, are naturally leaning along the conducting walls of the box, which should be equipotential.

Even more surprisingly, the image charge method works very efficiently not only for the rectilinear geometries, but also for spherical ones. Indeed, let us consider a point charge $q$ at some distance $d$ from the center of a conducting, grounded sphere of radius $R$ (Fig. 27a), and try to satisfy the boundary condition $\phi=0$ for the electrostatic potential on sphere's surface using an imaginary charge $q$ ' located at some point located beyond the surface, i.e. inside the sphere.

(b)


Fig. 2.27. Method of charge images for a conducting sphere: (a) the idea, and (b) the resulting potential distribution for particular case $d=2 R$.

From problem's symmetry, it is clear that the point should be at the line passing through the real charge and the sphere's center, at some distance $d^{\prime}$ from the center. Then the total potential created by the two charges at an arbitrary point with $r \geq R$ (Fig. 27a) is

$$
\begin{equation*}
\phi(r, \theta)=\frac{1}{4 \pi \varepsilon_{0}}\left[\frac{q}{\left(r^{2}+d^{2}-2 r d \cos \theta\right)^{1 / 2}}+\frac{q^{\prime}}{\left(r^{2}+d^{\prime 2}-2 r d^{\prime} \cos \theta\right)^{1 / 2}}\right] \tag{2.197}
\end{equation*}
$$

It is easy to see that we can make the two fractions to be equal and opposite at all points on the sphere's surface (i.e. for any $\theta$ at $r=R$ ), if we take ${ }^{62}$

$$
\begin{equation*}
d^{\prime}=\frac{R^{2}}{d}, \quad q^{\prime}=-\frac{R}{d} q \tag{2.198}
\end{equation*}
$$

Since the solution to any Poisson boundary problem is unique, Eqs. (197) and (198) give us such solution for this problem. Figure 27b shows a typical equipotential pattern calculated using Eqs. (197) and (198). It is surprising how formulas that simple may describe such a nontrivial field distribution.

Now let us calculate the total charge $Q$ induced by charge $q$ on conducting sphere's surface. We could do this, as we have done for the conducting plane, by the brute force integration of the surface charge density $\sigma=-\varepsilon_{0} \partial \phi /\left.\partial r\right|_{r=R}$. It is more elegant, however, to use the following Gauss law argument. Expression (197) is valid (at $r \geq R$ ) regardless whether we are dealing with our real problem (charge $q$ and the conducting sphere) or with the equivalent charge configuration (point charges $q$ and $q^{\prime}$, with no sphere at all). Hence, according to Eq. (1.16), the Gaussian integral over a surface with radius $r=R+0$, and the total charge inside the sphere should be also the same. Hence we immediately get

$$
\begin{equation*}
Q=q^{\prime}=-\frac{R}{d} q \tag{2.199}
\end{equation*}
$$

The similar argumentation may be used to find the charge-to-sphere interaction force:

$$
\begin{equation*}
F=q E_{\mathrm{image}}(d)=q \frac{q^{\prime}}{4 \pi \varepsilon_{0}\left(d-d^{\prime}\right)^{2}}=-\frac{q^{2}}{4 \pi \varepsilon_{0}} \frac{R}{d} \frac{1}{\left(d-R^{2} / d\right)^{2}}=-\frac{q^{2}}{4 \pi \varepsilon_{0}} \frac{R d}{\left(d^{2}-R^{2}\right)^{2}} . \tag{2.200}
\end{equation*}
$$

(Note that this expression is legitimate only at $d>R$.) At large distances, $d / R \gg 1$, this attractive force decreases as $1 / d^{3}$. This unusual dependence arises because, as Eq. (198) specifies, the induced charge of the sphere, responsible for the force, is not constant but decreases as $Q \propto 1 / d$.

All the previous formulas referred to a sphere that is grounded to keep its potential equal to zero. But what if we keep the sphere galvanically insulated, so that its net charge is fixed, e.g., equals zero? Instead of solving the problem from the scratch, let us use (again!) the linear superposition principle. For that, we may add to the previous problem an additional charge, equal to $(-Q)$, to the sphere, and argue that this addition gives an additional potential that does not depend of the potential induced by charge $q$. For the interaction force, such addition yields

[^210]\[

$$
\begin{equation*}
F=\frac{q q^{\prime}}{4 \pi \varepsilon_{0}\left(d-d^{\prime}\right)^{2}}+\frac{q Q}{4 \pi \varepsilon_{0} d^{2}}=-\frac{q^{2}}{4 \pi \varepsilon_{0}}\left[\frac{R d}{\left(d^{2}-R^{2}\right)^{2}}-\frac{R}{d^{3}}\right] . \tag{2.201}
\end{equation*}
$$

\]

At large distances, the two terms proportional to $1 / d^{3}$ cancel each other, giving $F \propto 1 / d^{5}$. Such a rapid force decay is due to the fact that the field of the uncharged sphere is equivalent to that of two (equal and opposite) induced charges $+Q$ and $-Q$, and the distance between them ( $d^{\prime}=R^{2} / d$ ) tends to zero at $d$ $\rightarrow \infty$. The potential energy of such interaction behaves as $U \propto 1 / d^{6}$ at $d \rightarrow \infty$; in the next chapter we will see that this is the general law of the induced dipole interaction.

### 2.7. Green's functions

I have spent so much time/space discussing the potential distributions created by a single point charge in various conductor geometries, because, for any geometry, the generalization of these results to the arbitrary distribution $\rho(\mathbf{r})$ of free charges is straightforward. Namely, if a single charge $q$, located at point $\mathbf{r}$ ', created electrostatic potential

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} q G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \tag{2.202}
\end{equation*}
$$

then, due to the linear superposition principle, an arbitrary charge distribution creates potential

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \sum_{j} q_{j} G\left(\mathbf{r}, \mathbf{r}_{j}\right)=\frac{1}{4 \pi \varepsilon_{0}} \int \rho\left(\mathbf{r}^{\prime}\right) G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) d^{3} r^{\prime} \tag{2.203}
\end{equation*}
$$

Spatial Green's
function

Kernel $G(\mathbf{r}, \mathbf{r}$ ') is called the (spatial) Green's function - the notion very popular in all fields of physics. ${ }^{63}$ Evidently, as Eq. (1.35) shows, in the unlimited free space

$$
\begin{equation*}
G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \tag{2.204}
\end{equation*}
$$

i.e. the Green's function depends only on one scalar argument - the distance between the field observation point $\mathbf{r}$ and the field-source (charge) point $\mathbf{r}$ '. However, as soon as there are conductors around, the situation changes. In this course we will only deal with Green's functions that are defined in the space between conductors, and that vanish as soon as the radius-vector $\mathbf{r}$ points to the surface of any conductor: ${ }^{64}$

$$
\begin{equation*}
\left.G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)\right|_{\mathbf{r} \in A}=0 . \tag{2.205}
\end{equation*}
$$

With this definition, it is straightforward to deduce the Green's functions for the solutions of the last section's problems in which conductors were grounded ( $\phi=0$ ). For example, for a semi-space $z \geq 0$ limited by a conducting plane (Fig. 24), Eq. (185) yields

$$
\begin{equation*}
G=\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}-\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime \prime}\right|}, \quad \text { with } \rho^{\prime \prime}=\rho^{\prime} \text { and } z^{\prime \prime}=-z^{\prime} \tag{2.206}
\end{equation*}
$$

[^211]We see that in the presence of conductors (and, as we will see later, any other polarizable media), the Green's function may depend not only on the difference $\mathbf{r}-\mathbf{r}$ ', but in a specific way from each of these two arguments.

So far, this looked just like re-naming our old results. The really non-trivial result of the Green's function application to electrostatics is that, somewhat counter-intuitively, the knowledge of the Green's function for a system with grounded conductors (Fig. 28a) allows one to calculate the field created by voltage-biased conductors (Fig. 28b), with the same geometry.
(a)


(b)


Fig. 2.28. Green's function method allows the solution of a simpler boundary problem (a) to be used to find the solution of a more complex problem (b), for the same conductor geometry.

In order to show that, let us use the so-called Green's theorem of the vector calculus. ${ }^{65}$ The theorem states that for any two scalar, differentiable functions $f(\mathbf{r})$ and $g(\mathbf{r})$, and any volume $V$,

$$
\begin{equation*}
\int_{V}\left(f \nabla^{2} g-g \nabla^{2} f\right) d^{3} r=\oint_{S}(f \nabla g-g \nabla f)_{n} d^{2} r, \tag{2.207}
\end{equation*}
$$

where $S$ is the surface limiting the volume. Applying the theorem to the electrostatic potential $\phi(\mathbf{r})$ and the Green's function $G$ (also considered as a function of $\mathbf{r}$ ), let us use the Poisson equation (1.41) to replace $\nabla^{2} \phi$ with $\left(-\rho / \varepsilon_{0}\right)$, and notice that $G$, considered as a function of $\mathbf{r}$, obeys the Poisson equation with the $\delta$-functional source:

$$
\begin{equation*}
\nabla^{2} G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=-4 \pi \delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \tag{2.208}
\end{equation*}
$$

(Indeed, according to its definition (202), this function may be formally considered as the field of a point charge $q=4 \pi \varepsilon_{0}$.) Now swapping the notation of radius-vectors, $\mathbf{r} \leftrightarrow \mathbf{r}$ ', and using the Green's function symmetry, $G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=G\left(\mathbf{r}^{\prime}, \mathbf{r}\right),{ }^{66}$ we get

$$
\begin{equation*}
-4 \pi \phi(\mathbf{r})-\int_{V}\left(-\frac{\rho\left(\mathbf{r}^{\prime}\right)}{\varepsilon_{0}}\right) G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) d^{3} r^{\prime}=\oint_{S}\left[\phi\left(\mathbf{r}^{\prime}\right) \frac{\partial G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)}{\partial n^{\prime}}-G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \frac{\partial \phi\left(\mathbf{r}^{\prime}\right)}{\partial n^{\prime}}\right] d^{2} r^{\prime} \tag{2.209}
\end{equation*}
$$

Let us apply this relation to volume $V$ of free space between the conductors, and the boundary $A$ slightly outside of their surface. In this case, by its definition, the Green's function $G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)$ vanishes at the conductor surface ( $\mathbf{r} \in S$ ) - see Eq. (205). Now changing the sign of $\partial n^{\prime}$ (so that it would be the outer normal for conductors, rather than free space volume $V$ ), dividing all terms by $4 \pi$, and partitioning

[^212]the total surface $A$ into the parts (numbered by index $j$ ) corresponding to different conductors (possibly, kept at different potentials $\phi_{k}$ ), we finally arrive at the famous result: ${ }^{67}$
\[

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int_{V} \rho\left(\mathbf{r}^{\prime}\right) G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) d^{3} r^{\prime}+\frac{1}{4 \pi} \sum_{k} \phi_{k} \oint_{S_{k}} \frac{\partial G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)}{\partial n^{\prime}} d^{2} r^{\prime} \tag{2.210}
\end{equation*}
$$

\]

Potential via Green's function

While the first term in the right-hand part of this relation is a direct and evident expression of the superposition principle, given by Eq. (203), the second term is highly non-trivial: it describes the effect of conductors with nonvanishing potentials $\phi_{k}$ (Fig. 28b) using the Green's function calculated for the similar system with grounded conductors, i.e. with all $\phi_{k}=0$ (Fig. 28a). Let me emphasize that since our volume $V$ excludes conductors, the first term in the right-hand part of Eq. (210) includes only the "freestanding" charges of the system (in Fig. 28, marked $q_{1}, q_{2}$, etc.), but not the surface charges of the conductors - which are taken into account, implicitly, by the second term.

In order to illustrate what a powerful tool Eq. (210) is, let us use to calculate the electrostatic field in two systems. In the first of them, a circular disk, separated with a very thin cut from a conducting plane, is biased with potential $\phi=V$, while the rest of the plane is grounded - see Fig. 29.


Fig. 2.29. Voltage-biased conducting circle inside a grounded conducting plane.

If the width of the gap between the circle and rest of the plane is negligible, we may apply Eq. (210) with $\rho\left(\mathbf{r}^{\prime}\right)=0$, and the Green's function for the uncut plane - see Eq. (206). ${ }^{68}$ In the cylindrical coordinates, the function may be rewritten as

$$
\begin{equation*}
G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=\frac{1}{\left(\rho^{2}+\rho^{\prime 2}-2 \rho \rho^{\prime} \cos \left(\varphi-\varphi^{\prime}\right)+\left(z-z^{\prime}\right)^{2}\right)^{1 / 2}}-\frac{1}{\left(\rho^{2}+\rho^{\prime 2}-2 \rho \rho^{\prime} \cos \left(\varphi-\varphi^{\prime}\right)+\left(z+z^{\prime}\right)^{2}\right)^{1 / 2}} . \tag{2.211}
\end{equation*}
$$

(The sum of the first three terms under the square roots of Eq. (211) is just the squared distance between the horizontal projections $\rho$ and $\rho$ ' of vectors $\mathbf{r}$ and $\mathbf{r}$ ' (or $\mathbf{r}$ "), correspondingly, while the last terms are the squares of their vertical spacings.)

Now we can readily calculate the necessary derivative:

[^213]\[

$$
\begin{equation*}
\left.\frac{\partial G}{\partial n^{\prime}}\right|_{S}=\left.\frac{\partial G}{\partial z^{\prime}}\right|_{z^{\prime}=+0}=\frac{2 z}{\left(\rho^{2}+\rho^{\prime 2}-2 \rho \rho^{\prime} \cos \left(\varphi-\varphi^{\prime}\right)+z^{2}\right)^{3 / 2}} . \tag{2.212}
\end{equation*}
$$

\]

Due the axial symmetry of the system, we can take $\varphi$ for zero. With this, Eqs. (210) and (212) yield

$$
\begin{equation*}
\phi=\frac{V}{4 \pi} \oint_{S} \frac{\partial G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)}{\partial n^{\prime}} d^{2} r^{\prime}=\frac{V z}{2 \pi} \int_{0}^{2 \pi} d \varphi^{\prime} \int_{0}^{R} \frac{\rho^{\prime} d \rho^{\prime}}{\left(\rho^{2}+\rho^{\prime 2}-2 \rho \rho^{\prime} \cos \varphi^{\prime}+z^{2}\right)^{3 / 2}} . \tag{2.213}
\end{equation*}
$$

This integral is not too pleasing, but may be readily worked out for points on the symmetry axis $(\rho=0)$ :

$$
\begin{equation*}
\phi=V z \int_{0}^{R} \frac{\rho^{\prime} d \rho^{\prime}}{\left(\rho^{\prime 2}+z^{2}\right)^{3 / 2}}=\frac{V^{R^{2} / z^{2}}}{2} \int_{0}^{\frac{d \xi}{(\xi+1)^{3 / 2}}=V\left[1-\frac{z}{\left(R^{2}+z^{2}\right)^{1 / 2}}\right] . . . . . . .} \tag{2.214}
\end{equation*}
$$

This expression shows that if $z \rightarrow 0$, the potential tends to $V$ (as it should), while at $z \gg R$,

$$
\begin{equation*}
\phi \rightarrow V \frac{R^{2}}{2 z^{2}} . \tag{2.215}
\end{equation*}
$$

This asymptotic behavior is typical for electric dipoles - see the next chapter.
Now, let us use the same Eq. (210) to solve the (in :-)famous problem of the cut sphere (Fig. 30). Again, if the gap between the two conducting semi-spheres is very thin $(t \ll R)$, we may use the Green's function for the grounded (and uncut) sphere. For a particular case $\mathbf{r}^{\prime}=d \mathbf{n}_{z}$, this function is given by Eqs. (197)-(198); generalizing the former relation for an arbitrary direction of vector $\mathbf{r}$ ', we get

$$
\begin{equation*}
G=\frac{1}{\left(r^{2}+r^{\prime 2}-2 r r^{\prime} \cos \gamma\right)^{1 / 2}}-\frac{R / r^{\prime}}{\left(r^{2}+\left(R^{2} / r^{\prime}\right)^{2}-2 r\left(R^{2} / r^{\prime}\right) \cos \gamma\right)^{1 / 2}}, \quad \text { for } r, r^{\prime} \geq R . \tag{2.216}
\end{equation*}
$$

where $\gamma$ is the angle between vectors $\mathbf{r}$ and $\mathbf{r}^{\prime}$, and hence $\mathbf{r}$ " (Fig. 30).


Fig. 2.30. A system of two, oppositely biased semispheres.

Now, finding the Green's function's derivative,

$$
\begin{equation*}
\left.\frac{\partial G}{\partial r^{\prime}}\right|_{r^{\prime}=R+0}=-\frac{\left(r^{2}-R^{2}\right)}{R\left[r^{2}+R^{2}-2 R r \cos \gamma\right]^{3 / 2}}, \tag{2.217}
\end{equation*}
$$

and plugging it into Eq. (210), we see that the integration is easy only for the field on the symmetry axis $\left(\mathbf{r}=r \mathbf{n}_{z}, \gamma=\theta\right)$, giving

$$
\begin{equation*}
\phi=\frac{V}{2}\left[1-\frac{z^{2}-R^{2}}{z\left(z^{2}+R^{2}\right)^{1 / 2}}\right] . \tag{2.218}
\end{equation*}
$$

For $z \rightarrow R, \phi \rightarrow V / 2$ (just checking :-), while for $z \gg R$,

$$
\begin{equation*}
\phi \rightarrow V \frac{3 R^{2}}{4 z^{2}} \tag{2.219}
\end{equation*}
$$

so this is also an electric dipole field - see the next chapter.

### 2.8. Numerical methods

Despite the richness of analytical methods, for many boundary problems (especially in geometries without high degree of symmetry), numerical methods is the only way to the solution. Despite the current abundance of software codes and packages offering their automatic numerical solution, ${ }^{69}$ it is important to an educated physicist to understand "what is under their hood", at least because most universal programs exhibit mediocre performance in comparison with custom codes written for particular problems, and sometimes do not converge at all, especially for fast-changing (say, exponential) functions.

The simplest of the numerical methods of solution of partial differential equations is the finitedifference method ${ }^{70}$ in which the sought function of $N$ scalar arguments $f\left(r_{1}, r_{2}, \ldots r_{N}\right)$ is represented by its values in discrete points of a rectangular grid (also called mesh) of the corresponding dimensionality (Fig. 31).


Fig. 2.31. General idea of the finite-difference method in (a) one, (b) two, and (c) three dimensions.

Each partial second derivative of the function is approximated by the formula that readily follows from the linear approximations for the function $f$ and then its partial derivatives - see Fig. 31a:

$$
\begin{equation*}
\frac{\partial^{2} f}{\partial r_{j}^{2}}=\frac{\partial}{\partial r_{j}}\left(\frac{\partial f}{\partial r_{j}}\right) \approx \frac{1}{h}\left(\left.\frac{\partial f}{\partial r_{j}}\right|_{r_{j}+h / 2}-\left.\frac{\partial f}{\partial r_{j}}\right|_{r_{j}-h / 2}\right) \approx \frac{1}{h}\left[\frac{f_{\rightarrow}-f}{h}-\frac{f-f_{\leftarrow}}{h}\right]=\frac{f_{\rightarrow}+f_{\leftarrow}-2 f}{h^{2}} \tag{2.220}
\end{equation*}
$$

[^214]where $f_{\rightarrow} \equiv f\left(r_{j}+h\right)$ and where $f_{\leftarrow} \equiv f\left(r_{j}-h\right)$. (The relative error of this approximation is of the order of $h^{4} \partial^{4} f / \partial r_{j}^{4}$.) As a result, a 2D Laplace operator may be presented as
\[

$$
\begin{equation*}
\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}=\frac{f_{\rightarrow}+f_{\leftarrow}-2 f}{h^{2}}+\frac{f_{\uparrow}+f_{\downarrow}-2 f}{h^{2}}=\frac{f_{\rightarrow}+f_{\leftarrow}+f_{\uparrow}+f_{\downarrow}-4 f}{h^{2}}, \tag{2.221}
\end{equation*}
$$

\]

while the 3D operator as

$$
\begin{equation*}
\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}+\frac{\partial^{2} f}{\partial z^{2}}=\frac{f_{\rightarrow}+f_{\leftarrow}+f_{\uparrow}+f_{\downarrow}+f_{\otimes}+f_{\times}-6 f}{h^{2}} . \tag{2.222}
\end{equation*}
$$

(The notation used in these formulas should be clear from Figs. 31b and 31c, respectively.)
Let us apply this scheme to find the electrostatic potential distribution inside of a cylindrical box with conducting walls and square cross-section, using an extremely coarse mesh with step $h=a / 2$ (Fig. 32). In this case our function, the electrostatic potential, equals zero on the side walls and the bottom, and equals to $V_{0}$ at the top lid, so that, according to Eq. (221), the Laplace equation may be approximated as

$$
\begin{equation*}
\frac{0+0+V_{0}+0-4 \phi}{(a / 2)^{2}}=0 \tag{2.223}
\end{equation*}
$$

The resulting value for the potential in the center of the box is $\phi=V_{0} / 4$. Surprisingly, this is the exact value! This may be proved by solving this problem by the variable separation method, just as this has been done for the similar 3D problem in Sec. 4 above. The result is

$$
\phi(x, y)=\sum_{n=1}^{\infty} c_{n} \sin \frac{\pi n x}{a} \sinh \frac{\pi n y}{a}, \quad c_{n}=\frac{4 V_{0}}{\pi n \sinh (\pi n)} \times\left\{\begin{array}{l}
1, \text { if } n \text { is odd }  \tag{2.224}\\
0, \text { otherwise } .
\end{array}\right.
$$

so that at the central point $(x=y=a / 2)$,

$$
\begin{equation*}
\phi=\frac{4 V_{0}}{\pi} \sum_{j=0}^{\infty} \frac{\sin [\pi(2 j+1) / 2] \sinh [\pi(2 j+1) / 2]}{(2 j+1) \sinh [\pi(2 j+1)]}=\frac{2 V_{0}}{\pi} \sum_{j=0}^{\infty} \frac{(-1)^{j}}{(2 j+1) \cosh [\pi(2 j+1) / 2]} . \tag{2.225}
\end{equation*}
$$

The last series equals exactly to $\pi / 8$, so that $\phi=V_{0} / 4$.


Fig. 2.32. Numerical solution of the internal 2D boundary problem for a conducting, cylindrical box with square crosssection, using a very coarse mesh (with $h=a / 2$ ).

For a similar 3D problem (a cubic box) we can use Eq. (222) to get

$$
\begin{equation*}
\frac{0+0+V_{0}+0+0+0-6 \phi}{(a / 2)^{2}}=0 \tag{2.226}
\end{equation*}
$$

so that $\phi=V_{0} / 6$. Unbelievably enough, this result is also exact! (This follows from our variable separation result expressed by Eqs. (95) and (99).)

Though such exact results should be considered as a happy coincidence rather than the norm, they still show that numerical methods, with a relatively crude mesh, may be more computationally efficient than the "analytical" approaches, like the variable separation method with its infinite-sum results that, in most cases, require computers anyway - at least for the result's comprehension and analysis.

A more powerful (but also much more complex for implementation) approach is the finiteelement method in which the discrete point mesh, typically with triangular cells, is (automatically) generated in accordance with the system geometry. Such mesh generators provide higher point concentration near sharp convex parts of conductor surfaces, where the field concentrates and hence the potential changes faster, and thus ensure better accuracy-to-performance trade-off than the finitedifference methods on a uniform grid. The price to pay for this improvement is the algorithm complexity that makes manual adjustments much harder. Unfortunately I do not have time for going into the details of that method, and have to refer the reader to the special literature on this subject. ${ }^{71}$

### 2.9. Exercise problems

2.1. Calculate the force (per unit area) exerted on a conducting surface by an electric field. Compare the result with the definition of the electric field, given by Eq. (1.5).
2.2. A thin plane film, carrying a uniform electric charge density $\sigma$, is placed inside a plane capacitor whose plates are connected by a wire - see Fig. on the right. Neglecting the edge effects, calculate the surface charges of the plates, and the net force acting on the film (per unit area).

2.3. Following the discussion of two weakly coupled spheres in Sec. 2, find an approximate expression for the mutual capacitance (per unit length) between two very thin, parallel wires, both with a round cross-section, but each with its own diameter. Compare the result with that for two small spheres, and interpret the difference.
2.4. Use the Gauss law to calculate the mutual capacitance of the following 2 -electrode systems, with the cross-section shown in Fig. 5 (reproduced on the right):
(i) a conducting sphere inside a concentric spherical cavity in another conductor, and
(ii) a conducting cylinder inside a coaxial cavity in another conductor.


[^215](In this case, we speak about the capacitance per unit length).
Compare the results with those obtained in Sec. 2.2, using the Laplace equation solution.
2.5. Calculate the electrostatic potential distribution around two barely separated conductors in the form of coaxial, round cones (see Fig. on the right), with voltage $V$ between them. Compare the result with that of a similar 2D problem, with the cones replaced by plane-face wedges. Can you calculate the mutual capacitance between the conductors in any of these systems? If not, can you estimate it?

2.6. A system of two thin conducting plates is located over a ground plane as shown in Fig. on the right, where $A$ ' and $A$ '" are plate part areas, while $d^{\prime}$ and $d^{\prime \prime}$ are distances between them. Neglecting the fringe effects, calculate:
(i) the effective capacitance of each plate, and
(ii) their mutual capacitance.

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2.7. Using the results for a single thin round disk, obtained in Sec. 4, consider a system of two such disks at a small distance $d \ll R$ from each other see Fig. on the right. In particular, calculate:

(i) the reciprocal capacitance matrix of the system,
(ii) the mutual capacitance between the disks,
(iii) the partial capacitance, and
(iv) the effective capacitance of one disk,
(all in the first non-vanishing approximations in $d / R \ll 1$ ). Compare the results (ii)-(iv) and interpret their similarities and differences.
2.8. ${ }^{*}$ Calculate the mutual capacitance (per unit length) between two cylindrical conductors forming a system with the cross-section shown in Fig. on the right, in the limit $t \ll w \ll R$.

Hint: You may like to use elliptical (not "ellipsoidal"!) coordinates $\{\alpha, \beta\}$ defined by the following equation:

$$
\begin{equation*}
x+i y=c \cosh (\alpha+i \beta) \tag{*}
\end{equation*}
$$

with the appropriate choice of constant $c$. In these orthogonal 2D coordinates, the Laplace operator is very simple: ${ }^{72}$

$$
\nabla^{2}=\frac{1}{c^{2}\left(\cosh ^{2} \alpha-\cos ^{2} \beta\right)}\left(\frac{\partial^{2}}{\partial \alpha^{2}}+\frac{\partial^{2}}{\partial \beta^{2}}\right)
$$

[^216]2.9. Formulate 2D electrostatic problems that can be solved using each of the following analytic functions of the complex variable $z \equiv x+i y$ :
(i) $\boldsymbol{w}=\ln \boldsymbol{z}$,
(ii) $\boldsymbol{\omega}=\boldsymbol{z}^{1 / 2}$,
and solve these problems.
2.10. On each wall of a cylindrical volume with a rectangular cross-section $a \times b$, with no electric charges inside it, the electric field is uniform, normal to the wall plane, and opposite to that on opposite side - see Fig. on the right. Calculate the distribution of the electric potential inside the volume, provided that the field magnitude on the vertical walls equals $E$.

2.11. Complete the solution of the problem shown in Fig. 10, by calculating the distribution of the surface charge of the semi-planes. Can you calculate the mutual capacitance between the plates (per unit length)? If not, can you estimate it?
2.12.* A straight, long, thin, round-cylindrical metallic pipe has been cut, along its axis, into two equal parts - see Fig. on the right.
(i) Use the conformal mapping method to calculate the distribution of the electrostatic potential, created by voltage $V$ applied between the two parts, both outside and inside the pipe, and of the surface charge.
(ii) Calculate the mutual capacitance between pipe's halves (per unit length), taking into account a small width $2 t \ll R$ of the cut.

Hints: In Task (i), you may like to use the following complex function:


$$
\boldsymbol{u}=\ln \left(\frac{R+z}{R-z}\right)
$$

while in Task (ii), it is advisable to use the solution of the previous problem.
2.13. Solve Task (i) of the previous problem using the variable separation method, and compare the results.
2.14. Use the variable separation method to calculate the potential distribution above the plane surface of a conductor, with a strip of width $w$ separated by very thin cuts, and biased with voltage $V-$ see Fig. below.

2.15. In the Fig. of the previous problem, the cut-out and voltage-biased part of the conducting plane is now not a strip, but a square with side $w$. Calculate the potential distribution above conductor's surface.
2.16. Complete the cylinder problem started in Sec. 5 (see Fig. 15), for the cases when voltage on the top lid is fixed as follows:
(i) $V=V_{0} J_{1}\left(\xi_{11} \rho / R\right) \sin \varphi$, where $\xi_{11} \approx 3.832$ is the first root of function $J_{1}(x)$, and
(ii) $V=V_{0}=$ const.

For both cases, calculate the electric field in the centers of the lower and upper lids. (For assignment (ii), an answer including series and/or integrals is satisfactory.)
2.17. Each electrode of a large plane capacitor is cut into long strips of equal width $l$, with very narrow gaps between them. These strips are kept at the alternating potentials as shown in Fig. on the right. Use the variable separation method to calculate the electrostatic potential distribution. Explore the limit $l \ll d$.

2.18. Solve the problem shown in Fig. 19. In particular:
(i) calculate and sketch the distribution of the electrostatic potential inside the system for various values of ratio $R / h$, and
(ii) simplify the results for the limit $R / h \rightarrow 0$.
2.19. Use the variable separation method to find the potential distribution inside and outside of a thin spherical shell of radius $R$, with fixed potential $\phi(R, \theta, \varphi)=V_{0} \sin \theta \cos \varphi$.
2.20. A thin spherical shell carries charge with areal density $\sigma=\sigma_{0} \cos \theta$. Calculate the spatial distribution of the electrostatic potential and field.
2.21. Use the variable separation method to calculate the potential distribution both inside and outside of a thin spherical shell of radius $R$, separated with a very thin cut, along plane $\mathrm{z}=0$, into two halves, with voltage $V$ applied between them - see Fig. on the right. Analyze the solution; in particular, compare the field at axis $z$, for $z>R$, with Eq. (2.218), obtained by the Green's function method.

Hint: You may like to use the following integral of a Legendre polynomial with odd index $l=1,3,5 \ldots=2 n-1:^{73}$


[^217]$$
I_{n} \equiv \int_{0}^{1} P_{2 n-1}(\xi) d \xi=\frac{1}{n!} \cdot\left(\frac{1}{2}\right) \cdot\left(-\frac{3}{2}\right) \cdot\left(-\frac{5}{2}\right) \cdots\left(\frac{3}{2}-n\right) \equiv(-1)^{n-1} \frac{(2 n-3)!!}{2 n(2 n-2)!!} .
$$
2.22. A small conductor (in this context, usually called the single-electron box or single-electron island) is placed between two conducting electrodes, with voltage $V$ applied between them. The gap between one of the electrodes and the box is so narrow that electrons may tunnel quantum-mechanically through this gap ("weak tunnel junction") - see Fig. on the right. Neglecting thermal fluctuations, calculate the equilibrium charge of the island as a function of $V$.

Hint: To solve this problem, you do not need to know much about quantum-mechanical tunneling through weak junctions, ${ }^{74}$ besides that such
 tunneling of an electron, and its subsequent energy relaxation inside the conductor, may be considered as a single inelastic (energy-dissipating) event. In the absence of thermal agitation, such event takes place when (and only when) it decreases the potential energy of the system.
2.23. Calculate the total surface charges induced in the plates of a very broad plane capacitor of thickness $D$ by a point charge $q$ separated from one of the electrodes by distance $d$.
2.24. Prove the statement, made in Sec. 6, that the 2D boundary problem shown in Fig. on the right can be solved using a finite number of image charges if angle $\beta$ equals $\pi / n$, where $n=1,2, \ldots$

2.25. Use the image charge method to calculate the energy of electrostatic interaction between a point charge placed in the center of a spherical cavity that was carved inside a grounded conductor, and the conductor's walls. Looking at the result, could it be obtained in a simpler way (or ways)?
2.26. Use the method of images to find the Green's function of the system shown in Fig. on the right, where the bulge on the conducting plane has the shape of a semi-sphere of radius $R$.
2.27.* Use the fact of spherical inversion, expressed by Eq. (198), to develop an iterative method for more and more precise calculation of the mutual capacitance between two similar metallic spheres of radius $R$, with centers separated by distance $d>2 R$.

[^218]2.28.* A metallic sphere of radius $R_{1}$, carrying electric charge $Q$, is placed inside a spherical cavity of radius $R_{2}>R_{1}$, cut inside another metal. Calculate the force exerted on the sphere if is center is displaced by a small distance $\delta \ll R_{1}, R_{2}-R_{1}$ from that of the cavity - see Fig. on the right.

2.29. Within the simple model of electric field screening in conductors, discussed in Sec. 2.1, analyze the partial screening of the electric field of a point charge $q$ by a plane, uniform conducting film of thickness $t \ll \lambda$, where $\lambda$ is (depending on charge carrier statistics) either the Debye or the ThomasFermi screening length - see, respectively, Eqs. (2.8) or (2.10). Assume that the distance $d$ between the charge and plane is much larger than $t$.
2.30. Suggest a convenient definition of 2D Green's function for electrostatic problems, and calculate it for:
(i) the unlimited free space, and
(ii) the free space above a conducting plane.

Use the latter result to re-solve Problem 14.
2.31. Find the 2D Green's function for the free space
(i) outside a round conducting cylinder,
(ii) inside a round cylindrical hole in a conductor.
2.32. Solve Task (i) of Problem 12 (see also Problem 13), using the Green's function method.

Hints: You may like to use the 2D Green's function derived in the solution of Problem 2.27(ii), and the following table integral: ${ }^{75}$

$$
\int \frac{d \xi}{a+b \cos \xi}=\frac{2}{\left(a^{2}-b^{2}\right)^{1 / 2}} \tan ^{-1}\left[\frac{(a-b)}{\left(a^{2}-b^{2}\right)^{1 / 2}} \tan \frac{\xi}{2}\right], \quad \text { if } a^{2}-b^{2}>0 .
$$

2.33. Solve the same 2D boundary problem that was discussed in Sec. 6 (Fig. 32) using:
(i) the finite difference method, with a finer square mesh, $h=a / 3$, and
(ii) the variable separation method.

Compare the results (at the mesh points only) and comment.

[^219]

## Chapter 3. Polarization of Dielectrics

In the last chapter, we have discussed the electric polarization of conductors. In contrast to those materials, in dielectrics the charge motion is limited to the interior of an atom or a molecule, so that the electric polarization of these materials by external field takes a different form. This issue is the main subject of this chapter. In preparation to the analysis of dielectrics, we have to start with a more general discussion of the electric field of a spatially-restricted system of charges.

### 3.1. Electric dipole

Let us consider a localized system of charges, of a linear size scale $a$, and calculate a simple but approximate expression for the electrostatic field induced by the system at a distant point $\mathbf{r}$. For that, let us select a reference frame with the origin either somewhere inside the system, or at a distance of the order of $a$ from it (Fig. 1).


Fig. 3.1. Deriving the approximate expression (5) for the electrostatic field of a localized system of charges at a distant point $(r \gg r \prime \sim a)$.

Then positions of all charges of the system satisfy the following condition

$$
\begin{equation*}
r^{\prime} \ll r . \tag{3.1}
\end{equation*}
$$

Using this condition, we can expand the general expression (1.38) for the electrostatic potential $\phi(\mathbf{r})$ of the system into the Taylor series in small parameter $\mathbf{r}^{\prime} \equiv\left\{r^{\prime}{ }_{1}, r^{\prime}{ }_{2}, r^{\prime}{ }_{3}\right\}$. For any spatial function of the type $f\left(\mathbf{r}-\mathbf{r}^{\prime}\right)$, the expansion may be presented as ${ }^{1}$

$$
\begin{equation*}
f\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \approx f(\mathbf{r})-\sum_{j=1}^{3} r_{j}^{\prime} \frac{\partial f}{\partial r_{j}}(\mathbf{r})+\frac{1}{2!} \sum_{j, j^{\prime}=1}^{3} r_{j}^{\prime} r_{j^{\prime}}^{\prime} \frac{\partial^{2} f}{\partial r_{j} \partial r_{j^{\prime}}}(\mathbf{r})-\ldots \tag{3.2}
\end{equation*}
$$

The two leading terms of this expansion, sufficient for our current purposes, may be rewritten in the vector form: ${ }^{2}$

$$
\begin{equation*}
f\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \approx f(\mathbf{r})-\mathbf{r}^{\prime} \cdot \nabla f(\mathbf{r})+\ldots \tag{3.3}
\end{equation*}
$$

Let us apply this approximate formula to the free-space Green's function (2.204), which weighs the charge density contributions in Eq. (1.38). The gradient of such a spherically-symmetric function $f(r)=$ $1 / r$ is just $\mathbf{n}_{r} d f / d r$, so that

[^220]\[

$$
\begin{equation*}
\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \approx \frac{1}{r}-\mathbf{r}^{\prime} \cdot \mathbf{n}_{r} \frac{d}{d r}\left(\frac{1}{r}\right)=\frac{1}{r}+\mathbf{r}^{\prime} \cdot \frac{\mathbf{r}}{r^{3}} . \tag{3.4}
\end{equation*}
$$

\]

Plugging this dipole expansion into Eq. (1.38), we get

$$
\begin{equation*}
\phi(\mathbf{r}) \approx \frac{1}{4 \pi \varepsilon_{0}}\left[\frac{1}{r} \int \rho\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime}+\frac{\mathbf{r}}{r^{3}} \cdot \int \rho\left(\mathbf{r}^{\prime}\right) \mathbf{r}^{\prime} d^{3} r^{\prime}\right]=\frac{1}{4 \pi \varepsilon_{0}}\left(\frac{Q}{r}+\frac{\mathbf{r} \cdot \mathbf{p}}{r^{3}}\right), \tag{3.5}
\end{equation*}
$$

where $Q$ is the net charge of the system, while the vector

$$
\begin{equation*}
\mathbf{p} \equiv \int \rho\left(\mathbf{r}^{\prime}\right) \mathbf{r}^{\prime} d^{3} r^{\prime} \tag{3.6}
\end{equation*}
$$

with magnitude $p$ of the order of $Q a$, is called its (electric) dipole moment. ${ }^{3}$
If $Q \neq 0$, the second term in the right-hand part of Eq. (5) is just a small correction to the first one, and in many cases may be ignored. (Remember, Eq. (5) is only valid in the limit $r / a \rightarrow \infty$ ). However, the net charge of many systems is exactly zero. The most important example is a neutral atom or a neutral molecule, in which the negative charge of electrons exactly compensates the positive charge of protons in nuclei. For such neural systems, the second (dipole-moment) term, $\phi_{d}$, in Eq. (5) is the leading one. Due to its importance, let us rewrite this expression in two other, equivalent forms:

$$
\begin{equation*}
\phi_{d} \equiv \frac{1}{4 \pi \varepsilon_{0}} \frac{\mathbf{r} \cdot \mathbf{p}}{r^{3}}=\frac{1}{4 \pi \varepsilon_{0}} \frac{p \cos \theta}{r^{2}}=\frac{1}{4 \pi \varepsilon_{0}} \frac{p z}{\left[x^{2}+y^{2}+z^{2}\right]^{3 / 2}}, \tag{3.7}
\end{equation*}
$$

Electric dipole's potential
that are more convenient for some applications. Here $\theta$ is the angle between vectors $\mathbf{p}$ and $\mathbf{r}$, and in the last (Cartesian) presentation, axis $z$ is directed along vector $\mathbf{p}$. Figure 2a shows equipotential surfaces of the dipole field (or rather their cross-sections by a plane in which vector $\mathbf{p}$ resides).


Fig. 3.2. Dipole field: (a) equipotential surfaces and (b) electric field lines, for vertical vector $\mathbf{p}$.

[^221]The simplest example of the dipole (that gave such systems their name) is a system of two equal but opposite point charges, $+q$ and $-q$, with radius-vectors, respectively, $\mathbf{r}_{+}$and $\mathbf{r}_{\text {.: }}$

$$
\begin{equation*}
\rho(\mathbf{r})=(+q) \delta\left(\mathbf{r}-\mathbf{r}_{+}\right)+(-q) \delta\left(\mathbf{r}-\mathbf{r}_{-}\right) . \tag{3.8}
\end{equation*}
$$

For this system, Eq. (6) yields

$$
\begin{equation*}
\mathbf{p}=(+q) \mathbf{r}_{+}+(-q) \mathbf{r}_{-}=q\left(\mathbf{r}_{+}-\mathbf{r}_{-}\right)=q \mathbf{a}, \tag{3.9}
\end{equation*}
$$

where $\mathbf{a}$ is the vector connecting points $\mathbf{r}_{-}$and $\mathbf{r}_{+}$. Note that in this case (and for all systems with $Q=0$ ), the dipole moment does not depend on the reference frame origin choice.

A less trivial example is a conducting sphere of radius $R$ in a uniform external electric field $\mathbf{E}_{0}$. As a reminder, we have solved this problem in Sec. 2.5(iv) and obtained Eq. (2.176) as a result. The first term in the parentheses of that relation describes the external field (2.173), so that the field of the sphere itself (meaning the field of its surface charge induced by $\mathbf{E}_{0}$ ) is given by the second term:

$$
\begin{equation*}
\phi_{s}=\frac{E_{0} R^{3}}{r^{2}} \cos \theta \tag{3.10}
\end{equation*}
$$

Comparing this expression with the second form of Eq. (7), we see that the sphere has an induced dipole moment

$$
\begin{equation*}
\mathbf{p}=4 \pi \varepsilon_{0} \mathbf{E}_{0} R^{3} \tag{3.11}
\end{equation*}
$$

This is an interesting example of a purely dipole field - in all points outside the sphere $(r>R)$, the field has no higher moments. ${ }^{4}$

Returning to the general properties of the dipole field, let us calculate its characteristics. First of all, we may use Eq. (7) to calculate the electric field of a dipole:

$$
\begin{equation*}
\mathbf{E}_{d}=-\nabla \phi_{d}=-\frac{1}{4 \pi \varepsilon_{0}} \nabla\left(\frac{\mathbf{r} \cdot \mathbf{p}}{r^{3}}\right)=-\frac{1}{4 \pi \varepsilon_{0}} \nabla\left(\frac{p \cos \theta}{r^{2}}\right) \tag{3.12}
\end{equation*}
$$

The differentiation is easiest in spherical coordinates, using the following well-known expression for the gradient of a scalar function in these coordinates ${ }^{5}$ and taking axis $z$ parallel to vector $\mathbf{p}$. From the last form of Eq. (12) we immediately get

$$
\begin{equation*}
\mathbf{E}_{d}=\frac{p}{4 \pi \varepsilon_{0} r^{3}}\left(2 \mathbf{n}_{r} \cos \theta+\mathbf{n}_{\theta} \sin \theta\right)=\frac{1}{4 \pi \varepsilon_{0}} \frac{3 \mathbf{r}(\mathbf{r} \cdot \mathbf{p})-\mathbf{p} r^{2}}{r^{5}} \tag{3.13}
\end{equation*}
$$

Figure $2 b$ shows the electric field lines given by Eqs. (13).
Next, let us calculate the potential energy of interaction between a fixed dipole and a external electric field, using Eq. (1.54). Assuming that the external field does not change much at distances of the order of $a$ (Fig. 1), we may expand the external potential $\phi_{\text {ext }}(\mathbf{r})$ into the Taylor series, just as Eq. (3) prescribes, and keep only its two leading terms:

[^222]\[

$$
\begin{equation*}
U=\int \rho(\mathbf{r}) \phi_{\mathrm{ext}}(\mathbf{r}) d^{3} r \approx \int \rho(\mathbf{r})\left[\phi_{\mathrm{ext}}(0)+\mathbf{r} \cdot \nabla \phi_{\mathrm{ext}}(0)\right] d^{3} r=Q \phi_{\mathrm{ext}}(0)-\mathbf{p} \cdot \mathbf{E}_{\mathrm{ext}} . \tag{3.14}
\end{equation*}
$$

\]

The first term is the potential energy the system would have if it were a point charge. If the net charge $Q$ is zero, that term disappears, and the leading contribution is due to the dipole moment:

$$
\begin{equation*}
U=-\mathbf{p} \cdot \mathbf{E}_{\mathrm{ext}} . \tag{3.15}
\end{equation*}
$$

Note, however, that Eq. (15) is only valid for a fixed dipole, with $\mathbf{p}$ independent of $\mathbf{E}_{\text {ext }}$. In the opposite limit, when the dipole is induced by the field, i.e. $\mathbf{p} \propto \mathbf{E}_{\text {ext }}$ (see Eq. (11) as an example), we can repeat the discussion that accompanied Fig. 1.6 to show that Eq. (15) acquires an additional factor $1 / 2$.

In particular, combining Eqs. (13) and Eq. (15), we may get the following important formula for interaction of two independent dipoles

$$
\begin{equation*}
U=\frac{1}{4 \pi \varepsilon_{0}} \frac{\mathbf{p}_{1} \cdot \mathbf{p}_{2} r^{2}-3\left(\mathbf{r} \cdot \mathbf{p}_{1}\right)\left(\mathbf{r} \cdot \mathbf{p}_{2}\right)}{r^{5}}=\frac{1}{4 \pi \varepsilon_{0}} \frac{p_{1 x} p_{2 x}+p_{1 y} p_{2 y}-2 p_{1 z} p_{2 z}}{r^{3}}, \tag{3.16}
\end{equation*}
$$

where $\mathbf{r}$ is the vector connecting the dipoles, and axis $z$ is directed along this vector. If each moment is due to the polarization of the dipole by the electric field of its counterpart: $\mathbf{p}_{1,2} \propto \mathbf{E}_{2,1} \propto 1 / r^{3}$, this expression (which is valid for this case with the additional factor $1 / 2$ ) the potential is always negative and proportional to $1 / r^{6}$. Such potential describes, in particular, the long-range, attractive part (the so-called London dispersion force) of the interaction between electrically neutral atoms and molecules. ${ }^{6}$

According to Eq. (15), in order to reach the minimum of $U$, the electric field "tries" to align the dipole direction along its own. The quantitative expression of this effect is the torque $\tau$ exerted by the field. The simplest way to calculate it is to sum up all the elementary torques $d \tau=\mathbf{r} \times d \mathbf{F}_{\text {ext }}=$ $\mathbf{r} \times \mathbf{E}_{\text {ext }}(\mathbf{r}) \rho(\mathbf{r}) d^{3} r$ exerted on all elementary charges of the system:

$$
\begin{equation*}
\boldsymbol{\tau}=\int \mathbf{r} \times \mathbf{E}_{\mathrm{ext}}(\mathbf{r}) \rho(\mathbf{r}) d^{3} r \approx \mathbf{p} \times \mathbf{E}_{\mathrm{ext}}(0), \tag{3.17}
\end{equation*}
$$

where at the last transition we have again neglected the spatial dependence of the external field.
The spatial dependence of $\mathbf{E}_{\text {ext }}$ cannot, however, be ignored at the calculation of the total force exerted by the field on the dipole (with $Q=0$ ). Indeed, Eq. (15) shows that if the field is constant, the dipole energy is the same at all spatial points, and hence the net force is zero. However, if the field has a finite gradient, a total force does appear:

$$
\begin{equation*}
\mathbf{F}=-\nabla U=\nabla\left(\mathbf{p} \cdot \mathbf{E}_{\mathrm{ext}}\right), \tag{3.18}
\end{equation*}
$$

where the derivative has to be taken at the dipole's position (in our notation, at $\mathbf{r}=0$ ). If the dipole that is being moved in a field retains its magnitude and orientation, then the last formula is equivalent to ${ }^{7}$

$$
\begin{equation*}
\mathbf{F}=(\mathbf{p} \cdot \nabla) \mathbf{E}_{\mathrm{ext}} . \tag{3.19}
\end{equation*}
$$

Alternatively, the last expression may be obtained similarly to Eq. (14):

$$
\begin{equation*}
\mathbf{F}=\int \rho(\mathbf{r}) \mathbf{E}_{\mathrm{ext}}(\mathbf{r}) d^{3} r \approx \int \rho(\mathbf{r})\left[\mathbf{E}_{\mathrm{ext}}(0)+(\mathbf{r} \cdot \nabla) \mathbf{E}_{\mathrm{ext}}\right] d^{3} r=Q \mathbf{E}_{\mathrm{ext}}(0)+(\mathbf{p} \cdot \nabla) \mathbf{E}_{\mathrm{ext}} \tag{3.20}
\end{equation*}
$$

[^223]Finally, let me add a note on the so-called coarse-grain model of the dipole. The dipole approximation explored above is asymptotically correct at large distances, $r \gg a$. However, for some applications (including the forthcoming discussion in Sec. 5 of molecular field effects) it is important to have an expression that would be approximately valid everywhere in space, though maybe without exact details at $r \sim a$, and also give the correct result for the space-average of the electric field,

$$
\begin{equation*}
\overline{\mathbf{E}} \equiv \frac{1}{V} \int_{V} \mathbf{E} d^{3} r \tag{3.21}
\end{equation*}
$$

where $V$ is a regularly-shaped volume much larger than $a^{3}$, for example a sphere of radius $R \gg a$, with the dipole at its center. For the field $\mathbf{E}_{d}$ given by Eq. (13), such average is zero. Indeed, let us consider Cartesian components of that vector in the coordinate system with axis $z$ directed along vector $\mathbf{p}$. Due to the axial symmetry of the field, the averages of components $E_{x}$ and $E_{y}$ evidently vanish. Let us use Eq. (13) to spell out the "vertical" component of the field (parallel to the dipole moment vector):

$$
\begin{equation*}
E_{z} \equiv \mathbf{E}_{d} \cdot \frac{\mathbf{p}}{p}=\frac{1}{4 \pi \varepsilon_{0} r^{3}}\left(2 \mathbf{n}_{r} \cdot \mathbf{p} \cos \theta-\mathbf{n}_{\theta} \cdot \mathbf{p} \sin \theta\right)=\frac{p}{4 \pi \varepsilon_{0} r^{3}}\left(2 \cos ^{2} \theta-\sin ^{2} \theta\right) . \tag{3.22}
\end{equation*}
$$

Integrating this expression over the whole solid angle $\Omega=4 \pi$, at fixed $r$, using a convenient variable substitution $\cos \theta \equiv \xi$, we get

$$
\begin{equation*}
\oint_{4 \pi} E_{z} d \Omega=2 \pi \int_{0}^{\pi} E_{z} \sin \theta d \theta=\frac{p}{2 \varepsilon_{0} r^{3}} \int_{0}^{\pi}\left(2 \cos ^{2} \theta-\sin ^{2} \theta\right) \sin \theta d \theta=\frac{p}{2 \varepsilon_{0} r^{3}} \int_{-1}^{+1}\left(3 \xi^{3}-\xi\right) d \xi=0 \tag{3.23}
\end{equation*}
$$

On the other hand, the exact electric field of an arbitrary charge distribution, having the total dipole moment $\mathbf{p}$, satisfies the following condition,

$$
\begin{equation*}
\int_{V} \mathbf{E}(\mathbf{r}) d^{3} r=-\frac{\mathbf{p}}{3 \varepsilon_{0}} \tag{3.24}
\end{equation*}
$$

where the integration is over any sphere containing all the charges. A proof of this formula for the general case requires a somewhat cumbersome, though straightforward integration, ${ }^{8}$ but later in the course we will see that it is correct for several particular cases. The origin of the difference between Eqs. (23) and (24) is illustrated in Fig. 3 on the example of a dipole created by two equal but opposite charges - see Eqs. (8)-(9). The zero average of the dipole field (13) does not take into account the contribution of the field in the region between the charges (where Eq. (13) is not valid), which is directed mostly against the dipole vector (9).

Thus in order to be used as a reasonable coarse-grain model, Eq. (13) should be modified as follows:

$$
\begin{equation*}
\mathbf{E}_{c g}=\frac{1}{4 \pi \varepsilon_{0}}\left[\frac{3 \mathbf{r}(\mathbf{r} \cdot \mathbf{p})-\mathbf{p} r^{2}}{r^{5}}-\frac{4 \pi}{3} \mathbf{p} \delta(\mathbf{r})\right] . \tag{3.25}
\end{equation*}
$$

Evidently, such modification does not change the field at large distances $r \gg a$, i.e. in the region where the expansion (3) and hence Eq. (13) are valid.

[^224]

Fig. 3.3. Illustrating the origin of Eq. (24). (The field lines are very approximate.)

### 3.2. Dipole media

Let us generalize equation (7) to the case of several (possibly, many) dipoles $\mathbf{p}_{j}$ located at arbitrary points $\mathbf{r}_{j}$. Using the linear superposition principle, we get

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \sum_{j} \mathbf{p}_{j} \cdot \frac{\mathbf{r}-\mathbf{r}_{j}}{\left|\mathbf{r}-\mathbf{r}_{j}\right|^{3}} . \tag{3.26}
\end{equation*}
$$

If our system (medium) contains many similar dipoles, distributed in space with density $n(\mathbf{r})$, we may use the same standard argumentation that has led us from Eq. (1.5) to Eq. (1.8), to rewrite the last sum as an integral

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int \mathbf{P}\left(\mathbf{r}^{\prime}\right) \cdot \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} d^{3} r^{\prime}, \tag{3.27}
\end{equation*}
$$

where vector $\mathbf{P}(\mathbf{r}) \equiv n(\mathbf{r}) \mathbf{p}$, called electric polarization has the physical meaning of the net dipole moment per unit volume. Note again that since Eq. (26) does not describe that field at distances comparable to the dipole size, and hence Eq. (27), and all the following formulas of this section, describes the so-called macroscopic electric field, i.e. the dipole field averaged over the microscopic (dipole-size) distances.

Now comes a very impressive mathematical trick. Just as has been done in the previous section (just with the appropriate sign change), Eq. (27) may be rewritten in the equivalent form

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int \mathbf{P}\left(\mathbf{r}^{\prime}\right) \cdot \nabla^{\prime} \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} \tag{3.28}
\end{equation*}
$$

where $\nabla$ ' means the del operator (in this particular case, the gradient) acting in the "source space" of vectors $\mathbf{r}$ '. The right-hand part of Eq. (28), applied to any volume $V$ limited by surface $S$, may be integrated by parts in the following way: ${ }^{9}$

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \oint_{S} P_{n}\left(\mathbf{r}^{\prime}\right) \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{2} r^{\prime}-\frac{1}{4 \pi \varepsilon_{0}} \int_{V} \frac{\nabla^{\prime} \cdot \mathbf{P}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} . \tag{3.29}
\end{equation*}
$$

[^225]If the surface does not carry an infinitely dense ( $\delta$-functional) sheet of additional dipoles, or it is just very far, the first term in the right-hand part is negligible. Now comparing the second term with the basic equation (1.38) for the electric potential, we see that this term may be interpreted as the field of certain effective electric charges with density

Effective
charge density

$$
\begin{equation*}
\rho_{\mathrm{ef}}=-\nabla \cdot \mathbf{P} \tag{3.30}
\end{equation*}
$$

Figure 4 illustrates the physics of this relation for a cartoon model of a multi-dipole system: a layer of uniformly-distributed two-point-charge units oriented perpendicular to the layer surface. (In this case $\nabla \cdot \mathbf{P}=d P / d x$.) One can see that $\rho_{\text {ef }}$, defined by Eq. (30), may be interpreted as the density of uncompensated surface charges of polarized elementary dipoles.


Fig. 3.4. Spatial distributions of the polarization and effective charges in a layer of similar elementary dipoles (schematically).

Next, from Sec. 1.2, we already know that Eq. (1.38) is equivalent to the inhomogeneous Maxwell equation (1.27) for the electric field. This is why Eq. (30) implies that if, besides the compensated charges of the dipoles, the system also has certain stand-alone charges (not a part of the dipoles!) distributed in space with density $\rho(\mathbf{r})$, the average electric field obeys, instead of Eq. (1.27), the following generalized equation

$$
\begin{equation*}
\nabla \cdot \mathbf{E}=\frac{1}{\varepsilon_{0}}\left(\rho+\rho_{\mathrm{ef}}\right)=\frac{1}{\varepsilon_{0}}(\rho-\nabla \cdot \mathbf{P}) . \tag{3.31}
\end{equation*}
$$

It is evidently tempting (and very convenient for applications!) to carry over the dipole-related term of this equation over to the left-hand part of Eq. (31), and rewrite the resulting equality as the so-called macroscopic Maxwell equation

$$
\begin{equation*}
\nabla \cdot \mathbf{D}=\rho \tag{3.32}
\end{equation*}
$$

where a new vector, called the electric displacement, is defined as ${ }^{10}$

[^226]\[

$$
\begin{equation*}
\mathbf{D} \equiv \varepsilon_{0} \mathbf{E}+\mathbf{P} \tag{3.33}
\end{equation*}
$$

\]

The comparison of Eqs. (32) and (1.27) shows that $\mathbf{D}$ may be interpreted as the "would-be" electric field that would be created by stand-alone charges in the absence of the dipole medium polarization. In contrast, $\mathbf{E}$ is the actual electric field - though, as was mentioned above, space-averaged over a volume much larger that of an elementary dipole. ${ }^{11}$

To complete the general analysis of the multi-dipole systems, let us rewrite the macroscopic Maxwell equation (32) in the integral form. Applying the divergence theorem to an arbitrary volume $V$ limited by surface $S$, we get the following macroscopic Gauss law:

$$
\begin{equation*}
\oint_{S} D_{n} d^{2} r=\int_{V} \rho d^{3} r \equiv Q \tag{3.34}
\end{equation*}
$$

where $Q$ is the total stand-alone charge inside volume $V$.
Let me emphasize again that the key Eq. (27), and hence all the following equations of this section, only to the macroscopic field, i.e. the electric field averaged over its rapid variations at the atomic space scale. Such macroscopic description is valid as soon as we are not concerned with the inter-atomic field variations - for whose description the classical physics is inadequate in any case.

### 3.3. Linear dielectrics

The general equations derived above are broadly used to describe any dielectrics - materials with bound electric charges (and hence with no dc electric conduction). The polarization properties of these materials may be described by the dependence between vectors $\mathbf{P}$ and $\mathbf{E}$. In the most materials, in the absence of external electric field, the elementary dipoles $\mathbf{p}$ either equal zero or have a random orientation in space, so that the net dipole moment of each macroscopic volume (still containing many such dipoles) equals zero: $\mathbf{P}=0$.

Moreover, if the field changes are sufficiently slow, most materials may be characterized by a unique dependence of $\mathbf{P}$ on $\mathbf{E}$. Then using the Taylor expansion of function $\mathbf{P}(\mathbf{E})$, we may argue that in relatively low electric fields the function should be well approximated by a linear dependence between these two vectors. In an isotropic media, the coefficient of proportionality should be just a scalar. ${ }^{12}$ In SI units, this constant is defined by the following relation:

$$
\begin{equation*}
\mathbf{P}=\chi_{e} \varepsilon_{0} \mathbf{E} \tag{3.35}
\end{equation*}
$$

Electric susceptibility definition
with the dimensionless constant $\chi_{e}$ called the electric susceptibility. However, it is much more common to use, instead of $\chi_{e}$, another parameter,

$$
\begin{equation*}
\varepsilon_{r} \equiv 1+\chi_{e}, \tag{3.36}
\end{equation*}
$$

[^227]which is sometimes called the relative electric permittivity, but much more often, the dielectric constant. ${ }^{13}$ This parameter is very convenient, because combining Eqs. (35) and (36),
\[

$$
\begin{equation*}
\mathbf{P}=\left(\varepsilon_{r}-1\right) \varepsilon_{0} \mathbf{E} . \tag{3.37}
\end{equation*}
$$

\]

and then plugging the resulting relation into the general Eq. (33), we get simply ${ }^{14}$

Electric permittivity

$$
\begin{equation*}
\mathbf{D}=\varepsilon \mathbf{E}, \quad \text { with } \varepsilon \equiv \varepsilon_{0} \varepsilon_{r}=\varepsilon_{0}\left(1+\chi_{e}\right) \tag{3.38}
\end{equation*}
$$

where $\varepsilon$ is called the electric permittivity of the material. Table 1 gives values of the dielectric constant for several representative materials.

Table 3.1. Dielectric constants of a few representative (and/or practically important) dielectrics

| Material | $\varepsilon_{r}$ |
| :---: | :---: |
| Air (at ambient conditions) | 1.00054 |
| Teflon (polytetrafluoroethylene, $\mathrm{C}_{n} \mathrm{~F}_{2 n}$ ) | 2.1 |
| Silicon dioxide (amorphous) | 3.9 |
| Glasses (of various compositions) | $3.7-10$ |
| Castor oil | 4.5 |
| Silicon | 11.7 |
| Water (at $100^{\circ} \mathrm{C}$ ) | 55.3 |
| Water (at $20^{\circ} \mathrm{C}$ ) | 80.1 |
| Barium titanate $\left(\mathrm{BaTiO}_{3}\right.$ at $20^{\circ} \mathrm{C}$ ) | $\sim 1,600$ |

In order to get some feeling of the physics behind these values, let us consider a very common model of a media whose elementary dipoles do not interact, so that in the relation $\mathbf{P}=n \mathbf{p}$ the elementary dipole moments $\mathbf{p}$ may be calculated independently of each other. This means that in a linear dielectric, in which Eq. (35) holds, each induced dipole moment $\mathbf{p}$ has to be proportional to the applied field $\mathbf{E}$ as well. Let us write this dependence in the following traditional form,

Molecular polarizability

$$
\begin{equation*}
\mathbf{p}=4 \pi \varepsilon_{0} \alpha_{\mathrm{mol}} \mathbf{E} \tag{3.39}
\end{equation*}
$$

where $\alpha_{\text {mol }}$ is called the molecular (or, sometimes, "atomic") polarizability, so that

$$
\begin{equation*}
\mathbf{P} \equiv n \mathbf{p}=4 \pi \varepsilon_{0} \alpha_{\mathrm{mol}} n \mathbf{E} . \tag{3.40}
\end{equation*}
$$

Comparing this relation with Eq. (35), we get $\chi_{e}=4 \pi \alpha_{\text {mol }} n$, so that Eq. (36) yields ${ }^{15}$

[^228]\[

$$
\begin{equation*}
\varepsilon_{r}=1+4 \pi \alpha_{\mathrm{mol}} n \tag{3.41}
\end{equation*}
$$

\]

Now let us consider the following toy model of a dielectric: ${ }^{16}$ a set of similar conducting spheres of radius $R$, spread apart with small density $n \ll 1 / R^{3}$. At such low density of the spheres, their electrostatic interaction is negligible, and we can use Eq. (11) for the induced dipole moment of a single sphere. Then the polarizability definition (39) yields $\alpha_{\text {mol }}=R^{3}$, so that $\chi_{e}=4 \pi n R^{3}$, and

$$
\begin{equation*}
\varepsilon_{r}=1+4 \pi R^{3} n \tag{3.42}
\end{equation*}
$$

Let us use this result for a crude estimate of the dielectric constant of air at the so-called ambient conditions, meaning the normal atmospheric pressure, and temperature $T=300 \mathrm{~K}$. At these conditions the molecular density $n$ may be, with a few-percent accuracy, found from the equation of state of an ideal gas: ${ }^{17} n \approx P / k_{\mathrm{B}} T \approx\left(1.013 \times 10^{5}\right) /\left(1.38 \times 10^{-23} \times 300\right) \approx 2.5 \times 10^{25} \mathrm{~m}^{-3}$. The main component of air, molecular nitrogen $\mathrm{N}_{2}$, has a van-der-Waals radius ${ }^{18}$ of $155 \mathrm{pm}=1.55 \times 10^{-10} \mathrm{~m}$. Using it for $R$, from our crude model we get $\varepsilon_{r} \approx 1.001$. Comparing this number with the first line of Table 1 , we see that our crude model gives surprisingly reasonable results: in order to get the exact experimental value, it is sufficient to decrease $R$ by just $\sim 25 \%$.

This result may encourage us to try using Eq. (42) for larger density $n$, i.e., beyond the range of its quantitative applicability. For example, as a crude model for solid and liquids let us assume that spheres form a simple cubic lattice with period $a=2 R$ (i.e., the neighboring spheres almost touch). With this $n=1 / a^{3}=1 / 8 R^{3}$, Eq. (33) yields $\varepsilon_{r}=1+4 \pi / 8 \approx 2.5$. Due to the crude nature of this estimate, we may conclude that it provides a reasonable explanation for the values of $\varepsilon_{r}$, listed in first few lines of Table 1. Still, it is clear that such model cannot even approximately describe dielectric properties of either water or barium titanate (and similar materials), as well as their strong temperature dependence. Such high values may be explained by the molecular field effect: each elementary dipole is polarized not only by the external field (as in our current toy model), but by the field of neighboring dipoles as well.

Before analyzing this effect (in the next section), let us review how are the most important results of electrostatics modified by a uniform linear dielectric medium that obeys Eq. (38) with a spaceindependent dielectric constant $\varepsilon_{r}$. The simplest problem of this kind is a set of free charges of density $\rho(\mathbf{r})$, inserted into the medium. For this case, we can combine Eqs. (32) and (38) to write

$$
\begin{equation*}
\nabla \cdot \mathbf{E}=\frac{\rho}{\varepsilon}, \quad \text { i.e. } \nabla^{2} \phi=-\frac{\rho}{\varepsilon} \tag{3.43}
\end{equation*}
$$

For charges in vacuum, we had similar equations (1.27) and (1.41), but with a different constant, $\varepsilon_{0}=$ $\varepsilon / \varepsilon_{r}$. Hence all the results discussed in Chapter 1 are valid, with both $\mathbf{E}$ and $\phi$ reduced by the factor of $\varepsilon_{r}$. Thus, the most straightforward result of the induced polarization of a dielectric media is the electric field reduction. This is a very important effect, especially taken into account the very high values of $\varepsilon_{r}$ in such dielectrics as water - see Table 1 . Indeed, this is the reduction of the attraction between positive

[^229]and negative ions (called, respectively, cations and anions) in water that enables their substantial dissociation and hence almost all biochemical reactions, which are the basis of biological cell functions and hence of the life itself.

Now, what if the electric field in a uniform dielectric is induced by charges located on conductors - with potentials rather than charge density fixed? Then, with the substitution of the electrostatic potential definition $\mathbf{E} \equiv-\nabla \phi$, Eq. (43) in the space between the conductors is reduced to the Laplace equation, and the boundary problem remains exactly the same as formulated in Chapter 2 - see Eqs. (2.35). Hence the potential distribution $\phi(\mathbf{r})$ is related to the conductor potential in exactly the same way as in vacuum (see, e.g., any problem discussed in Chapter 2), without any effect of the medium polarization. However, in order to find, from that distribution, the density $\sigma$ of charges on conductor surfaces, we need to use the macroscopic Gauss law (34). Applying this equation to a pillbox-shaped volume on the conductor surface, we get the following relation,

$$
\begin{equation*}
\sigma=D_{n}=\varepsilon E_{n}=-\varepsilon \frac{\partial \phi}{\partial n}, \tag{3.44}
\end{equation*}
$$

which differs from Eq. (2.3) only by the replacement $\varepsilon_{0} \rightarrow \varepsilon=\varepsilon_{r} \varepsilon_{0}$. Hence the charge density, calculated for the vacuum case, should be increased by the factor of $\varepsilon_{r}-$ that's it. In particular, this means that all the capacitances that had been calculated in vacuum, should be increased by that factor. For example, for planar capacitor filled with linear dielectric $\varepsilon_{r}$, we get the well-known formula

$$
\begin{equation*}
C_{m}=\frac{\varepsilon_{r} \varepsilon_{0} A}{d}=\frac{\varepsilon A}{d} \tag{3.45}
\end{equation*}
$$

(As a reminder, this increase of $C_{m}$ by $\varepsilon_{r}$ has been already used in Sec. 2.2 for capacitance estimates.)
Now let us discuss more complex situations in which the dielectric medium is not uniform, for example when it contains a boundary separating two regions filled by different uniform dielectrics. (The analysis is clearly applicable to a dielectric/vacuum boundary as well, with one of the dielectric constants set to 1.) For that, let us apply the macroscopic Gauss law (34) to a pillbox formed at the interface between two dielectrics, with no surface charges - see the solid lines in Fig. 5.


Fig. 3.5. Deriving boundary conditions on the interface between two dielectrics: a Gauss pillbox and a circulation contour. $\mathbf{n}$ and $\tau$ are the unit vectors which are, respectively, normal and tangential to the interface.

This immediately gives $\left(D_{n}\right)_{1}=\left(D_{n}\right)_{2}$, so that Eq. (38) yields

Boundary condition for $E_{n}$

$$
\begin{equation*}
\left(\varepsilon E_{n}\right)_{1}=\left(\varepsilon E_{n}\right)_{2}, \quad \text { i.e. } \varepsilon_{1} \frac{\partial \phi_{1}}{\partial n}=\varepsilon_{2} \frac{\partial \phi_{2}}{\partial n} \tag{3.46}
\end{equation*}
$$

Now, what about the tangential component $\left(E_{\tau}\right)$ of the electric field? In dielectrics, static electric field is still potential, hence we can still use Eq. (1.28). Integrating this equation along to a narrow contour stretched along the interface (see the dashed line in Fig. 5), we get

$$
\begin{equation*}
\left(E_{\tau}\right)_{1}=\left(E_{\tau}\right)_{2}, \quad \text { i.e. } \frac{\partial \phi_{1}}{\partial \tau}=\frac{\partial \phi_{2}}{\partial \tau} . \tag{3.47}
\end{equation*}
$$

Note that this condition is compatible with (and may be derived follows from) the continuity of the electrostatic potential itself, $\phi_{1}=\phi_{2}$, at each point of the interface. That relation may be derived from the electric field definition as the gradient of $\phi$-see Eq. (1.33). Indeed, if the potential leaped at the border, the electric field would be infinite.

Let us apply the boundary conditions (46)-(47), for example, to two thin ( $t \ll d$ ) vacuum slits cut in a uniform dielectric with an initially uniform ${ }^{19}$ electric field $\mathbf{E}_{0}$ (Fig. 6). In both cases, a slit with $t$ $\rightarrow 0$ cannot modify the field distribution outside it substantially.


Fig. 3.6. Fields inside narrow slits cut in a linear dielectric.

For slit (a), normal to the applied field, we may apply Eq. (46) to the "major" (broad) interfaces, shown horizontal in Fig. 6, we see that $D$ should be continuous. But according to Eq. (33), this means that inside the gap (i. e. in the vacuum, with $\mathbf{P}=0$ ) the electric field equals $\mathbf{D} / \varepsilon_{0}$. This field, and hence D, may be measured, showing that the electric displacement is not a purely mathematical construct. Superficially, this result violates the boundary condition (47) on the vertical ("minor") interfaces of the slit. Note, however, that the electric field within the gap is $\varepsilon_{r}$ times higher than in the dielectric outside it. Hence the slit deforms the equipotential surfaces around it to concentrate the field inside itself. The curving of the surfaces near the minor interfaces takes care of the fulfillment of Eq. (47) at the minor interfaces.

On the contrary, for slit (b) parallel to the applied field, we may apply Eq. (47) to the major (now, vertical) interfaces of the slit, to see that it is electric field $\mathbf{E}$ that is continuous now, while the electric displacement $\mathbf{D}=\varepsilon_{0} \mathbf{E}$ inside the gap is a factor of $\varepsilon_{r}$ lower than its value in the dielectric. (Any perturbation of the field uniformity, caused by the compliance with Eq. (46) at the minor interfaces, is settled at distances $\sim t$ from these interfaces.)

[^230]For problems with piecewise-constant $\varepsilon$ but more complex geometries we may need to apply the methods studied in Chapter 2. As in vacuum, in the simplest cases we can select such a set of orthogonal coordinates that the electrostatic potential depends on just one of them. Consider, for example, two types of plane capacitor filling with two different dielectrics - see Fig. 7.

In case (a), voltage $V$ between the electrodes is the same for each part of the capacitor, and at least far from the dielectric interface, the electric field is vertical, uniform, and similar ( $E=V / d$ ). Hence the boundary condition (47) is satisfied even if such a distribution is valid near the surface as well, i.e. at any point of the system. The only effect of different values of $\varepsilon$ in the two parts is that the electric displacement $D=\varepsilon E$ and hence electrodes' surface charge density $\sigma=D$ are different in the two parts. Thus we can calculate the electrode charges $Q_{1,2}$ of the two parts independently, in each case using Eq. (44), and then add up the results to get the total capacitance

$$
\begin{equation*}
C_{m}=\frac{Q_{1}+Q_{2}}{V}=\frac{1}{d}\left(\varepsilon_{1} A_{1}+\varepsilon_{2} A_{2}\right) . \tag{3.48}
\end{equation*}
$$

Note that this formula may be interpreted as the total capacitance of two separate capacitors connected (by conducting wires) in parallel. This is natural, because we may cut the system along the dielectric interface, without any effect on the fields in either part, and then connect the corresponding electrodes by external wires, again without any effect on the system - besides very close to capacitor's edges.

(b)

Fig. 3.7. Plane capacitors filled with two different dielectrics.

Case (b) may be analyzed by applying Eq. (34) to a Gaussian pillbox with the lower lid inside the (for example) bottom electrode, and the top lid in any of the layers. From this we see that $D$ anywhere inside the system should be equal to the surface charge density $\sigma$ of the lower electrode, i.e. constant. Hence, in the top dielectric layer the electric field is constant: $E_{1}=D_{1} / \varepsilon_{1}=\sigma / \varepsilon_{1}$, while in bottom layer, similarly, $E_{2}=D_{2} / \varepsilon_{2}=\sigma / \varepsilon_{2}$. Integrating $E$ across the whole capacitor, we get

$$
\begin{equation*}
V=\int_{0}^{d_{1}+d_{2}} E(z) d z=E_{1} d_{1}+E_{2} d_{2}=\left(\frac{d_{1}}{\varepsilon_{1}}+\frac{d_{2}}{\varepsilon_{2}}\right) \sigma, \tag{3.49}
\end{equation*}
$$

so that the mutual capacitance per unit area

$$
\begin{equation*}
\frac{C_{m}}{A} \equiv \frac{\sigma}{V}=\left[\frac{d_{1}}{\varepsilon_{1}}+\frac{d_{2}}{\varepsilon_{2}}\right]^{-1} \tag{3.50}
\end{equation*}
$$

Note that this result is equivalent to the total capacitance of an in-series connection of two plane capacitors based on each of the layers. This is natural, because we could insert an uncharged thin conducting sheet (rather than a cut as in the previous case) at the layer interface, which is an
equipotential surface, without changing the field distribution in the system. Then we could thicken the conducting sheet as much as we like (turning it into a wire), also without changing the fields and hence the capacitance.

In order to warm up for more complex problems, let us see how the last problem could be solved using the Laplace equation approach. Due to the symmetry of the system, the electrostatic potential in each layer may only depend on one (in Fig. 7b, vertical) coordinate $z$, so that the Laplace equation in each uniform part of the system is reduced to $d^{2} \phi / d^{2} z=0$. Hence in each layer the electrostatic potential changes linearly, though possibly with different coefficients: $\phi_{1}=c_{11} Z+c_{12}$, and $\phi_{2}=c_{21} Z+c_{22}$. Selecting the electrode potentials as $\phi(0)=0$ and $\phi\left(d_{1}+d_{2}\right)=V$, from those boundary conditions we get $c_{12}=0, c_{21}\left(d_{1}+d_{2}\right)+c_{22}=V$, so that we need two more equations to find all four coefficients $c_{j j}$. These additional equations come from the conditions of continuity of the potential ( $c_{11} d_{1}+c_{12}=c_{21} d_{1}+c_{22}$ ) and displacement $\left(\varepsilon_{1} c_{11}=\varepsilon_{2} c_{21}\right)$ at the interface $z=d_{1}$. Solving these equations, we can readily find the electric field and displacement in both layers, then the surface charge densities

$$
\begin{equation*}
\sigma(0)=\left.D\right|_{z=0}=-\left.\varepsilon_{1} \frac{d \phi_{1}}{d z}\right|_{z=0}, \quad \sigma\left(d_{1}+d_{2}\right)=\left.D\right|_{z=d_{1}+d_{2}}=-\left.\varepsilon_{2} \frac{d \phi_{2}}{d z}\right|_{z=d_{1}+d_{2}} \tag{3.51}
\end{equation*}
$$

(which in this case are equal and opposite) and finally the capacitance per unit area, with (of course) the same result (50).

Let us apply the same approach to a more complex problem, shown in Fig. 8a: a dielectric sphere placed into a uniform external electric field $\mathbf{E}_{0}$.


Fig. 3.8. Dielectric sphere in an initially uniform electric field: (a) the problem, and (b) the equipotential surfaces, as given by Eq. (55), for $\varepsilon_{r}=3$.

In this case the Laplace equation is not one-dimensional, and hence invites the variable separation method discussed in Sec. 2.5. From that discussion we already know, in particular, the general solution (2.172) of the Laplace equation outside of the sphere. To satisfy the uniform-field condition at $r \rightarrow \infty$, it reduces to

$$
\begin{equation*}
\phi_{r \geq R}=-E_{0} r \cos \theta+\sum_{l=1}^{\infty} \frac{b_{l}}{r^{l+1}} \mathcal{P}_{l}(\cos \theta) . \tag{3.52}
\end{equation*}
$$

Inside the sphere we can only use the radial functions that are finite at $r \rightarrow 0$ :

$$
\begin{equation*}
\phi_{r \leq R}=\sum_{l=1}^{\infty} a_{l} r^{l} \mathcal{P}_{l}(\cos \theta) . \tag{3.53}
\end{equation*}
$$

Now, writing the boundary conditions (46) and (47) at $r=R$, we see that for all coefficients $a_{l}$ and $b_{l}$ with $l \geq 2$ we (just like for the conducting sphere in vacuum) get homogeneous equations that have only trivial solutions. Hence, all these terms may be dropped, while for the only surviving angular harmonic, proportional to $\mathcal{P}_{1}(\cos \theta)=\cos \theta$, Eqs. (46)-(47) yield two equations:

$$
\begin{equation*}
-E_{0}-\frac{2 b_{1}}{R^{3}}=\varepsilon_{r} a_{1}, \quad-E_{0} R+\frac{b_{1}}{R^{2}}=a_{1} R . \tag{3.54}
\end{equation*}
$$

Solving this simple system for $a_{1}$ and $b_{1}$, we get the final solution of the problem:

$$
\begin{equation*}
\phi_{r \geq R}=E_{0}\left(-r+\frac{\varepsilon_{r}-1}{\varepsilon_{r}+2} \frac{R^{3}}{r^{2}}\right) \cos \theta, \quad \phi_{r \leq R}=-E_{0} \frac{3}{\varepsilon_{r}+2} r \cos \theta . \tag{3.55}
\end{equation*}
$$

Figure 8 b shows the equipotential surfaces given by this solution, for a particular value off the dielectric constant $\varepsilon_{r}$. Note that, just like for a conducting sphere, at $r \geq R$ the dielectric sphere produces (on the top of the uniform external field) a purely dipole field, with $\mathbf{p}=4 \pi R^{3} \varepsilon_{0} \mathbf{E}_{0}\left(\varepsilon_{r}-1\right) /\left(\varepsilon_{r}+2\right)$ - an evident generalization of Eq. (11), to which our result tends at $\varepsilon_{r} \rightarrow \infty$. By the way, this property is common: from the point of view of their electrostatic (but not transport!) properties, conductors may be adequately described as dielectrics with $\varepsilon_{r} \rightarrow \infty$.

Another remarkable feature of Eqs. (55) is that the electric field inside the sphere is uniform ${ }^{20}$ with $R$-independent values

$$
\begin{equation*}
\mathbf{E}=\frac{3}{\varepsilon_{r}+2} \mathbf{E}_{0}, \quad \mathbf{D} \equiv \varepsilon_{r} \varepsilon_{0} \mathbf{E}=\varepsilon_{0} \frac{3 \varepsilon_{r}}{\varepsilon_{r}+2} \mathbf{E}_{0}, \quad \mathbf{P} \equiv \mathbf{D}-\varepsilon_{0} \mathbf{E}=3 \varepsilon_{0} \frac{\varepsilon_{r}-1}{\varepsilon_{r}+2} \mathbf{E}_{0} . \tag{3.56}
\end{equation*}
$$

In the limit $\varepsilon_{r} \rightarrow 1$ (the "vacuum sphere", i.e. no sphere at all), the electric field inside the sphere naturally tends to the external one, and its polarization disappears. In the opposite limit and $\varepsilon_{r} \rightarrow \infty$ the electric field inside the sphere vanishes, and the field outside the sphere approaches that we have found for the conducting sphere - see Eq. (2.176).

To complete the discussion of this example, note a very curious result: the field $\mathbf{E}_{\text {self }}$, created by the dielectric sphere inside itself, is related to its polarization vector by a simple equation independent of either the dielectric constant or sphere's size:

$$
\begin{equation*}
\mathbf{E}_{\text {self }} \equiv \mathbf{E}-\mathbf{E}_{0}=-\frac{\varepsilon_{r}-1}{\varepsilon_{r}+2} \mathbf{E}_{0}=-\frac{1}{3 \varepsilon_{0}} \mathbf{P}, \tag{3.57}
\end{equation*}
$$

where factor 3 stems sphere's dimensionality. (For a round cylinder in a normal external field, the similar relation is valid, but with factor 2.) This equality is just the particular manifestation of the general relation (24). Indeed, if summed over all $N=n V$ similar dipoles $\mathbf{p}$, distributed inside the sphere with constant density $\mathbf{n}$ (so that the polarization vector $\mathbf{P}=n \mathbf{p}$ is constant), Eq. (24) yields

[^231]\[

$$
\begin{equation*}
\int_{V} \mathbf{E}_{\text {self }}(\mathbf{r}) d^{3} r=-\frac{\mathbf{P}}{3 \varepsilon_{0}} V, \tag{3.58}
\end{equation*}
$$

\]

so that after division by $V$, and taking into account the field uniformity in our particular case, it coincides with Eq. (57). ${ }^{21}$ We will use these results in the following section to discuss the molecular field effect.

Before doing that, let me briefly revisit the method of charge images that was discussed in Sec. 2.6, to find its new features pertaining to dielectrics. As the simplest example, consider a point charge near a dielectric half-space - see Fig. 9 (cf. Fig. 2.24).


Fig. 3.9. Charge images for a dielectric half-space.

The Laplace equations in the upper half-space $z>0$ (besides the charge point $\rho=0, z=d$ ) may still be satisfied using a single image charge $q$ ' at point $\rho=0, z=-d$, but now $q$ ' may differ from ( $-q$ ). In addition, in contrast to the conducting plane case, we should also find the field inside the dielectric ( $z$ $\leq 0$ ). This field cannot be contributed by the image charge, because it would provide a potential divergence at its location. Thus, in that half-space we should try to use the real point source only, but maybe with a re-normalized charge $q$ " rather than the genuine charge $q$ - see Fig. 9. As a result, we may look for the potential distribution in the form

$$
\phi(\rho, z)=\frac{1}{4 \pi \varepsilon_{0}} \times \begin{cases}{\left[\frac{q}{\left(\rho^{2}+(z-d)^{2}\right)^{1 / 2}}+\frac{q^{\prime}}{\left(\rho^{2}+(z+d)^{2}\right)^{1 / 2}}\right],} & \text { for } z \geq 0  \tag{3.59}\\ \frac{q^{\prime \prime}}{\left(\rho^{2}+(z-d)^{2}\right)^{1 / 2}}, & \text { for } z \leq 0\end{cases}
$$

at this stage with unknown $q^{\prime}$ and $q$ ". Plugging this solution into the boundary conditions (46) and (47) at $z=0$ (with $\partial / \partial n=\partial / \partial z$ ), we see that they are indeed satisfied (so that Eqs. (59) express the unique solution of the boundary problem) if the effective charges $q$ ' and $q$ '' obey the following relations:

[^232]\[

$$
\begin{equation*}
q-q^{\prime}=\varepsilon_{r} q^{\prime \prime}, \quad q+q^{\prime}=q^{\prime \prime} . \tag{3.60}
\end{equation*}
$$

\]

Solving this simple system of linear equations, we get

$$
\begin{equation*}
q^{\prime}=-\frac{\varepsilon_{r}-1}{\varepsilon_{r}+1} q, \quad q^{\prime \prime}=\frac{2}{\varepsilon_{r}+1} q . \tag{3.61}
\end{equation*}
$$

If $\varepsilon_{r} \rightarrow 1$, then $q^{\prime} \rightarrow 0$, and $q^{\prime \prime} \rightarrow q$ - both facts very natural, because in this limit (no polarization!) we have to recover the unperturbed field of the initial point charge in both semi-spaces. In the opposite limit $\varepsilon_{r} \rightarrow \infty$ (which, according to our discussion of the last problem, should correspond to a conducting plane), $q^{\prime} \rightarrow q$ (repeating the result we have discussed in very much detail in Sec. 2.6) and $q \prime \rightarrow 0$. According to the second of Eqs. (3.59), the last result means the field in the dielectric tends to zero in this limit, as it should.

Finally, following the logic of Chapter 2, at this point it would be appropriate to discuss the Green's function method. However, due to the time/space restrictions, I will skip this discussion, especially because the all the method's philosophy remains absolutely the same as for the vacuum case, so that the generalization to the case of dielectrics is straightforward.

### 3.4. Molecular field effects

In 1850, O.-F. Mossotti and (probably, independently, but almost 30 years later!) R. Clausius made an interesting experimental observation known now, rather unfairly, as the Clausius-Mossotti relation: if density $n$ of molecules in a chemical compound may be changed without changing its molecular structure, then the following ratio,

$$
\begin{equation*}
\frac{\varepsilon_{r}-1}{\varepsilon_{r}+2} \tag{3.62}
\end{equation*}
$$

is approximately proportional to $n$. For $\varepsilon_{r} \rightarrow 1$, i.e., $n \rightarrow 0$, there is no surprise here: according to Eq. (41), for independent molecular dipoles $\varepsilon_{r}-1=4 \pi \alpha_{\text {mol }} n \propto \propto n$. However, at larger density $n$, the effective field $\mathbf{E}_{\text {ef }}$, acting on each dipole, includes not only the external field $\mathbf{E}_{0}$, but also a substantial "molecular field" $\mathbf{E}_{\text {mol }}$ of the surrounding dipoles:

$$
\begin{equation*}
\mathbf{E}_{\mathrm{ef}}=\mathbf{E}_{0}+\mathbf{E}_{\mathrm{mol}}(0), \tag{3.63}
\end{equation*}
$$

where the position of the particular dipole we are discussing is taken for $\mathbf{r}=0$. Let us calculate $\mathbf{E}_{\text {mol }}(0)$, using a very simple model: a regular cubic lattice of identical dipoles (Fig. 10). In a Cartesian coordinate system with axes directed along the lattice vectors, coordinates of the dipoles are

$$
\begin{equation*}
x_{j k l}=a j, \quad y_{j k l}=a k, \quad z_{j k l}=a l, \tag{3.64}
\end{equation*}
$$

where $j, k$, and $l$ are the integers numbering the dipoles. Now we may use the last form of Eq. (13), and the linear superposition principle, to calculate one of the Cartesian components (say, along axis $x$ ) of the molecular field induced by all other dipoles of the lattice:

$$
\begin{equation*}
\left(E_{\mathrm{mol}}\right)_{x}(0)=\frac{1}{4 \pi \varepsilon_{0} a^{3}} \sum_{j, k, l=-\infty}^{+\infty} \frac{3 j\left(j p_{x}+k p_{y}+l p_{z}\right)-p_{x}\left(j^{2}+k^{2}+l^{2}\right)}{\left(j^{2}+k^{2}+l^{2}\right)^{5 / 2}} \tag{3.65}
\end{equation*}
$$

with excluded term $j=k=l=0$ is excluded. The sums of all cross-terms, proportional to $j k$ and $j l$, vanish due to system symmetry, so that Eq. (65) reduces to

$$
\begin{equation*}
\left(E_{\mathrm{mol}}\right)_{x}(0)=\frac{1}{4 \pi \varepsilon_{0} a^{3}} \sum_{j, k, l=-\infty}^{+\infty} \frac{\left[3 j^{2}-\left(j^{2}+k^{2}+l^{2}\right)\right]}{\left(j^{2}+k^{2}+l^{2}\right)^{5 / 2}} p_{x} \tag{3.66}
\end{equation*}
$$

Since all the sums participating in this expression are equal,

$$
\begin{equation*}
\sum_{j, k, l=-\infty}^{+\infty} \frac{j^{2}}{\left(j^{2}+k^{2}+l^{2}\right)^{5 / 2}}=\sum_{j, k, l=-\infty}^{+\infty} \frac{k^{2}}{\left(j^{2}+k^{2}+l^{2}\right)^{5 / 2}}=\sum_{j, k, l=-\infty}^{+\infty} \frac{l^{2}}{\left(j^{2}+k^{2}+l^{2}\right)^{5 / 2}}, \tag{3.67}
\end{equation*}
$$

we get $\left(E_{\text {mol }}\right)_{x}(0)=0$. Due to the system symmetry, the same result is valid for all other components of the dipole field. Hence, $\mathbf{E}_{\text {mol }}(0)=0$, and (due to the equivalence of all the dipoles of the system), the molecular field vanishes at the location of each dipole, so that Eq. (3.63) is reduced to $\mathbf{E}_{\text {ef }}=\mathbf{E}_{0}$.


Fig. 3.10. Cubic lattice of similar dipoles.

In order to relate the external field $\mathbf{E}_{0}$ and the average dipole ${ }^{22}$ field $\mathbf{E}$ in the medium, we may use Eq. (56) for a uniform, macroscopic sphere ${ }^{23}$ with a radius much larger then the inter-dipole distance $a$, so that our assumption of infinite limits of the rapidly converging sum (65) is not substantially affected:

$$
\begin{equation*}
\mathbf{E}=\frac{3}{\varepsilon_{r}+2} \mathbf{E}_{0}=\frac{3}{\varepsilon_{r}+2} \mathbf{E}_{\mathrm{ef}} \tag{3.68}
\end{equation*}
$$

Now we may plug this relation into the general formula (37) for linear dielectrics:

$$
\begin{equation*}
\mathbf{P}=\left(\varepsilon_{r}-1\right) \varepsilon_{0} \mathbf{E}=\frac{3\left(\varepsilon_{r}-1\right)}{\varepsilon_{r}+2} \varepsilon_{0} \mathbf{E}_{\mathrm{ef}} . \tag{3.69}
\end{equation*}
$$

This "macroscopic" relation has to give the same result as the "microscopic" Eq. (40) - with the replacement $\mathbf{E} \rightarrow \mathbf{E}_{\text {ef }}$ which reflects the fact that in the general case each dipole is polarized by the effective field (63) rather than the average field $\mathbf{E}$ :

$$
\begin{equation*}
\mathbf{P}=4 \pi \varepsilon_{0} \alpha_{\mathrm{mol}} n \mathbf{E}_{\mathrm{ef}} \tag{3.70}
\end{equation*}
$$

[^233]The comparison yields the so-called Lorentz-Lorenz formula, ${ }^{24}$

Lorentz-
Lorenz
formula

$$
\begin{equation*}
\frac{4 \pi \alpha_{\mathrm{mol}}}{3} n=\frac{\varepsilon_{r}-1}{\varepsilon_{r}+2} \tag{3.71}
\end{equation*}
$$

that complies with the Clausius-Mossotti observation, provided that the molecular polarizability $\alpha_{\text {mol }}$ is independent of density. (This is a good approximation at least for weak "molecular" bonding.)

It is somewhat surprising how many dielectric materials obey Eq. (71) rather well, because of its approximate nature. Indeed, its derivation is based on the assumption of a specific crystal lattice and, more importantly, that the molecules are localized exactly in the crystal lattice nodes, and the field of each molecule may be expressed by the dipole approximation. In reality, atom's electrons, which participate in the dipole moment formation, are spread in space due to quantum-mechanical uncertainty on a scale that may be comparable with distances between the molecules.

Solving Eq. (71) for the dielectric constant, we get

$$
\begin{equation*}
\varepsilon_{r}=\frac{1+8 \pi \alpha_{\mathrm{mol}} n / 3}{1-4 \pi \alpha_{\mathrm{mol}} n / 3} . \tag{3.72}
\end{equation*}
$$

If the dipole density is low, $\alpha_{\text {mol }} n \ll 1$, we get our old result (41) corresponding to independent dipoles, and hence to $\mathbf{E}_{\text {ef }}=\mathbf{E}$. However, at high dipole density and/or polarizability, the effective field acting on the each dipole,

$$
\begin{equation*}
\mathbf{E}_{\mathrm{ef}}=\frac{\varepsilon_{r}+2}{3} \mathbf{E}=\frac{\mathbf{E}}{1-4 \pi \alpha_{\mathrm{mol}} n / 3}, \tag{3.73}
\end{equation*}
$$

may be substantially larger than the average field $\mathbf{E}$, due to the molecular field contribution. Note $\varepsilon_{r}$, the $\mathbf{E}_{\mathrm{ef}} / \mathbf{E}$ ratio, and hence the electric susceptibility

$$
\begin{equation*}
\chi_{e} \equiv \frac{\mathbf{P}}{\varepsilon_{0} \mathbf{E}}=\varepsilon_{r}-1=\frac{4 \pi \alpha_{\mathrm{mol}} n}{1-4 \pi \alpha_{\mathrm{mol}} n / 3}, \tag{3.74}
\end{equation*}
$$

all diverge when the density-polarizability product approaches the critical value $\alpha_{\mathrm{mol}} n=3 / 4 \pi$.
This is essentially a rudimentary ${ }^{25}$ description of the transition from linear dielectrics to the socalled ferroelectrics with self-sustained (spontaneous) polarization even in the absence of external

[^234]electric field. These materials are typically recognized by the hysteretic behavior of their polarization as a function of applied electric field - see, for example, Fig. 11.

Ferroelectric materials are being actively explored as the active materials for nonvolatile random-access memories (dubbed either FRAM or FeRAM). ${ }^{26}$ In cells of this memory, binary information is stored in the form of one of two possible directions of spontaneous polarization at $\mathbf{E}=0-$ see, e.g., Fig.11, and is read out by the effect of the average electric field on a nearby semiconductor field-effect transistor. Unfortunately, most materials suitable for fabrication of ferroelectric thin films are rather complex and incompatible with standard processes of microelectronics. In addition, the time of spontaneous depolarization of ferroelectric thin films is typically well below than 10 years - the industrial standard for data retention in nonvolatile memories, and this time may be decreased even more by "fatigue" from repeated polarization recycling. Due to these reasons, industrial production of FRAM is currently just a tiny, few-percent fraction of the nonvolatile memory market (which is currently dominated by floating-gate memories - see Sec. 4.2).


Fig. 3.11. Ferroelectric hysteretic loops: (a) for various material types (schematically), and (b) for several amplitudes of the applied ac electric field. (Panel b, showing recent (2013) experimental results by S.-W. Jung et al. for an inkjet-printed layer of organic semiconductor PC12TV12T, is adapted from http://etrij.etri.re.kr/etrij/journal/article/article.do?volume=35\&issue=4\&page=734.)

Other polarization effects can also be met, possible, e.g., antiferroelectricity or helielectricity. Unfortunately, we will not have time for a discussion of these exotic phenomena in this course; ${ }^{27}$ the main reason I am mentioning them is to emphasize again that the "material relation" $\mathbf{P}=\mathbf{P}(\mathbf{E})$ is by no means exact or fundamental, though most material, in practicable fields, behave as linear dielectrics.

[^235]
### 3.5. Energy of electric field in a dielectric

In Chapter 1, we have obtained two key results for the electrostatic energy: Eq. (1.54) for a charge interaction with an independent ("external") field, and a similarly structured formula (1.62), but with an additional factor $1 / 2$, for the field is produced by the charges under consideration. Both relations could be merged and rewritten in a "local" form involving energy density $u$ - see Eq. (1.67). These equations are of course always valid for dielectrics as well if the charge density includes all charges (including those bound into dipoles), but it is convenient to recast them unto a form depending on density $\rho(\mathbf{r})$ of only "stand-alone" charges.

If a field is created only by stand-alone charges under consideration, and is proportional to $\rho(\mathbf{r})$ (requiring that we deal with a linear dielectric!), we can repeat all the argumentation of the beginning of Sec. 1.3, and again arrive at Eq. (1.62), provided that $\phi$ is calculated correctly, i.e., with a due account of the dielectric. Now we can recast this result in terms of fields - essentially as this was done in Eqs. (1.64)-(1.66), but now making a clear difference between the electric field $\mathbf{E}$ (that still equals $-\nabla \phi$ ) and the electric displacement field $\mathbf{D}$ that obeys the macroscopic Maxwell equation (32). Plugging $\rho(\mathbf{r})$, expressed from that equation, into Eq. (1.62), we get

$$
\begin{equation*}
U=\frac{1}{2} \int(\nabla \cdot \mathbf{D}) \phi d^{3} r . \tag{3.75}
\end{equation*}
$$

Using the fact ${ }^{28}$ that for any differentiable functions $\phi$ and $\mathbf{D}$,

$$
\begin{equation*}
(\nabla \cdot \mathbf{D}) \phi=\nabla \cdot(\phi \mathbf{D})-(\nabla \phi) \cdot \mathbf{D} \tag{3.76}
\end{equation*}
$$

we may rewrite Eq. (75) as

$$
\begin{equation*}
U=\frac{1}{2} \int \nabla \cdot(\phi \mathbf{D}) d^{3} r-\frac{1}{2} \int(\nabla \phi) \cdot \mathbf{D} d^{3} r . \tag{3.77}
\end{equation*}
$$

The divergence theorem, applied to first term, reduces it to a surface integral of $\phi D_{n}$. (As a reminder, in Eq. (1.65) the integral was of $\phi(\nabla \phi)_{n} \propto \phi E_{n}$.) If the surface of the volume we consider is sufficiently far, this surface integral vanishes. On the other hand, the gradient in the second term of Eq. (77) is just (minus) field $\mathbf{E}$, so that it gives

$$
\begin{equation*}
U=\frac{1}{2} \int \mathbf{E} \cdot \mathbf{D} d^{3} r=\frac{1}{2} \int E(\mathbf{r}) \cdot \varepsilon(\mathbf{r}) E(\mathbf{r}) d^{3} r=\frac{\varepsilon_{0}}{2} \int \varepsilon_{r}(\mathbf{r}) E^{2}(\mathbf{r}) d^{3} r . \tag{3.78}
\end{equation*}
$$

This expression is a natural generalization of Eq. (1.67) and shows that we can, like we did in vacuum, present the electrostatic energy in a local form ${ }^{29}$

Field energy in a linear dielectric

$$
\begin{equation*}
U=\int u(\mathbf{r}) d^{3} r, \quad u=\frac{1}{2} \mathbf{E} \cdot \mathbf{D}=\frac{\varepsilon}{2} E^{2}=\frac{D^{2}}{2 \varepsilon} \tag{3.79}
\end{equation*}
$$

Again, this expression is not valid for nonlinear dielectrics, because our starting point, Eq. (1.62), is only valid if $\phi$ is proportional to $\rho$. In order to make our calculation more general, we should

[^236]intercept our calculations in Sec. 1.3 at an earlier stage, at which we have not yet used this proportionality. For example, Eq. (1.54) may be rewritten, in the continuous limit, as
\[

$$
\begin{equation*}
\delta U=\int \phi(\mathbf{r}) \delta \rho(\mathbf{r}) d^{3} r \tag{3.80}
\end{equation*}
$$

\]

where symbol $\delta$ means a small variation of the function - e.g., its change in time, sufficiently slow to ignore the relativistic and magnetic-field effects. Applying such variation to Eq. (32), and plugging the resulting $\delta \rho=\nabla \cdot \delta \mathbf{D}$ into Eq. (80), we get

$$
\begin{equation*}
\delta U=\int(\nabla \cdot \delta \mathbf{D}) \phi d^{3} r . \tag{3.81}
\end{equation*}
$$

(Note that in contrast to Eq. (75), this expression does not have factor $1 / 2$.) Now repeating the same calculations as in the linear case, for the energy density variation we get a remarkably simple (and general!) expression,

$$
\begin{equation*}
\delta u=\mathbf{E} \cdot \delta \mathbf{D} . \tag{3.82}
\end{equation*}
$$

This is as far as we can go for the general dependence $\mathbf{D}(\mathbf{E})$. If the dependence is linear and isotropic, as in Eq. (38), then $\delta \mathbf{D}=\varepsilon \delta \mathbf{E}$ and

$$
\begin{equation*}
\delta u=\varepsilon \mathbf{E} \cdot \delta \mathbf{E} \tag{3.83}
\end{equation*}
$$

Integration of this expression over variations, from zero field to a certain final distribution $\mathbf{E}(\mathbf{r})$, brings us back to Eq. (79).

Another important role of Eq. (82) is that it shows that Cartesian coordinates of $\mathbf{E}$ may be interpreted as generalized forces, and those of $\mathbf{D}$ as generalized coordinates (per unit volume). ${ }^{30}$ This allows one to form the proper Gibbs potential energy ${ }^{31}$ of a system inside some volume $V$, placed in an external electric field $\mathbf{E}_{\text {ext }}$ :

$$
\begin{equation*}
g=\int_{V} g(\mathbf{r}) d^{3} r, \quad g(\mathbf{r})=u(\mathbf{r})-\mathbf{E}_{\mathrm{ext}} \cdot \mathbf{D} . \tag{3.84}
\end{equation*}
$$

As an analytical mechanics reminder, if a generalized external force (in our case, $\mathbf{E}_{\text {ext }}$ ) is fixed, the stable equilibrium of the system corresponds to the minimum of $g$, rather than of the potential energy $U$ as such - in our case, that of the field:

$$
\begin{equation*}
U=\int_{V} u(\mathbf{r}) d^{3} r, \quad u(\mathbf{r})=\int \mathbf{E} \cdot \delta \mathbf{D} . \tag{3.85}
\end{equation*}
$$

In order to illustrate this important point, let us return to the simple case of a system with linear dielectric(s), in which $\delta \mathbf{D} \propto \delta \mathbf{E} \propto \delta \mathbf{E}_{\text {ext }}$, so that Eq. (85) may be explicitly integrated over the external field variation, to reproduce the second of Eqs. (79):

[^237]General energy variation

$$
\begin{equation*}
u(\mathbf{r})=\frac{1}{2} \mathbf{E} \cdot \mathbf{D} . \tag{3.86}
\end{equation*}
$$

In this case, Eq. (84) yields

$$
\begin{equation*}
g(\mathbf{r})=\frac{1}{2} \mathbf{E} \cdot \mathbf{D}-\mathbf{E}_{\mathrm{ext}} \cdot \mathbf{D}=\frac{\varepsilon}{2} E^{2}-\varepsilon \mathbf{E} \cdot \mathbf{E}_{\mathrm{ext}} \equiv \frac{\varepsilon}{2}\left(\mathbf{E}-\mathbf{E}_{\mathrm{ext}}\right)^{2}+\mathrm{const} \tag{3.87}
\end{equation*}
$$

where the constant may depend on the external field, but not on the resulting field distribution. As a sanity check, let us apply this result to a volume $V$ well inside a long dielectric cylinder placed into a uniform external field $\mathbf{E}_{\text {ext }}$ parallel to cylinder's axis. (Such orientation is important to ignore the geometric effects discussed in Sec. 3 - see, e.g., Fig. 6 and its discussion.) Then $\mathbf{E}$ has to be uniform in the dominating part of the cylinder, so that Eq. (84) may be explicitly integrated over the volume, giving

$$
\begin{equation*}
g=\frac{\varepsilon}{2}\left(\mathbf{E}-\mathbf{E}_{\mathrm{ext}}\right)^{2} V+\text { const } . \tag{3.88}
\end{equation*}
$$

The minimum of this function is achieved at the evidently correct result $\mathbf{E}=\mathbf{E}_{\text {ext }}$ - in contrast to the unphysical result $\mathbf{E}=0$ (meaning electric field's expulsion from the volume) that we would get minimizing $U$.

### 3.6. Exercise problems

3.1.* Prove the following extension of Eq. (5):

$$
\phi(\mathbf{r}) \approx \frac{1}{4 \pi \varepsilon_{0}}\left(\frac{1}{r} Q+\frac{1}{r^{3}} \sum_{j=1}^{3} r_{j} p_{j}+\frac{1}{2 r^{5}} \sum_{j, j^{\prime}=1}^{3} r_{j} r_{j^{\prime}} Q_{i j j^{\prime}}\right),
$$

where $Q$ is a scalar - the total charge of the system, $p_{j}$ are the Cartesian components of a vector system's dipole moment (6), and $\mathscr{Q}_{j j}$, are Cartesian components of a tensor - system's quadrupole moment:

$$
Q=\int \rho\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime}, \quad p_{j}=\int \rho\left(\mathbf{r}^{\prime}\right) r_{j}^{\prime} d^{3} r^{\prime}, \quad Q_{j j j^{\prime}}=\int \rho\left(\mathbf{r}^{\prime}\right)\left(3 r_{j}^{\prime} r_{j^{\prime}}^{\prime}-r^{\prime 2} \delta_{i j^{\prime}}\right) d^{3} r^{\prime}
$$

3.2. A plane, thin ring of radius $R$ is charged with a constant linear density $\lambda$. Calculate the exact electrostatic potential distribution along the symmetry axis of the ring, and prove that at large distances, $r \gg R$, it is indeed described by the multipole expansion spelled out in Problem 1.
3.3. Without carrying out an exact calculation, can you predict the spatial dependence of the interaction between various electric multipoles, including point charges (in this context, frequently called monopoles), dipoles, and quadrupoles? Based on these predictions, what is the functional dependence of the interaction between dumbbell-shaped diatomic molecules such as $\mathrm{H}_{2}, \mathrm{~N}_{2}, \mathrm{O}_{2}$, etc., on the distance between them, if the distance is much larger than the molecular size?
3.4. In suitable reference frames, calculate the dipole and quadrupole moments of the following systems (see Figs. below):
(i) 4 point charges of the same magnitude, but alternating signs, placed in the corners of a square;
(ii) a similar system, but with a pair charge sign alternation; and
(iii) a point charge in the center of a thin ring carrying a similar but opposite charge, uniformly distributed along its circumference.

(ii)

(iii)

3.5. Two similar electric dipoles, of fixed magnitude $p$, located at fixed distance $r$ from each other, are free to rotate, changing their directions. What stable equilibrium position(s) may they take as a result of their electrostatic interaction?
3.6. An electric dipole is located above an infinite conducting plane (see Fig. on the right). Calculate:
(i) the distribution of the induced charge in the conductor,
(ii) the dipole-to-plane interaction energy, and
(ii) the force and the torque acting on the dipole.

3.7. Use two different approaches to calculate the energy of interaction between a grounded conductor and an electric dipole $\mathbf{p}$, placed in the center of a spherical cavity of radius $R$, carved in the conductor.
3.8. A plane separating two parts of otherwise free space is densely and uniformly (with constant areal density $n$ ) filled with dipoles, with their dipole moments $\mathbf{p}$ oriented in a direction normal to the plane.
(i) Calculate the boundary conditions for the electrostatic potential on both sides of the plane.
(ii) Use the result of Task (i) to calculate the potential distribution created in space by a spherical surface, with radius $R$, densely and uniformly filled with radially-oriented dipoles.
(iii) What condition that should be imposed on the dipole density $n$ for your results to be qualitatively valid?
3.9. A plane capacitor, with zero voltage between its conducting plates (as may be fixed, e.g., with an external wire - see Fig. on the right), is partly filled with a material

with spontaneous, constant polarization $\mathbf{P}_{0} .{ }^{32}$ Find the distributions of the electric field, electric displacement, and the surface charge density of each plate.
3.10. A sphere of radius $R$ is made of a material with a uniform, fixed polarization $\mathbf{P}_{0}$.
(i) Calculate the electric field everywhere in space - both inside and outside the sphere.
(ii) Explore the limit $R \rightarrow 0$, keeping $P_{0} R^{3}=$ const, and compare the result with Eq. (25).
3.11. Discuss the physics of Eq. (3.85) of the lecture notes, in particular the physical nature of the potential energy $U$ in a dipole medium. Apply your conclusion to a material with fixed (fieldindependent) polarization $\mathbf{P}_{0}$, and calculate the electric field energy of the uniformly polarized sphere considered in the previous problem.
3.12. Experimental plots in Fig. on the right show that the polarization of $\mathrm{EuMn}_{2} \mathrm{O}_{5}$, a typical ferroelectric/paraelectric material, becomes almost linear at 50 K . Use the plot to calculate (with an accuracy better than $10 \%$ ) its dielectric constant $\varepsilon_{r}$ at this temperature.

3.13. In two separate experiments, a thin, plane sheet of a linear dielectric with $\varepsilon_{r}=$ const is placed into a uniform external electric field $\mathbf{E}_{0}$ :
(i) with sheet's surface parallel to the electric field, and
(ii) the surface perpendicular to the field.

For each case, find the electric field $\mathbf{E}$, the electric displacement $\mathbf{D}$, and the polarization vector $\mathbf{P}$ inside the dielectric (far from sheet's edges).
3.14. A point charge $q$ is located at distance $r \gg R$ from the center of a uniform sphere of radius $R$, made of a uniform linear dielectric. In the first nonvanishing approximation in small parameter $R / r$, calculate the interaction force, and the energy of interaction between the sphere and the charge.
3.15. A fixed dipole $\mathbf{p}$ is placed in the center of a spherical cavity of radius $R$, cut inside a uniform, linear dielectric. Calculate the electric field distribution everywhere in the system (both for $r<$ $R$ and $r>R$ ).

Hint: You may start with the assumption that the field at $r>R$ has a distribution typical for a dipole (but be ready for surprises :-).

[^238]3.16. A spherical capacitor (see Fig. on the right) is filled with a linear dielectric whose permittivity $\varepsilon$ depends on spherical angles $\theta$ and $\varphi$, but not on the distance $r$ from system's center. Give an explicit expression for its capacitance $C$.

3.17. For each of the two capacitors shown in Fig. 3.7 of the lecture notes, calculate the electric forces (per unit area) on the boundaries of two uniform dielectrics, in terms of the electric fields.
3.18. A uniform electric field $\mathbf{E}_{0}$ has been created (by external sources) inside a uniform linear dielectric. Find the change of the electric field, created by cutting out a cavity in the shape of a round cylinder of radius $R$, with the axis perpendicular to the external field - see Fig. on the right.

3.19. Small linear-dielectric particles of spherical shape are dispersed in free space with low concentration $n \ll 1 / R^{3}$, where $R$ is particle's radius. Calculate the average dielectric constant of such a medium. Compare the result with the apparent, but incomplete answer
$$
\overline{\varepsilon_{r}}-1=\left(\varepsilon_{r}-1\right) n V,
$$
(where $\varepsilon_{r}$ is the dielectric constant of particle's material and $V=(4 \pi / 3) R^{3}$ is its volume), and explain the origin of the difference.
3.20.* Calculate the spatial distribution of the electric potential induced by a point charge $q$ is placed at distance $d$ from a very wide parallel plate, of thickness $D$, made of a linear dielectric - see Fig. on the right.


## Chapter 4. DC Currents

In this chapter I discuss the laws governing the distribution of constant ("dc") currents inside conducing media, with a focus on the linear ("Ohmic") conductivity. In most cases, the partial differential equation governing the distribution may be reduced to the same Laplace and Poisson equations whose solution methods have been discussed in detail in Chapter 2. Due to this fact, this chapter is rather short.

### 4.1. Continuity equation and the Kirchhoff laws

Until this point, our discussion of conductors has been limited to the cases when they are separated with insulators (meaning either vacuum or dielectric media) preventing any continuous motion of charges from one conductor to another, even if there is a voltage difference (and hence electric field) between them - see Fig. 1a.


Fig. 4.1. Two oppositely charged conductors: (a) at the electrostatic situation, (b) at charge relaxation through an additional narrow conductor ("wire"), and (c) a system sustaining dc current in the wire.

Now let us connect two conductors galvanically, say with a wire - a thin, elongated conductor (Fig. 1b). Then the electric field causes the motion of charges in the wire - from a conductor with a higher electrostatic potential toward that with a lower potential, until the potentials equilibrate. Such process is called charge relaxation. The main equation governing this process may be obtained from the experimental fact (already mentioned in Sec. 1.1) that electric charges cannot appear or disappear (though opposite charges may recombine with the conservation of the net charge.) As a result the change of charge $Q$ in one conductor may change only due to the current $I$ through the wire: ${ }^{1}$

$$
\begin{equation*}
\frac{d Q}{d t}=-I . \tag{4.1}
\end{equation*}
$$

[^239]Let us express this law in a differential form, introducing the notion of current density vector $\mathbf{j}(\mathbf{r})$. This vector may be defined via the following relation for current $d I$ crossing an elementary area $d A$ (Fig. 2)

$$
\begin{equation*}
d I=j d A \cos \theta=(j \cos \theta) d A=j_{n} d A, \tag{4.2}
\end{equation*}
$$

where $\theta$ is the angle between the normal to the surface and the carrier motion direction (which is taken for the direction of vector $\mathbf{j}$ ).


Fig. 4.2. Current density vector.

With that definition, Eq. (1) may be re-written as

$$
\begin{equation*}
\frac{d}{d t} \int_{V} \rho d^{3} r=-\oint_{S} j_{n} d^{2} r \tag{4.3}
\end{equation*}
$$

where $V$ is an arbitrary stationary volume limited by the closed surface $S$. Applying to this volume the same divergence theorem as was repeatedly used in previous chapters, we get

$$
\begin{equation*}
\int_{V}\left[\frac{\partial \rho}{\partial t}+\nabla \cdot \mathbf{j}\right] d^{3} r=0 \tag{4.4}
\end{equation*}
$$

Since volume $V$ if arbitrary, this equation may be true only if

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}+\nabla \cdot \mathbf{j}=0 \tag{4.5}
\end{equation*}
$$

Continuity equation

This is the fundamental continuity equation - which is true even for the time-dependent phenomena. ${ }^{2}$
The charge relaxation is of course a dynamic, time-dependent process. However, electric currents may also exist in stationary situations, when a current source, for example a battery, replenishes the conductor charges and hence sustains currents at a certain time-independent level - see Fig. 1c. (As we will see below, in most cases this process requires a persistent replenishment of the electrostatic energy from either a source or storage of energy of a different kind - say, the chemical energy of the battery.) Let us discuss the laws governing the distribution of such dc currents. In this case $(\partial / \partial t=0)$, Eq. (5) reduces to a very simple equation

$$
\begin{equation*}
\nabla \cdot \mathbf{j}=0 \tag{4.6}
\end{equation*}
$$

This equation acquires an even a simpler form in the particular but important case of electric circuits (Fig. 3), the systems may be presented as an electric connection of components of two types:

[^240](i) small-size (lumped) circuit elements (also called "two-terminal devices"), meaning a passive resistor, a current source, etc. - generally, any black box with two wires sticking out of it, and
(ii) perfectly conducting wires, with negligible voltage drop along them, that are galvanically connected at certain points, called nodes (or "junctions").


Fig. 4.3. Typical system obeying the Kirchhoff laws.

In the standard circuit theory, the electric charges of the nodes are considered negligible, and we may integrate Eq. (6) over the closed surface drawn around any node to get

$$
\begin{equation*}
\sum_{j} I_{j}=0, \tag{4.7a}
\end{equation*}
$$

where the summation is over all the wires (numbered with index $j$ ) connected in the node. On the other hand, according to its definition (2.25), voltage drop $V_{k}$ across each circuit element may be presented as the difference of potentials of the adjacent nodes, $V_{k}=\phi_{k}-\phi_{k-1}$. Summing such differences around any closed loop of the circuit (Fig. 3), we get all terms cancelled, so that

$$
\begin{equation*}
\sum_{k} V_{k}=0 . \tag{4.7b}
\end{equation*}
$$

These relations are called, respectively, the $1^{\text {st }}$ and $2^{\text {nd }}$ Kirchhoff laws - or sometimes the node rule and the loop rule. They may seem elementary, and the genuine power of the Kirchhoff approach is in the fact a set of Eqs. (7), covering every node and every circuit element of the system, gives a system of equations sufficient for the calculation of all currents and voltages in it - provided that the relation between current and voltage in known for each circuit element.

It is almost evident that in the absence of current sources, the system of equations (7) has only a trivial solution: $I_{j}=0, V_{k}=0$ - with the exotic exception of superconductivity, to be discussed in Sec. 6.3. The current sources, that allow non-vanishing current flows, may be described by their electromotive forces (e.m.f.) $v_{k}$, having the dimensionality of voltage, which have to be taken into account in the corresponding terms $V_{k}$ of sum (7b). Let me hope that the reader has some experience of using Eqs. (7) for the analysis of simple circuits - say consisting of several resistors and dc batteries so I may save time on a discussion of these simple problems.

### 4.2. The Ohm law

As was mentioned above, the relations spelled out in Sec. 1 are sufficient for forming a closed system of equations for finding currents and electric field in a system only if they are complemented
with material equations relating scalars $I$ and $V$ in each circuit element, i.e. vectors $\mathbf{j}$ and $\mathbf{E}$ in each point of the medium of such an element. The simplest, and most frequently met relation of this kind is the famous Ohm law whose differential form is

$$
\begin{equation*}
\mathbf{j}=\sigma \mathbf{E} \tag{4.8}
\end{equation*}
$$

where $\sigma$ is a constant called conductivity. ${ }^{3}$ Though this is not a fundamental relation, and is approximate for any conducting media, we can argue that if:
(i) there is no current at $\mathbf{E}=0$ (mind superconductors!),
(ii) the medium is isotropic or almost isotropic (a notable exception: some organic conductors),
(iii) the mean free path $l$ of current carriers is much smaller than the characteristic scale $a$ of the spatial variations of $\mathbf{j}$ and $\mathbf{E}$,
then the Ohm law may be viewed as a result of the Taylor expansion of the local relation $\mathbf{j}(\mathbf{E})$ in relatively small fields, and thus is very common.

Table 1 gives the experimental values of dc conductivity for some practically important (or just representative) materials. The reader can see that the range of its values is very broad, covering more that 30 orders of magnitude, even without going to such extremes as very pure metallic crystals at very low temperatures, where $\sigma$ may reach $\sim 10^{12} \mathrm{~S} / \mathrm{m}$.

Table 4.1. Ohmic conductivities for some representative (or practically important) materials at $20^{\circ} \mathrm{C}$.

| Material | $\sigma(\mathrm{S} / \mathrm{m})$ |
| :---: | :---: |
| Teflon $\left(\left[\mathrm{C}_{2} \mathrm{~F}_{4}\right]_{n}\right)$ | $10^{-22}-10^{-24}$ |
| Silicon dioxide | $10^{-16}-10^{-19}$ |
| Various glasses | $10^{-10}-10^{-14}$ |
| Deionized water | $\sim 10^{-6}$ |
| Sea water | 5 |
| Silicon $n$-doped to $10^{16} \mathrm{~cm}^{-3}$ | $2.5 \times 10^{2}$ |
| Silicon $n$-doped to $10^{19} \mathrm{~cm}^{-3}$ | $1.6 \times 10^{4}$ |
| Silicon $p$-doped to $10^{19} \mathrm{~cm}^{-3}$ | $1.1 \times 10^{4}$ |
| Nichrome (alloy $80 \% \mathrm{Ni}+20 \% \mathrm{Cr})$ | $0.9 \times 10^{6}$ |
| Aluminum | $3.8 \times 10^{7}$ |
| Copper | $6.0 \times 10^{7}$ |
| Zinc crystal along $a$-axis | $1.65 \times 10^{7}$ |
| Zinc crystal along $c$-axis | $1.72 \times 10^{7}$ |

[^241]In order to get some feeling what do these values mean, let us consider a very simple system (Fig. 4): a plane capacitor of area $A \gg d^{2}$, filled with a material that has not only a dielectric constant $\varepsilon_{r}$, but also some Ohmic conductivity $\sigma$, with much more conductive plate electrodes.


Fig. 4.4. "Leaky" plane capacitor.

Assuming that these properties are compatible with each other, ${ }^{4}$, we may assume that the distribution of electric potential (not too close to the capacitor edges) still obeys Eq. (2.39), so that the electric field is vertical and uniform, with $E=V / d$. Then, according to Eq. (6) the current density is also uniform, $j=\sigma E=\sigma V / d$. From here, the total current between the plates is

$$
\begin{equation*}
I=j A=\sigma E A=\sigma \frac{V}{d} A . \tag{4.9}
\end{equation*}
$$

On the other hand, from Eqs. (2.26) and (3.45), the instant value of plate charge is $Q=C_{m} V=$ $\left(\varepsilon_{r} \varepsilon_{0} A / d\right) V$. Plugging these relations into Eq. (1), we see that the speed of charge (and voltage) relaxation does not depend on the geometric parameters $A$ and $d$ :

$$
\begin{equation*}
\frac{d V}{d t}=-\frac{V}{\tau_{r}}, \quad \tau_{r} \equiv \frac{\varepsilon_{r} \varepsilon_{0}}{\sigma}, \tag{4.10}
\end{equation*}
$$

where parameter $\tau_{r}$ has the sense of the relaxation time constant. As we know (see Table 3.1), for most practical materials the dielectric constant is within one order of magnitude from 10 , so that the numerator of Eq. (10) is of the order of $10^{-10}$. As a result, according to Table 1, the charge relaxation time ranges from $\sim 10^{14} \mathrm{~s}$ (more than a million years!) for best insulators like teflon, to $\sim 10^{-18} \mathrm{~s}$ for the least resistive metals.

What is the physics behind these values of $\sigma$ and why, for some materials, Table 1 gives them with such a large uncertainty? If charge carriers move as classical particles (e.g., in plasmas or nondegenerate semiconductors), a reasonable description of conductivity is given by the famous Drude formula. ${ }^{5}$ In his picture, due to weak electric field, the charge carriers are accelerated in its direction (possibly on the top of their random motion in all directions, i.e. with a vanishing average velocity vector):

$$
\begin{equation*}
\frac{d \mathbf{v}}{d t}=\frac{q}{m} \mathbf{E}, \tag{4.11}
\end{equation*}
$$

and as a result their velocity acquires an the average value

$$
\begin{equation*}
\langle\mathbf{v}\rangle=\frac{d \mathbf{v}}{d t} \tau=\frac{q}{m} \mathbf{E} \tau \tag{4.12}
\end{equation*}
$$

[^242]where the phenomenological parameter $\tau=l / v$ (not to be confused with $\tau_{r}$ !) may be understood as the effective average time between carrier scattering events. From here, the current density:
\[

$$
\begin{equation*}
\mathbf{j}=q n\langle\mathbf{v}\rangle=\frac{q^{2} n \tau}{m} \mathbf{E}, \quad \text { i.e. } \sigma=\frac{q^{2} n \tau}{m} \tag{4.13a}
\end{equation*}
$$

\]

(Notice the independence of $\sigma$ of the carrier charge sign.) Another form of the same result, more popular in the physics of semiconductors, is

$$
\begin{equation*}
\sigma=q^{2} n \mu, \quad \text { with } \mu=\frac{\tau}{m} \tag{4.13b}
\end{equation*}
$$

where parameter $\mu$, defined by relation $\langle\mathbf{v}\rangle \equiv \mu \mathbf{E}$, is called the charge carrier mobility.
Most good conductors (e.g., metals) are essentially degenerate Fermi gases (or liquids), in which the average thermal energy of a particle, $k_{\mathrm{B}} T$ is much lower that the Fermi energy $\varepsilon_{\mathrm{F}}$. In this case, a quantum theory is needed for the calculation of $\sigma$. Such theory was developed by the quantum physics’ godfather A. Sommerfeld in 1927 (and is sometimes called the Drude-Sommerfeld model). I have no time to discuss it in this course, ${ }^{6}$ and here I will only notice that for an ideal, isotropic Fermi gas the result is reduced to Eq. (13), with a certain effective value of $\tau$, so it may be used for estimates of $\sigma$, with due respect to the quantum theory of scattering. In a typical metal, $n$ is very high ( $\sim 10^{23} \mathrm{~cm}^{-3}$ ) and is fixed by the atomic structure, so that the sample quality may only affect $\sigma$ via the scattering time $\tau$.

At room temperature, the scattering of electrons by thermally-excited lattice vibrations (phonons) dominates, so that $\tau$ and $\sigma$ are high but finite, and do not change much from one sample to another. (Hence, the more accurate values given for metals in Table 1.) On the other hand, at $T \rightarrow 0$, a perfect crystal should not exhibit scattering at all, and conductivity should be infinite. In practice, this is never true (for example, due to electron scattering from imperfect boundaries of finite-size samples), and the effective conductivity $\sigma$ is infinite (or practically infinite, at least above the measurable value $\sim 10^{20} \mathrm{~S} / \mathrm{m}$ ) only in superconductors. ${ }^{7}$

On the other hand, the conductivity of quasi-insulators (including deionized water) and semiconductors depends mostly of the carrier density $n$ that is much lower than in metals. From the point of view of quantum mechanics, this happens because the ground-state eigenenergies of charge carriers are localized within an atom (or molecule), and separated from excited states, with spaceextended wavefunctions, by a large energy gap (called bandgap). For example, in $\mathrm{SiO}_{2}$ the bandgap approaches 9 eV , equivalent to $\sim 4,000 \mathrm{~K}$. This is why, even at room temperatures the density of thermally-excited free charge carriers in good insulators is negligible. In these materials, $n$ is determined by impurities and vacancies, and may depend on a particular chemical synthesis or other fabrication technology, rather than on fundamental properties of the material. (On the contrary, the carrier mobility $\mu$ in these materials is almost technology-independent.)

The practical importance of the technology may be illustrated on the following example. In cells of the so-called floating-gate memories, in particular the flash memories, which currently dominate the nonvolatile digital memory technology, data bits are stored as small electric charges ( $Q \sim 10^{-16} \mathrm{C}$ ) of

[^243]highly doped silicon islands (so-called floating gates) separated from the rest of the integrated circuit with a $\sim 10-n m$-thick layer of silicon dioxide, $\mathrm{SiO}_{2}$. Such layers are fabricated by high-temperature oxidation of virtually perfect silicon crystals. The conductivity of the resulting high-quality (though amorphous) material is so low, $\sigma \sim 10^{-19} \mathrm{~S} / \mathrm{m}$, that the relaxation time $\tau_{r}$, defined by Eq. (10), is well above 10 years - the industrial standard for data retention in non-volatile memories. In order to appreciate how good this technology is, the cited value should be compared with the typical conductivity $\sigma \sim 10^{-16} \mathrm{~S} / \mathrm{m}$ of the usual, bulk $\mathrm{SiO}_{2}$ ceramics. ${ }^{8}$

### 4.3. Boundary problems

For an Ohmic conducting media, we may combine Eqs. (6) and (8) the following differential equation

$$
\begin{equation*}
\nabla \cdot(\sigma \nabla \phi)=0 \tag{4.14}
\end{equation*}
$$

For a uniform conductor ( $\sigma=$ const), Eq. (14) is reduced to the Laplace equation for the electrostatic potential $\phi$. As we already know from Chapters 2 and 3, its solution depends on the boundary conditions. These conditions depend on the interface type.
(i) Conductor-conductor interface. Applying the continuity equation (6) to a Gauss-type pillbox at the interface of two different conductors (Fig. 5), we get

$$
\begin{equation*}
\left(j_{n}\right)_{1}=\left(j_{n}\right)_{2}, \tag{4.15}
\end{equation*}
$$

so that if the Ohm law is valid inside each medium, then

$$
\begin{equation*}
\sigma_{1} \frac{\partial \phi_{1}}{\partial n}=\sigma_{2} \frac{\partial \phi_{2}}{\partial n} . \tag{4.16}
\end{equation*}
$$



Fig. 4.5. DC current "refraction" at the interface between two different conductors.

Also, since the electric field should be finite, its potential $\phi$ has to be continuous across the interface - the condition that may also be written as

[^244]\[

$$
\begin{equation*}
\frac{\partial \phi_{1}}{\partial \tau}=\frac{\partial \phi_{2}}{\partial \tau} \tag{4.17}
\end{equation*}
$$

\]

Both these conditions (and hence the solutions of the boundary problems using them) are similar to those for the interface between two dielectrics - cf. Eqs. (3.46)-(3.47).

Note that using the Ohm law, Eq. (17) may be rewritten as

$$
\begin{equation*}
\frac{1}{\sigma_{1}}\left(j_{\tau}\right)_{1}=\frac{1}{\sigma_{2}}\left(j_{\tau}\right)_{2} \tag{4.18}
\end{equation*}
$$

Comparing it with Eq. (15) we see that, generally, the current density magnitude changes at the interface: $j_{1} \neq j_{2}$. It is also curious that if $\sigma_{1} \neq \sigma_{2}$, the current line slope changes at the interface (Fig. 4), qualitatively to the refraction of light rays in optics - see Chapter 7.
(ii) Conductor-electrode interface. The definition of an electrode, or a "perfect conductor", is a medium with $\sigma \rightarrow \infty$. Then, at fixed current density at the interface, the electric field in the electrode tends to zero, and hence it may be described by equation

$$
\begin{equation*}
\phi=\phi_{j}=\text { const }, \tag{4.19}
\end{equation*}
$$

where constants $\phi_{j}$ may be different for different electrodes (numbered with index $j$ ). Note that with such boundary conditions the Laplace boundary problem becomes exactly the same as in electrostatics see Eq. (2.35) - and hence we can use all the methods (and some solutions :-) of Chapter 2 for finding dc current distribution.
(iii) Conductor-insulator interface. For the description of an insulator, we can use $\sigma=0$, so that Eq. (16) yields the following boundary condition,

$$
\begin{equation*}
\frac{\partial \phi}{\partial n}=0 \tag{4.20}
\end{equation*}
$$

for the potential derivative inside the conductor. From the Ohm law we see that this is just the very natural requirement for the dc current not to flow into an insulator.

Now, note that this condition makes the Laplace problem inside the conductor completely welldefined, and independent on the potential distribution in the adjacent insulator. On the contrary, due to the continuity of the electrostatic potential at the border, its distribution in the insulator has to follow that inside the conductor. Let us discuss this conceptual issue on the following (apparently, trivial) example: dc current in a long wire with a constant cross-section area $A$. The reader certainly knows the answer:

$$
\begin{equation*}
I=\frac{V}{R}, \quad \text { where } R \equiv \frac{V}{I}=\frac{l}{\sigma A}, \tag{4.21}
\end{equation*}
$$

where $l$ is the wire length, and constant $R$ is called the resistance. ${ }^{9}$ However, let us get this result formally from our theoretical framework. For the ideal geometry shown in Fig. 6a, this is easy to do. Here the potential evidently has a linear 1D distribution

[^245]\[

$$
\begin{equation*}
\phi=\text { const }-\frac{x}{l} V \text {, } \tag{4.22}
\end{equation*}
$$

\]

both in the conductor and the surrounding free space, with both boundary conditions (16) and (17) satisfied at the conductor-insulator interfaces, and condition (20) satisfied at the conductor-electrode interfaces. As a result, the electric field is constant and has only one component $E_{x}=V / l$, so that inside the conductor

$$
j_{x}=\sigma E_{x}, \quad I=j_{x} A,
$$

giving us the well-known Eq. (21).
(a)

(b)

Fig. 4.6. (a) Trivial and (b) not-so-trivial problems of the field distribution at dc current flow. (For the latter case, schematically.)

However, what about the geometry shown in Fig. 6b? In this case the field distribution in the insulator is dramatically different, but according to boundary problem defined by Eqs. (14) and (20), inside the conductor the solution is exactly the same as it was in the former case. Now, the Laplace equation in the surrounding insulator has to be solved with the boundary values of the electrostatic potential, "dictated" by the distribution of the current (and hence potential) in the conductor.

Let us solve a problem in that this conduction hierarchy may be followed analytically to the very end. Consider an empty spherical cavity cut in a conductor with an initially uniform current flow with constant density $\mathbf{j}_{0}=\mathbf{n}_{z} j_{0}$ (Fig. 7a). Following the conduction hierarchy, we have to solve the boundary problem in the conducting part of the system, i.e. outside the sphere ( $r \geq R$ ), first. Since the problem is evidently axially-symmetric, we already know the general solution of the Laplace equation - see Eq. (2.172). Moreover, we know that in order to match the uniform field at $r \rightarrow \infty$, all coefficients $a_{l}$ but one ( $a_{1}=-E_{0}=-j_{0} / \sigma$ ) have to be zero, and that the boundary conditions at $r=R$ will give zero solutions for all coefficients $b_{l}$ but one ( $b_{1}$ ), so that

$$
\begin{equation*}
\phi=-\frac{j_{0}}{\sigma} r \cos \theta+\frac{b_{1}}{r^{2}} \cos \theta, \quad \text { for } r \geq R . \tag{4.24}
\end{equation*}
$$

In order to find coefficient $b_{1}$, we have to use the boundary condition (20) at $r=R$ :

$$
\begin{equation*}
\left.\frac{\partial \phi}{\partial r}\right|_{r=R}=\left(-\frac{j_{0}}{\sigma}-\frac{2 b_{1}}{R^{3}}\right) \cos \theta=0 . \tag{4.25}
\end{equation*}
$$

This gives $b_{1}=-j_{0} R^{3} / 2 \sigma$, so that, finally,

$$
\begin{equation*}
\phi(r, \theta)=-\frac{j_{0}}{\sigma}\left(r+\frac{R^{3}}{2 r^{2}}\right) \cos \theta \tag{4.26}
\end{equation*}
$$

(Note that this potential distribution corresponds to the dipole moment $\mathbf{p}=-\mathbf{E}_{0} R^{3} / 2$. It is easy to check that if the empty sphere was cut in a dielectric, the potential distribution outside the cavity would be similar, with $\mathbf{p}=-\mathbf{E}_{0} R^{3}\left(\varepsilon_{r}-1\right) /\left(\varepsilon_{r}+2\right)$. In the limit $\varepsilon_{r} \rightarrow \infty$, these two results coincide, despite the rather different type of the problem: in the dielectric case, there is no current at all.)


Fig. 4.7. Spherical cavity in a uniform conductor: (a) the problem's geometry, and (b) the equipotential surfaces, as given by Eq. (26) and (28).

Now, as the second step in the conductivity hierarchy, we may find the electrostatic potential distribution $\phi(r, \theta)$ in the insulator, in this particular case inside the cavity ( $r \leq R$ ). It should also satisfy the Laplace equation with the boundary conditions at $r=R$, "dictated" by distribution (26):

$$
\begin{equation*}
\phi(R, \theta)=-\frac{3}{2} \frac{j_{0}}{\sigma} R \cos \theta \tag{4.27}
\end{equation*}
$$

We could again solve this problem by the formal variable separation (keeping in the general solution (2.172) only the term proportional to $b_{1}$, that does not diverge at $r \rightarrow 0$ ), but if we notice that boundary condition (27) depends on just one Cartesian coordinate, $z=R \cos \theta$, the solution may be just guessed:

$$
\begin{equation*}
\phi(r, \theta)=-\frac{3}{2} \frac{j_{0}}{\sigma} z=-\frac{3}{2} \frac{j_{0}}{\sigma} r \cos \theta, \quad \text { at } r \leq R . \tag{4.28}
\end{equation*}
$$

It evidently satisfies the Laplace equation and the boundary condition (27), and corresponds to a constant vertical electric field equal to $3 j_{0} / 2 \sigma$ - see Fig. 6b.

The conductivity hierarchy says that static electrical fields and charges outside conductors (e.g., electric wires) do not affect currents flowing in the wires, and it is physically clear why. For example, if
a charge in vacuum is slowly moved close to a wire, it (in accordance with the linear superposition principle) will only induce an additional surface charge (see Chapter 2) that screens the external charge's field, without participating in (or disturbing) the current flow inside the conductor.

Besides the conceptual discussion, the two examples given above may be considered as a demonstration of the application of the first two methods described in Chapter 2 (the orthogonal coordinates (Fig. 5) and variable separation (Fig. 6)) to dc current distribution problems. Continuing this review of the methods we know, let us discuss the analog of the method of charge images. Let us consider the spherically-symmetric potential distribution of the electrostatic potential, similar to that given by Eq. (1.35):

$$
\begin{equation*}
\phi=\frac{c}{r} . \tag{4.29}
\end{equation*}
$$

As we know from Chapter 1, this is a particular solution of the 3D Laplace equation at all points but $r=$ 0 , and hence is a legitimate solution in a current-carrying conductor as well. In vacuum, this distribution would correspond to a point charge $q=4 \pi \varepsilon_{0} c$; but what about the conductor? Calculating the corresponding electric field and current density,

$$
\begin{equation*}
\mathbf{E}=-\nabla \phi=\frac{c}{r^{3}} \mathbf{r}, \quad \mathbf{j}=\sigma \mathbf{E}=\sigma \frac{c}{r^{3}} \mathbf{r}, \tag{4.30}
\end{equation*}
$$

we see that the total current flowing from the point in the origin through a sphere of an arbitrary radius $r$ does not depend on the radius:

$$
\begin{equation*}
I=A j=4 \pi r^{2} j=4 \pi \sigma c \tag{4.31}
\end{equation*}
$$

Plugging the resulting c into Eq. (29), we get

$$
\begin{equation*}
\phi=\frac{I}{4 \pi \sigma r} . \tag{4.32}
\end{equation*}
$$

Hence the Coulomb-type distribution of the electric potential in a conductor is possible (at least at some distance from the singular point $r=0$ ), and describes dc current $I$ flowing out of a small-size electrode - or into such a point, if coefficient $c$ is negative. Such current injection may be readily implemented experimentally; think for example about an insulated wire with a small bare end, inserted into a poorly conducting soil - an important method in geophysical research. ${ }^{10}$

Now let the injection point $\mathbf{r}$ ' be close to a plane interface between the conductor and an insulator (Fig. 8). In this case, besides the Laplace equation, we should satisfy the boundary condition,

$$
\begin{equation*}
j_{n}=\sigma E_{n}=-\sigma \frac{\partial \phi}{\partial n}=0 . \tag{4.33}
\end{equation*}
$$

It is clear that this can be done by replacing the insulator for a conductor with an additional current injection point, at the mirror image point $\mathbf{r}$ ". Note, however, that in contrast to the charge images, the sign of the imaginary current has to be similar, not opposite, to the initial one, so that the total electrostatic potential inside the conducting semi-space is

[^246]\[

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{I}{4 \pi \sigma}\left(\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}+\frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime \prime}\right|}\right) \tag{4.34}
\end{equation*}
$$

\]

(Note that the image current's sign would be opposite if we discussed an interface between a conductor with a moderate conductivity and a perfect conductor ("electrode") whose potential should be virtually constant.)


Fig. 4.8. Method of images at dc conduction.

This result may be readily used, for example, to calculate the current density at the conductor's surface, as a function of distance $\rho$ from point 0 (the surface point closest to the current injection) - see Fig. 8. At the surface, Eq. (34) yields

$$
\begin{equation*}
\phi=\frac{I}{2 \pi \sigma} \frac{1}{\left(\rho^{2}+d^{2}\right)^{1 / 2}}, \tag{4.35}
\end{equation*}
$$

so that the current density is independent of $\sigma$.

$$
\begin{equation*}
j_{\rho}=\sigma E_{\rho}=-\sigma \frac{\partial \phi}{\partial \rho}=\frac{I}{2 \pi} \frac{\rho}{\left(\rho^{2}+d^{2}\right)^{3 / 2}} \tag{4.36}
\end{equation*}
$$

Deviations from Eqs. (35) and (36), which are valid for a uniform medium, may be used to find and characterize conductance inhomogeneities, say, those due to mineral deposits in the Earth crust. ${ }^{11}$

### 4.4. Dissipation power

Let me conclude this brief chapter with an ultra-short discussion of energy dissipation in conductors. In contrast to the electrostatics situations in insulators (vacuum or dielectrics), at dc conduction the electrostatic energy $U$ is "dissipated" (i.e. transferred to heat) at a certain rate $\mathcal{P} \equiv-$ $d U / d t$, called dissipation power. ${ }^{12}$ This rate may evaluated by calculating the power of electric field's work on a single moving charge:

[^247]\[

$$
\begin{equation*}
\mathcal{P}_{1}=\mathbf{F} \cdot \mathbf{v}=q \mathbf{E} \cdot \mathbf{v} . \tag{4.37}
\end{equation*}
$$

\]

After the summation over all charges, Eq. (37) gives us the dissipation power. If the charge density $n$ is uniform, multiplying by it both parts of this equation, and taking into account that $q n \mathbf{v}=\mathbf{j}$, for the power dissipated in a unit volume we get the Joule law

General Joule law

$$
\begin{equation*}
\mathfrak{p} \equiv \frac{\mathcal{P}}{V}=\frac{\mathcal{P}_{1} N}{V}=\mathcal{P}_{1} n=q \mathbf{E} \cdot \mathbf{v} n=\mathbf{E} \cdot \mathbf{j} . \tag{4.38}
\end{equation*}
$$

In the particular case of the Ohmic conductivity, this expression may be also rewritten in two other forms:

Joule law for Ohmic conductivity

$$
\begin{equation*}
p=\sigma E^{2}=\frac{j^{2}}{\sigma} \tag{4.39}
\end{equation*}
$$

At dc conduction, the energy is permanently replenished by a flow of power from the current source(s).
With our electrostatics background, it is straightforward (and hence left for reader's exercise) to prove that the dc current distribution in a uniform Ohmic conductor, at a fixed voltage applied at its borders, corresponds to the minimum of the total dissipation power

$$
\begin{equation*}
\mathcal{P}=\sigma \int_{V} E^{2} d^{3} r . \tag{4.40}
\end{equation*}
$$

### 4.5. Exercise problems

4.1. Find the resistance between two large conductors separated with a very thin, plane, insulating partition, with a circular hole of radius $R$ in it - see Fig. on the right.

Hint: You may like to use the degenerate ellipsoidal coordinates that had been used in Sec. 2.4 to find the self-capacitance of a round disk in vacuum.
4.2. Calculate the effective (average) conductivity $\sigma_{\mathrm{ef}}$ of a medium with many empty spherical cavities of radius $R$, carved at random points in a uniform Ohmic conductor (see Fig. on the right), in the limit of low density $n \ll R^{-3}$ of the spheres.

Hint: Try to use the analogy with a dipole media (Sec. 3.2).

4.3. In two separate experiments, a narrow gap, of irregular width, between two close metallic electrodes is filled with some material - in the first case, with a uniform linear insulator with an electric permittivity $\varepsilon$, and in the second case, with a uniform conducting material with an Ohmic conductivity $\sigma$. Neglecting the fringe effects, calculate the relation between the mutual capacitance $C$ between the electrodes (in the first case) and the dc resistance $R$ between them (in the second case).
4.4. Calculate the voltage drop $V$ across a uniform, wide resistive slab of thickness $t$, at distance $l$ from the points of injection/ejection of dc current $I$ that is passed across the slab - see Fig. on the right.

Hint: Try to use the dc current analog of the charge image method.

4.6. Calculate the distribution of dc current density in a thin, round, uniform resistive disk, if the current is inserted into a point at its rim, and picked up at the center.
4.7.* The simplest model of a vacuum diode consists of two plane, parallel metallic electrodes of area $A$, separated by a gap of thickness $d \ll A^{1 / 2}$ : a "cathode" which emits electrons to vacuum, and an "anode" which absorbs the electrons arriving at its surface. Calculate the dc $I-V$ curve of the diode, i.e. the stationary relation between current $I$ flowing between the electrodes and voltage $V$ applied between them, using the following simplifying assumptions:
(i) due to the effect of the negative space charge of the emitted electrons, current $I$ is much smaller than the emission ability of the cathode,
(ii) the initial velocity of the emitted electrons is negligible, and
(iii) the direct Coulomb interaction of electrons (besides the space charge effect) is negligible.
4.8.* Calculate the space-charge-limited current in a system with the same geometry, and using the same assumptions as in the previous problem, besides assuming now that the emitted charge carriers move not ballistically, but in accordance with the Ohm law, with the conductivity given by Eq. (4.13): $\sigma$ $=q^{2} \mu \pi$, with constant mobility $\mu$.

Hint: In order to get a realistic result, assume that the medium in which the carriers move ${ }^{13}$ has a certain dielectric constant $\varepsilon_{r}$.
4.9. Prove that the distribution of dc currents in a uniform Ohmic conductor, at fixed voltage applied at its boundaries, corresponds to the minimum of the total power dissipation ("Joule heat").

[^248]
## Chapter 5. Magnetism

Despite the fact that we are now starting to discuss a completely new type of electromagnetic interactions, its coverage (for the stationary case) will take just one chapter, because we will be able to recycle many ideas and methods of electrostatics, though with a twist or two.

### 5.1. Magnetic interaction of currents

DC currents in conductors usually leave them electroneutral, $\rho(\mathbf{r})=0$, with a very good precision, because any virtual misbalance of positive and negative charge density results in extremely strong Coulomb forces that restore their balance by an additional shift of free carriers. ${ }^{1}$ This is why let us start the discussion of magnetic interactions from the simplest case of two spatially-separated, current-carrying, electroneutral conductors (Fig. 1).


Fig. 5.1. Magnetic interaction of two currents.

According to the Coulomb law, there should be no force between them. However, several experiments carried out in the early $1820 \mathrm{~s}^{2}$ proved that such non-Coulomb forces do exist, and are the manifestation of another, magnetic interactions between the currents. In the contemporary used in this course, their results may be summarized with one formula, in SI units expressed as: ${ }^{3}$

$$
\begin{equation*}
\mathbf{F}=-\frac{\mu_{0}}{4 \pi} \int_{V} d^{3} r \int_{V^{\prime}} d^{3} r^{\prime}\left(\mathbf{j}(\mathbf{r}) \cdot \mathbf{j}^{\prime}\left(\mathbf{r}^{\prime}\right)\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} . \tag{5.1}
\end{equation*}
$$

Here coefficient $\mu_{0} / 4 \pi$ (where $\mu_{0}$ is called either the magnetic constant or the free space permeability), by definition, equals exactly $10^{-7}$ SI units, thus relating the electric current (and hence electric charge) definition to that of force - see below.

Note that the Coulomb law (1.1), with the account of the linear superposition principle, may be presented in a very similar form:

[^249]\[

$$
\begin{equation*}
\mathbf{F}=\frac{1}{4 \pi \varepsilon_{0}} \int_{V} d^{3} r \int_{V^{\prime}} d^{3} r^{\prime} \rho(\mathbf{r}) \rho^{\prime}\left(\mathbf{r}^{\prime}\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} . \tag{5.2}
\end{equation*}
$$

\]

Besides the different coefficient and sign, the "only" difference of Eq. (1) from Eq. (2) is the scalar product of current densities, evidently necessary because of the vector character of the current density. We will see that this difference will bring certain complications in applying the electrostatics approaches, discussed in the previous chapters, to magnetostatics.

Before going to their discussion, let us have one more glance at the coefficients in Eqs. (1) and (2). To compare them, let us consider two objects with uncompensated charge distributions $\rho(\mathbf{r})$ and $\rho^{\prime}(\mathbf{r})$, each moving parallel to each other as a whole certain velocities $\mathbf{v}$ and $\mathbf{v}^{\prime}$, as measured in an inertial "lab" frame. In this case, $\mathbf{j}(\mathbf{r})=\rho(\mathbf{r}) \mathbf{v}, \mathbf{j}(\mathbf{r}) \cdot \mathbf{j}{ }^{\prime}(\mathbf{r})=\rho(\mathbf{r}) \rho^{\prime}(\mathbf{r}) v v^{\prime}$, and the integrals in Eqs. (1) and (2) become functionally similar, and differ only by the factor

$$
\begin{equation*}
\frac{F_{\text {magnetic }}}{F_{\text {electric }}}=-\frac{\mu_{0} v v^{\prime}}{4 \pi} / \frac{1}{4 \pi \varepsilon_{0}}=-\frac{v v^{\prime}}{c^{2}} . \tag{5.3}
\end{equation*}
$$

(This expression hold in any consistent system of units.) We immediately see that magnetism is an essentially relativistic phenomenon, very weak in comparison with the electrostatic interaction at the human scale velocities, $v \ll c$, and may dominate only if the latter interaction vanishes - as it does in electroneutral systems. ${ }^{4}$

Also, Eq. (3) points at an interesting paradox. Consider two electron beams moving parallel to each other, with the same velocity $v$ with respect to a lab reference frame. Then, according to Eq. (3), the net force of their total (electric and magnetic) interaction is proportional to $\left(1-v^{2} / c^{2}\right)$, and tends to zero in the limit $v \rightarrow c$. However, in the reference frame moving together with electrons, they are not moving at all, i.e. $v=0$. Hence, from the point of view of such a moving observer, the electron beams should interact only electrostatically, with a repulsive force independent of velocity $v$. Historically, this had been one of several paradoxes that led to the development of the special relativity; its resolution will be discussed in Chapter 9, devoted to this theory.

Returning to Eq. (1), in some simple cases, the double integration in it may be carried out analytically. First of all, let us simplify this expression for the case of two thin, long conductors (wires) separated by a distance much larger than their thickness. In this case we may integrate the products $\mathbf{j} d^{3} r$ and $\mathbf{j}^{\prime} d^{3} r^{\prime}$ over wires' cross-sections first, neglecting the corresponding change of ( $\mathbf{r}-\mathbf{r}^{\prime}$ ). Since the integrals of the current density over the cross-sections of the wire are just the currents $I$ and $I^{\prime}$ in the wires, and cannot change along their lengths (correspondingly, $l$ and $l$ '), they may be taken out of the remaining integrals, reducing Eq. (1) to

$$
\begin{equation*}
\mathbf{F}=-\frac{\mu_{0} I I^{\prime}}{4 \pi} \oint_{l} \oint_{l^{\prime}}\left(d \mathbf{r} \cdot d \mathbf{r}^{\prime}\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} \tag{5.4}
\end{equation*}
$$

[^250]As the simplest example, consider two straight, parallel wires (Fig. 2), separated by distance $d$, with length $l \gg \rho$. In this case, due to symmetry, the vector of magnetic interaction force has to:
(i) lay in the same plane as the currents, and
(ii) be perpendicular to the wires - see Fig. 2.

Hence we can limit our calculations to just one component of the force. Using the fact that with the coordinate choice shown in Fig. 2, $d \mathbf{r} \cdot d \mathbf{r}^{\prime}=d x d x$ ', we get

$$
\begin{equation*}
F=-\frac{\mu_{0} I I^{\prime}}{4 \pi} \int_{-\infty}^{+\infty} d x \int_{-\infty}^{+\infty} d x^{\prime} \frac{\sin \theta}{d^{2}+\left(x-x^{\prime}\right)^{2}}=-\frac{\mu_{0} I I^{\prime}}{4 \pi} \int_{-\infty}^{+\infty} d x \int_{-\infty}^{+\infty} d x^{\prime} \frac{d}{\left[d^{2}+\left(x-x^{\prime}\right)^{2}\right]^{3 / 2}} \tag{5.5}
\end{equation*}
$$

Introducing, instead of $x^{\prime}$, a new, dimensionless variable $\xi \equiv\left(x-x^{\prime}\right) / \rho$, we may reduce the internal integral to a table integral which we have already met in this course:

$$
\begin{equation*}
F=-\frac{\mu_{0} I I^{\prime}}{4 \pi d} \int_{-\infty}^{+\infty} d x \int_{-\infty}^{+\infty} \frac{d \xi}{\left(1+\xi^{2}\right)^{3 / 2}}=-\frac{\mu_{0} I I^{\prime}}{2 \pi d} \int_{-\infty}^{+\infty} d x . \tag{5.6}
\end{equation*}
$$

The integral over $x$ is formally diverging, but this means merely that the interaction force per unit length of the wires is constant:

$$
\begin{equation*}
\frac{F}{l}=-\frac{\mu_{0} I I^{\prime}}{2 \pi d} . \tag{5.7}
\end{equation*}
$$

Note that the force drops rather slowly (only as $1 / d$ ) as the distance $d$ between the wires is increased, and is attractive (rather than repulsive as in the Coulomb law) if the currents are of the same sign.


Fig. 5.2. Magnetic force between two straight parallel currents. a current

This is an important result, ${ }^{5}$ but again, the problems solvable so simply are few and far between, and it is intuitively clear that we would strongly benefit from the same approach as in electrostatics, i.e., from breaking Eq. (1) into a product of two factors via the introduction of a suitable field. Such decomposition may done as follows:

[^251]where vector $\mathbf{B}$ is called the magnetic field (in our particular case, induced by current $\mathbf{j}$ '): ${ }^{6}$
\[

$$
\begin{equation*}
\mathbf{B}(\mathbf{r}) \equiv \frac{\mu_{0}}{4 \pi} \int_{V^{\prime}} \mathbf{j}^{\prime}\left(\mathbf{r}^{\prime}\right) \times \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} d^{3} r^{\prime} \tag{5.9}
\end{equation*}
$$

\]

BiotSavart law

The last equation is called the Biot-Savart law, while F expressed by Eq. (8) is sometimes called the Lorentz force. ${ }^{7}$ However, more frequently the later term is reserved for the full force,

$$
\begin{equation*}
\mathbf{F}=q(\mathbf{E}+\mathbf{v} \times \mathbf{B}) \tag{5.10}
\end{equation*}
$$

exerted by electric and magnetic fields field on a point charge $q$, moving with velocity $\mathbf{v}$. (The equivalence of Eq. (8) and the magnetic part of Eq. (10) follows from the summation of all forces acting on $n$ particles in a unit volume, moving with the same velocity $\mathbf{v}$, so that $\mathbf{j}=q n \mathbf{v}$.)

Now we have to prove that the new formulation (8)-(9) is equivalent to Eq. (1). At the first glance, this seems unlikely. Indeed, first of all, Eqs. (8) and (9) involve vector products, while Eq. (1) is based on a scalar product. More profoundly, in contrast to Eq. (1), Eqs. (8) and (9) do not satisfy the $3^{\text {rd }}$ Newton's law, applied to elementary current components $\mathbf{j} d^{3} r$ and $\mathbf{j}^{\prime} d^{3} r^{\prime}$, if these vectors are not parallel to each other. Indeed, consider the situation shown in Fig. 3. Here vector $\mathbf{j}$ ' is perpendicular to vector ( $\mathbf{r}$ $-\mathbf{r}$ '), and hence, according to Eq. (9), produces a nonvanishing contribution $d \mathbf{B}$ ' to the magnetic field, directed (in Fig. 3) perpendicular to the plane of drawing, i.e. is perpendicular to vector $\mathbf{j}$. Hence, according to Eq. (8), this field provides a nonvanishing contribution to $\mathbf{F}$. On the other hand, if we calculate the reciprocal force $\mathbf{F}$ ' by swapping indices in Eqs. (8) and (9), the latter equation immediately shows that $d \mathbf{B}\left(\mathbf{r}^{\prime}\right) \propto \mathbf{j} \times\left(\mathbf{r}-\mathbf{r}^{\prime}\right)=0$, because the two operand vectors are parallel (Fig. 3). Hence, the current component $\mathbf{j}^{\prime} d^{3} \mathbf{r}^{\prime}$ does exert a force on its counterpart, while $\mathbf{j} d^{3} \mathbf{r}$ does not.


Fig. 5.3. Apparent violation of the $3^{\text {rd }}$
Newton law in magnetism.

Despite this apparent problem, let us still go ahead and plug Eq. (9) into Eq. (8):

$$
\begin{equation*}
\mathbf{F}=\frac{\mu_{0}}{4 \pi} \int_{V} d^{3} r \int_{V^{\prime}} d^{3} r^{\prime} \mathbf{j}(\mathbf{r}) \times\left(\mathbf{j}^{\prime}\left(\mathbf{r}^{\prime}\right) \times \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}}\right) \tag{5.11}
\end{equation*}
$$

[^252]This double vector product may transformed into two scalar products, using the vector algebraic identity called the bac minus cab rule, $\mathbf{a} \times(\mathbf{b} \times \mathbf{c})=\mathbf{b}(\mathbf{a} \cdot \mathbf{c})-\mathbf{c}(\mathbf{a} \cdot \mathbf{b}) .{ }^{8}$ Applying this relation, with $\mathbf{a}=\mathbf{j}, \mathbf{b}=\mathbf{j}$, and $\mathbf{c}$ $=\mathbf{R} \equiv \mathbf{r}-\mathbf{r}^{\prime}$, to Eq. (11), we get

$$
\begin{equation*}
\mathbf{F}=\frac{\mu_{0}}{4 \pi} \int_{V^{\prime}} d^{3} r^{\prime} \mathbf{j}^{\prime}\left(\mathbf{r}^{\prime}\right)\left(\int_{V} d^{3} r \frac{\mathbf{j}(\mathbf{r}) \cdot \mathbf{R}}{R^{3}}\right)-\frac{\mu_{0}}{4 \pi} \int_{V} d^{3} r \int_{V^{\prime}} d^{3} r^{\prime} \mathbf{j}(\mathbf{r}) \cdot \mathbf{j}^{\prime}\left(\mathbf{r}^{\prime}\right) \frac{\mathbf{R}}{R^{3}} \tag{5.12}
\end{equation*}
$$

The second term in the right-hand part of this equation coincides with the right-hand part of Eq. (1), while the first term equals zero, because its the internal integral vanishes. Indeed, we may break volumes $V$ and $V^{\prime}$ into narrow current tubes, the stretched sub-volumes whose walls are not crossed by current lines $\left(j_{n}=0\right)$. As a result, the (infinitesimal) current in each tube, $d I=j d A=j d^{2} r$, is the same along its length, and, just as in a thin wire, $\mathbf{j} d^{2} r$ may be replaced with $d I d \mathbf{r}$. Because of this, each tube's contribution to the internal integral in the first term of Eq. (12) may be presented as

$$
\begin{equation*}
d I \oint_{l} d \mathbf{r} \cdot \frac{\mathbf{R}}{R^{3}}=-d I \oint_{l} d \mathbf{r} \cdot \nabla \frac{1}{R}=-d I \oint_{l} d r \frac{\partial}{\partial r} \frac{1}{R}, \tag{5.13}
\end{equation*}
$$

where operator $\nabla$ acts in the $\mathbf{r}$ space, and the integral is taken along tube's length $l$. Due to the current continuity, each loop should follow a closed contour, and an integral of a full differential of some scalar function (in our case, $1 / r_{12}$ ) along it equals zero.

So we have recovered Eq. (1). Returning for a minute to the paradox illustrated with Fig. 3, we may conclude that the apparent violation of the $3^{\text {rd }}$ Newton law was the artifact of our interpretation of Eqs. (8) and (9) as sums of independent elementary components. In reality, due to the dc current continuity expressed by Eq. (4.6), these components are not independent. For the whole currents, Eqs. (8)-(9) do obey the $3^{\text {rd }}$ law - as follows from their already proved equivalence to Eq. (1).

Thus we have been able to break the magnetic interaction into the two effects: the creation of the magnetic field $\mathbf{B}$ by one current (in our notation, $\mathbf{j}$ '), and the effect of this field on the other current ( $\mathbf{j}$ ). Now comes an additional experimental fact: other elementary components $\mathbf{j} d^{3} r$ ' of current $\mathbf{j}$ also contribute to the magnetic field (9) acting on component $\mathbf{j} d^{3} r$. ${ }^{9}$ This fact allows us to drop prime after $\mathbf{j}$ in Eq. (9), and rewrite Eqs. (8) and (9) as

$$
\begin{gather*}
\mathbf{B}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \int_{V^{\prime}} \mathbf{j}\left(\mathbf{r}^{\prime}\right) \times \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} d^{3} r^{\prime},  \tag{5.14}\\
\mathbf{F}=\int_{V} \mathbf{j}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}) d^{3} r, \tag{5.15}
\end{gather*}
$$

Again, the field observation point $\mathbf{r}$ and the field source point $\mathbf{r}$ ' have to be clearly distinguished. We immediately see that these expressions are similar to, but still different from the corresponding relations of the electrostatics, namely Eq. (1.8),

[^253]\[

$$
\begin{equation*}
\mathbf{E}(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \oint_{V^{\prime}} \rho\left(\mathbf{r}^{\prime}\right) \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{\prime}} d^{3} r^{\prime}, \tag{5.16}
\end{equation*}
$$

\]

and the distributed version of Eq. (1.6):

$$
\begin{equation*}
\mathbf{F}=\oint_{V} \rho(\mathbf{r}) \mathbf{E}(\mathbf{r}) d^{3} r \tag{5.17}
\end{equation*}
$$

(Note that the sign difference has disappeared, at the cost of the replacement of scalar-by-vector multiplications in electrostatics with cross-products of vectors in magnetostatics.)

For the frequent case of a field of a thin wire of length l', Eq. (14) may be re-written as

$$
\begin{equation*}
\mathbf{B}(\mathbf{r})=\frac{\mu_{0} I}{4 \pi} \oint_{l^{\prime}} d \mathbf{r}^{\prime} \times \frac{\mathbf{r}-\mathbf{r}^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} . \tag{5.18}
\end{equation*}
$$

Let us see how does the last formula work for the simplest case of a straight wire (Fig. 4a). The magnetic field contribution $d \mathbf{B}$ due to any small fragment $d \mathbf{r}$ ' of the wire's length is directed along the same line (perpendicular to both the wire and the perpendicular $d$ dropped from the observation point to the wire line), and its magnitude is

$$
\begin{equation*}
d B=\frac{\mu_{0} I}{4 \pi} \frac{d x^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{2}} \sin \theta=\frac{\mu_{0} I}{4 \pi} \frac{d x^{\prime}}{\left(d^{2}+x^{2}\right)} \frac{d}{\left(d^{2}+x^{2}\right)^{1 / 2}} . \tag{5.19}
\end{equation*}
$$

Summing up all such contributions, we get

$$
\begin{equation*}
B=\frac{\mu_{0} I \rho}{4 \pi} \int_{-\infty}^{\infty} \frac{d x}{\left(x^{2}+d^{2}\right)^{3 / 2}}=\frac{\mu_{0} I}{2 \pi d} . \tag{5.20}
\end{equation*}
$$



Fig. 5.4. Magnetic fields of: (a) a straight current, and (b) a current loop.
This is a simple but very important result. (Note that it is only valid for very long ( $l \gg d$ ), straight wires.) It is especially crucial to note the "vortex" character of the field: its lines go around the wire, forming round rings with the centers on the current line. This is in the sharp contrast to the electrostatic field lines that can only begin and end on electric charges and never form closed loops (otherwise the Coulomb force $q \mathbf{E}$ would not be conservative). In the magnetic case, the vortex field may be reconciled with the potential character of magnetic forces, which is evident from Eq. (1), due to the vector products in Eqs. (14)-(15).

Now we may use Eq. (15), or rather its thin-wire version

$$
\begin{equation*}
\mathbf{F}=I \oint_{l} d \mathbf{r} \times \mathbf{B}(\mathbf{r}), \tag{5.21}
\end{equation*}
$$

to apply Eq. (20) to the two-wire problem (Fig. 2). Since for the second wire vectors $\mathrm{d} \mathbf{r}$ and $\mathbf{B}$ are perpendicular to each other, we immediately arrive at our previous result (7).

The next important application of the Biot-Savart law (14) is the magnetic field at the axis of a circular current loop (Fig. 4b). Due to the problem symmetry, the net field $\mathbf{B}$ has to be directed along the axis, but each of its components $\mathrm{d} \mathbf{B}$ is tilted by angle $\theta=\tan ^{-1}(z / R)$ to this axis, so that its axial component

$$
\begin{equation*}
d B_{z}=d B \cos \theta=\frac{\mu_{0} I}{4 \pi} \frac{d r^{\prime}}{R^{2}+z^{2}} \frac{R}{\left(R^{2}+z^{2}\right)^{1 / 2}} \tag{5.22}
\end{equation*}
$$

Since the denominator of this expression remains the same for all wire components $d r$, in this case the integration is trivial $\left(\int d r^{\prime}=2 \pi R\right)$, giving finally

$$
\begin{equation*}
B=\frac{\mu_{0} I}{2} \frac{R^{2}}{\left(R^{2}+z^{2}\right)^{3 / 2}} . \tag{5.23}
\end{equation*}
$$

Note that the magnetic field in the loop's center (i.e., for $z=0$ ),

$$
\begin{equation*}
B=\frac{\mu_{0} I}{2 R} \tag{5.24}
\end{equation*}
$$

is $\pi$ times higher than that due to a similar current in a straight wire, at distance $d=R$ from it. This increase it readily understandable, since all elementary components of the loop are at the same distance $R$ from the observation point, while in the case of a straight wire, all its point but one are separated from the observation point by a distance larger than $d$.

Another notable fact is that at large distances $\left(z^{2} \gg R^{2}\right)$, field (23) is proportional to $z^{-3}$ :

$$
\begin{equation*}
B \approx \frac{\mu_{0} I}{2} \frac{R^{2}}{|z|^{3}}=\frac{\mu_{0}}{4 \pi} \frac{2 m}{|z|^{3}} \tag{5.25}
\end{equation*}
$$

just like the electric field of a dipole (along its direction), with the replacement of the electric dipole moment magnitude $p$ with $m=I A$, where $A=\pi R^{2}$ is the loop area. This is the best example of a magnetic dipole, with dipole moment $m$ - the notions to be discussed in more detail in Sec. 5 below.

### 5.2. Vector-potential and the Ampère law

The reader can see that the calculations of the magnetic field using Eq. (14) or (18) are still cumbersome even for the very simple systems we have examined. As we saw in Chapter 1, similar calculations in electrostatics, at least for several important systems of high symmetry, could be substantially simplified using the Gauss law (1.16). A similar relation exists in magnetostatics as well, but has a different form, due to the vortex character of the magnetic field. To derive it, let us notice that in an analogy with the scalar case, the vector product under integral (14) may be transformed as

$$
\begin{equation*}
\frac{j\left(\mathbf{r}^{\prime}\right) \times\left(\mathbf{r}-\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}}=\nabla \times \frac{\mathbf{j}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{\prime}}, \tag{5.26}
\end{equation*}
$$

where operator $\nabla$ acts in the $\mathbf{r}$ space. (This equality may be really verified by its Cartesian components, noticing that the current density is a function of $\mathbf{r}^{\prime}$ and hence its components are independent of $\mathbf{r}$.) Plugging Eq. (26) into Eq. (14), and moving operator $\nabla$ out of the integral over $\mathbf{r}$ ', we see that the magnetic field may be presented as the curl of another vector field: ${ }^{10}$

$$
\begin{equation*}
\mathbf{B}(\mathbf{r})=\nabla \times \mathbf{A}(\mathbf{r}), \tag{5.27}
\end{equation*}
$$

namely the so-called vector-potential:

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}) \equiv \frac{\mu_{0}}{4 \pi} \int_{V^{\prime}} \frac{\mathbf{j}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} \tag{5.28}
\end{equation*}
$$

Please note a wonderful analogy between Eqs. (27)-(28) and, respectively, Eqs. (1.33) and (1.38). This analogy implies that vector-potential A plays, for the magnetic field, essentially the same role as the scalar potential $\phi$ plays for the electric field (hence the name "potential"), with due respect to the vortex character of $\mathbf{A}$. I will discuss this notion in detail below.

Now let us see what equations we may get for the spatial derivatives of the magnetic field. First, vector algebra says that the divergence of any curl is zero. ${ }^{11}$ In application to Eq. (27), this means that

$$
\begin{equation*}
\nabla \cdot \mathbf{B}=0 . \tag{5.29}
\end{equation*}
$$

Comparing this equation with Eq. (1.27), we see that Eq. (29) may be interpreted as the absence of a magnetic analog of an electric charge on which magnetic field lines could originate or end. Numerous searches for such hypothetical magnetic charges, called magnetic monopoles, using very sensitive and sophisticated experimental setups, have never given a convincing evidence of their existence in Nature.

Proceeding to the alternative, vector derivative of the magnetic field (i.e., its curl), and using Eq. (28), we get

$$
\begin{equation*}
\nabla \times \mathbf{B}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \nabla \times\left(\nabla \times \int_{V^{\prime}} \frac{\mathbf{j}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime}\right) \tag{5.30}
\end{equation*}
$$

This expression may be simplified by using the following general vector identity: ${ }^{12}$

$$
\begin{equation*}
\nabla \times(\nabla \times \mathbf{c})=\nabla(\nabla \cdot \mathbf{c})-\nabla^{2} \mathbf{c} \tag{5.31}
\end{equation*}
$$

applied to vector $\mathbf{c}(\mathbf{r})=\mathbf{j}\left(\mathbf{r}^{\prime}\right) /\left|\mathbf{r}-\mathbf{r}^{\prime}\right|$ :

$$
\begin{equation*}
\nabla \times \mathbf{B}=\frac{\mu_{0}}{4 \pi} \nabla \int_{V^{\prime}} \mathbf{j}\left(\mathbf{r}^{\prime}\right) \cdot \nabla \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime}-\frac{\mu_{0}}{4 \pi} \int_{V^{\prime}} \mathbf{j}\left(\mathbf{r}^{\prime}\right) \nabla^{2} \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} \tag{5.32}
\end{equation*}
$$

As was already discussed during our study of electrostatics,

[^254]\[

$$
\begin{equation*}
\nabla^{2} \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}=-4 \pi \delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \tag{5.33}
\end{equation*}
$$

\]

so that the last term of Eq. (32) is just $\mu_{0} \mathbf{j}(\mathbf{r})$. On the other hand, inside the first integral we can replace $\nabla$ with ( $-\nabla^{\prime}$ ), where prime means differentiation in the space of radius-vector $\mathbf{r}^{\prime}$. Integrating that term by parts, we get

$$
\begin{equation*}
\nabla \times \mathbf{B}=-\frac{\mu_{0}}{4 \pi} \nabla \oint_{S^{\prime}} j_{n}\left(\mathbf{r}^{\prime}\right) \frac{1}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{2} r^{\prime}+\nabla \int_{V^{\prime}} \frac{\nabla^{\prime} \cdot \mathbf{j}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime}+\mu_{0} \mathbf{j}(\mathbf{r}) . \tag{5.34}
\end{equation*}
$$

Applying this equation to the volume $V^{\prime}$ limited by a surface $S^{\prime}$ sufficiently distant from the field concentration (or with no current crossing it), we may neglect the first term in the right-hand part of Eq. (34), while the second term always equals zero in statics, due to the dc charge continuity - see Eq. (4.6). As a result, we arrive at a very simple differential equation ${ }^{13}$

$$
\begin{equation*}
\nabla \times \mathbf{B}=\mu_{0} \mathbf{j} . \tag{5.35}
\end{equation*}
$$

This is (the dc form of) the inhomogeneous Maxwell equation, which in magnetostatics plays the role similar to the Poisson equation (1.27) in electrostatics. Let me display, for the first time in this course, this fundamental system of equations (at this stage, for statics only), and give the reader a minute to stare at their beautiful symmetry - that has inspired so much of the $20^{\text {th }}$ century physics:

Static Maxwell equations

$$
\begin{array}{ll}
\nabla \times \mathbf{E}=0, & \nabla \times \mathbf{B}=\mu_{0} \mathbf{j}, \\
\nabla \cdot \mathbf{E}=\frac{\rho}{\varepsilon_{0}}, & \nabla \cdot \mathbf{B}=0 . \tag{5.36}
\end{array}
$$

Their only asymmetry, two zeros in the right hand parts (for the magnetic field's divergence and electric field's curl), is due to the absence in Nature of, respectively, the magnetic monopoles and their currents. I will discuss these equations in more detail in Sec. 6.7, after the equations for field curls have been generalized to their full (time-dependent) versions.

Returning now to a more mundane but important task of calculating magnetic field induced by simple current configurations, we can benefit from an integral form of Eq. (35). For that, let us integrate this equation over an arbitrary surface $S$ limited by a closed contour $C$, applying to it the Stokes theorem. ${ }^{14}$ The resulting expression,

$$
\begin{equation*}
\oint_{C} \mathbf{B} \cdot d \mathbf{r}=\mu_{0} \oint_{S} j_{n} d^{2} r \equiv \mu_{0} I \tag{5.37}
\end{equation*}
$$

where $I$ is the net electric current crossing surface $S$, is called the Ampère law.
As the first example of its application, let us return to a current in a straight wire (Fig. 4a). With the Ampère law in our arsenal, we can readily pursue an even more ambitious goal - calculate the magnetic field both outside and inside of a wire of arbitrary radius $R$, with an arbitrary (albeit axiallysymmetric) current distribution $j(\rho)$ - see Fig. 5. Selecting two contours $C$ in the form of rings of some

[^255]radius $\rho$ in the plane perpendicular to the wire axis $z$, we have $\mathbf{B} \cdot d \mathbf{r}=B \rho(d \varphi)$, these $\varphi$ is the azimuthal angle, so that the Ampère law (37) yields:
\[

2 \pi \rho B=\mu_{0} \times $$
\begin{cases}2 \pi \int_{0}^{\rho} j\left(\rho^{\prime}\right) \rho^{\prime} d \rho^{\prime}, & \text { for } \rho \leq R  \tag{5.38}\\ 2 \pi \int_{0}^{R} j\left(\rho^{\prime}\right) \rho^{\prime} d \rho^{\prime} \equiv I, & \text { for } \rho \geq R\end{cases}
$$
\]

Thus we have not only recovered our previous result (20), with the notation replacement $d \rightarrow \rho$, in a much simpler way, but could also find the magnetic field distribution inside the wire. (In the most common case when the wire conductivity $\sigma$ is constant, and hence the current is uniformly distributed along its cross-section, $j(\rho)=$ const, the first of Eqs. (38) immediately yields $B \propto \rho$ for $\rho \leq R$ ).


Fig. 5.5. The simplest application of the Ampère law: dc current in a straight wire.

Another important example is a straight, long solenoid (Fig. 6a), with dense winding: $n^{2} A \gg 1$, where $n$ is the number of wire turns per unit length and $A$ is the area of solenoid's cross-section - not necessarily circular.

(a)
(b)


Fig. 5.6. Magnetic field of (a) straight and (b) toroidal solenoids.

From the symmetry of this problem, the longitudinal (in Fig. 6a, vertical) component $B_{z}$ of the magnetic field may only depend on the horizontal position $\rho$ of the observation point. First taking a plane Ampère contour $C_{1}$, with both long sides outside the solenoid, we get $B_{z}\left(\rho_{2}\right)-B_{z}\left(\rho_{1}\right)=0$, because the total current piercing the contour equals zero. This is only possible if $B_{z}=0$ at any $\rho$ outside of the
(infinitely long!) solenoid. ${ }^{15}$ With this result on hand, from contour $C_{2}$ we get the following relation for the only (z-) component of the internal field:

$$
\begin{equation*}
B l=\mu_{0} N I \tag{5.39}
\end{equation*}
$$

where $N$ is the number of wire turns passing through the contour of length $l$. This means that regardless of the exact position internal side of the contour, the result is the same:

$$
\begin{equation*}
B=\mu_{0} \frac{N}{l} I=\mu_{0} n I . \tag{5.40}
\end{equation*}
$$

Thus, the field inside an infinitely long solenoid is uniform; in this sense, a long solenoid is a magnetic analog of a wide plane capacitor.

As should be clear from its derivation, the obtained result, especially that the field outside of the solenoid equals zero, is conditional on the solenoid length being very large in comparison with its lateral size. (From Eq. (25), we may predict that for a solenoid of a finite length $l$, the external field is only a factor of $\sim A / l^{2}$ lower than the internal one.) Much better suppression of this external ("fringe") field may be obtained using the toroidal solenoid (Fig. 6b). The application of Ampère law to this geometry shows that, in the limit of dense winding ( $N \gg 1$ ), there is no fringe field at all - for any relation between two radii of the thorus, while inside the solenoid, and distance $\rho$ from the center,

$$
\begin{equation*}
B=\frac{\mu_{0} N I}{2 \pi \rho} . \tag{5.41}
\end{equation*}
$$

We see that a possible drawback of this system for practical applications is that internal field depends on $\rho$, i.e. is not quite uniform; however, if the thorus is thin, this problem is minor.

How should we solve the problems of magnetostatics for systems whose low symmetry does not allow getting easy results from the Ampère law? (The examples are of course too numerous to list; for example, we cannot use this approach even to reproduce Eq. (23) for a round current loop.) From the deep analogy with electrostatics, we may expect that in this case we could recover the field from the solution of a certain partial boundary problem for the field's potential, in this case the vector-potential A defined by Eq. (28). However, despite the similarity of this formula and Eq. (1.38) for $\phi$, that was emphasized above, there are two additional issues we should tackle in the magnetic case.

First, finding vector-potential distribution means determining three scalar functions (say, $A_{x}, A_{y}$, and $A_{z}$ ), rather than one $(\phi)$. Second, generally the differential equation satisfied by $\mathbf{A}$ is more complex than the Poisson equation for $\phi$. Indeed, plugging Eq. (27) into Eq. (35), we get

$$
\begin{equation*}
\nabla \times(\nabla \times \mathbf{A})=\mu_{0} \mathbf{j} . \tag{5.42}
\end{equation*}
$$

If we wrote the left-hand part of this equation in (say, Cartesian) components, we would see that they are much more interwoven than in the Laplace operator, and hence much less convenient for using the orthogonal coordinate approach or the variable separation method. In order to remedy the situation, let us apply to Eq. (42) the now-familiar identity (31). The result is

[^256]\[

$$
\begin{equation*}
\nabla(\nabla \cdot \mathbf{A})-\nabla^{2} \mathbf{A}=\mu_{0} \mathbf{j} . \tag{5.43}
\end{equation*}
$$

\]

We see that if we could kill the first term in the left-hand part, for example if $\nabla \cdot \mathbf{A}=0$, the second term would give us a set of independent Poisson equations for each Cartesian component of vector $\mathbf{A}$.

In this context, let us discuss what discretion do we have in the potentials' choice. In electrostatics, we might add to any function $\phi^{\prime}$, that satisfies Eq. (1.33), not only an arbitrary constant, but also an arbitrary function of time, without affecting the electric field:

$$
\begin{equation*}
-\nabla\left[\phi^{\prime}+f(t)\right]=-\nabla \phi^{\prime}=\mathbf{E} . \tag{5.44}
\end{equation*}
$$

Similarly, using the fact that curl of the gradient of any scalar function equals zero, ${ }^{16}$ we may add to any function $\mathbf{A}^{\prime}$, that satisfies Eq. (27) for a given field $\mathbf{B}$, not only a constant, but even a gradient of an arbitrary function $\chi(\mathbf{r}, t)$, because

$$
\begin{equation*}
\nabla \times\left(\mathbf{A}^{\prime}+\nabla \chi\right)=\nabla \times \mathbf{A}^{\prime}+\nabla \times(\nabla \chi)=\nabla \times \mathbf{A}^{\prime}=\mathbf{B} . \tag{5.45}
\end{equation*}
$$

Such additions, keeping the actual (observable) fields intact, are called gauge transformations. ${ }^{17}$ Let us see what such a transformation does to $\nabla \cdot \mathbf{A}^{\prime}$ ':

$$
\begin{equation*}
\nabla \cdot\left(\mathbf{A}^{\prime}+\nabla \chi\right)=\nabla \cdot \mathbf{A}^{\prime}+\nabla^{2} \chi \tag{5.46}
\end{equation*}
$$

Hence we can always choose a function $\chi$ in such a way that the right-hand part of this relation, and hence the divergence of the transformed vector-potential, $\mathbf{A} \equiv \mathbf{A}^{\prime}+\nabla \chi$, would vanish at all points. In this case, Eq. (43) is reduced to the vector Poisson equation

$$
\begin{equation*}
\nabla^{2} \mathbf{A}=-\mu_{0} \mathbf{j} \tag{5.47}
\end{equation*}
$$

As we know from the electrostatics (please compare Eqs. (1.38) and (1.41)), the vector-potential defined by Eq. (28) does satisfy this equation. So, the so-called Coulomb gauge condition,

$$
\begin{equation*}
\nabla \cdot \mathbf{A}=0 \tag{5.48}
\end{equation*}
$$

reduces the set of the functions $\mathbf{A}(\mathbf{r})$ that satisfy Eq. (27) to the actual vector-potential (28). However, this condition still leaves some liberty in the vector-potential selection. In order to demonstrate that, and also to get a better feeling of vector-potential's distribution in space, let us calculate it for two important particular cases.

First, let us revisit the straight wire problem (Fig. 5). As Eq. (28) shows, in this case vector A has just one component (along the axis $z$ ). Moreover, due to the problem's axial symmetry, its magnitude may only depend on the distance from the axis: $\mathbf{A}=\mathbf{n}_{z} A(\rho)$. Hence, the gradient of $\mathbf{A}$ is directed across axis $z$, so that Eq. (48) is satisfied even for this vector, i.e. the Poisson equation (47) is satisfied even for the original vector $\mathbf{A}$. For our symmetry $(\partial / \partial \varphi=\partial / \partial z=0)$, the Laplace operator, written in cylindrical coordinates, has just one term, ${ }^{18}$ reducing Eq. (47) to

$$
\begin{equation*}
\frac{1}{\rho} \frac{d}{d \rho}\left(\rho \frac{d A}{d \rho}\right)=-\mu_{0} j(\rho) \tag{5.49}
\end{equation*}
$$

[^257]Multiplying both parts of this equation by $\rho$ and integrating them over the coordinate once, we get

$$
\begin{equation*}
\rho \frac{d A}{d \rho}=-\mu_{0} \int_{0}^{\rho} j\left(\rho^{\prime}\right) \rho^{\prime} d \rho^{\prime}+\text { const } \tag{5.50}
\end{equation*}
$$

Since in the cylindrical coordinates, for our symmetry, ${ }^{19} B=-d A / d \rho$, Eq. (50) is nothing else than our old result (38) for the magnetic field. ${ }^{20}$ However, let us continue the integration, at least for the region outside the wire, where the function $A(\rho)$ depends only on the full current $I$ rather than on the current distribution inside the wire. Dividing both parts of Eq. (50) by $\rho$, and integrating them over that coordinate again, we get

$$
\begin{equation*}
A(\rho)=-\frac{\mu_{0} I}{2 \pi} \ln \rho+\text { const, where } I=2 \pi \int_{0}^{R} j(\rho) \rho d \rho . \tag{5.51}
\end{equation*}
$$

As a reminder, we had the similar logarithmic behavior for the electrostatic potential outside a uniformly charged straight line. This is natural, because the Poisson equations for both cases are similar.

Now let us find the vector-potential for the long solenoid (Fig. 6a), with its uniform magnetic field. Since Eq. (28) prescribes vector $\mathbf{A}$ to follow the direction of the current, we can start with looking for it in the form $\mathbf{A}=\mathbf{n}_{\varphi} A(\rho)$. (This is especially natural if the solenoid's cross-section is circular.) With this orientation of $\mathbf{A}$, the same general expression for the curl operator in cylindrical coordinates yields $\nabla \times \mathbf{A}=\mathbf{n}_{z}(1 / \rho) d(\rho A) / d \rho$. According to the definition (27) of $\mathbf{A}$, this expression should be equal to $\mathbf{B}$, in our case equal to $\mathbf{n}_{z} B$, with constant $B$ - see Eq. (40). Integrating this equality, and selecting such integration constant so that $A(0)$ is finite, we get

$$
\begin{equation*}
A(\rho)=\frac{B \rho}{2} . \tag{5.52}
\end{equation*}
$$

Plugging this result into the general expression for the Laplace operator in the cylindrical coordinates, ${ }^{21}$ we see that the Poisson equation (47) with $\mathbf{j}=0$ (i.e. the Laplace equation), is satisfied again - which is natural since for this distribution, $\nabla \cdot \mathbf{A}=0$. However, Eq. (52) is not the unique (or even the simplest) solution of the problem. Indeed, using the well-known expression for the curl operator in Cartesian coordinates, ${ }^{22}$ it is straightforward to check that either function $\mathbf{A}^{\prime}=\mathbf{n}_{y} B x$, or function $\mathbf{A}^{\prime \prime}=-\mathbf{n}_{\mathrm{x}} B y$, or any of their weighed sums, for example $\mathbf{A}^{\prime \prime \prime}=\left(\mathbf{A}^{\prime}+\mathbf{A}^{\prime \prime}\right) / 2=B\left(-\mathbf{n}_{\mathrm{x}} y+\mathbf{n}_{y} x\right) / 2$, also give the same magnetic field, and also evidently satisfy the Laplace equation. If such solutions do not look very natural due to their anisotropy in the $[x, y]$ plane, please consider the fact that they represent the uniform magnetic field regardless of its source (e.g., of the shape of long solenoid's crosssection). Such choices of vector-potential may be very convenient for some problems, for example for the analysis of the 2 D motion of a charged quantum particle in the perpendicular magnetic field, giving the famous Landau energy levels. ${ }^{23}$

[^258]
### 5.3. Magnetic energy, flux, and inductance

Considering currents flowing in a system as generalized coordinates, magnetic forces (1) between them are their unique functions, and in this sense the magnetic interaction energy $U$ may be considered a potential energy of the system. The apparent (but deceptive) way to guess the energy is to use the analogy between Eq. (1) and its electrostatic analog, Eq. (2). As we know from Chapter 1, if these densities describe the distribution of the same charge, i.e. if $\rho^{\prime}(\mathbf{r})=\rho(\mathbf{r})$, then the self-interaction of its elementary components correspond to the potential energy expressed by Eq. (1.61):

$$
\begin{equation*}
U=\frac{1}{4 \pi \varepsilon_{0}} \frac{1}{2} \int d^{3} r \int d^{3} r^{\prime} \frac{\rho(\mathbf{r}) \rho\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \tag{5.53}
\end{equation*}
$$

Using the analogy, for the magnetic interaction between elementary components of the same current, with density $\mathbf{j}(\mathbf{r})=\mathbf{j}$ ' $(\mathbf{r})$, we could guess that

$$
\begin{equation*}
U=\frac{\mu_{0}}{4 \pi} \frac{1}{2} \int d^{3} r \int d^{3} r^{\prime} \frac{\mathbf{j}(\mathbf{r}) \cdot \mathbf{j}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}, \tag{5.53}
\end{equation*}
$$

while for independent currents the coefficient $1 / 2$ should be removed. Now let me confess that this is a wrong way to get this correct result. Indeed, the sign in Eq. (1) is opposite to that in Eq. (2), so that following this argumentation we would get Eq. (53) with the minus sign. The reason of this paradox is fundamental: fixing electric charges does not require external interference (work), while the maintenance of currents generally does. Strictly speaking, a derivation of Eq. (53) required additional experimental fact, the Faraday induction law. However, I would like to defer its discussion until the beginning of the next chapter, and for now ask the reader to believe me that the sign in Eq. (53) is correct.

Due to the importance of this relation, let us rewrite it in several other forms, beneficial for different applications. First of all, just as in electrostatics, Eq. (54) may be recast into a potential-based form. Indeed, using definition (28) of the vector-potential $\mathbf{A}(\mathbf{r})$, Eq. (54) becomes ${ }^{24}$

$$
\begin{equation*}
U=\frac{1}{2} \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d^{3} r . \tag{5.55}
\end{equation*}
$$

This formula, that is a clear magnetic analog of Eq. (1.62) of electrostatics, is very popular among theoretical physicists, because it is very handy for the field theory manipulations. However, for many calculations it is more convenient to have a direct expression of energy via the magnetic field. Again, this may be done very similarly to what we have done in Sec. 1.3 for electrostatics, i.e. plugging into Eq. (55) the current density expressed from Eq. (35) to transform it as ${ }^{25}$

$$
\begin{equation*}
U=\frac{1}{2} \int \mathbf{j} \cdot \mathbf{A} d^{3} r=\frac{1}{2 \mu_{0}} \int \mathbf{A} \cdot(\nabla \times \mathbf{B}) d^{3} r=\frac{1}{2 \mu_{0}} \int \mathbf{B} \cdot(\nabla \times \mathbf{A}) d^{3} r-\frac{1}{2 \mu_{0}} \int \nabla \cdot(\mathbf{A} \times \mathbf{B}) d^{3} r . \tag{5.56}
\end{equation*}
$$

Now using the divergence theorem, the second integral may be transformed into a surface integral of product $(\mathbf{A} \times \mathbf{B})_{n}$. Equations (27)-(28) show that if the current distribution $\mathbf{j}(\mathbf{r})$ is localized, this product drops with distance $r$ faster than $1 / r^{2}$, so that if the integration volume is large enough, the surface

[^259]integral is negligible. In the remaining first integral, we may use Eq. (27) to recast $\nabla \times \mathbf{A}$ into the magnetic field. As a result, we get a very simple and fundamental formula.
\[

$$
\begin{equation*}
U=\frac{1}{2 \mu_{0}} \int B^{2} d^{3} r . \tag{5.57a}
\end{equation*}
$$

\]

Just as with the electric field, this expression may be interpreted as a volume integral of the magnetic energy density $u$ :

Magnetic field energy

$$
\begin{equation*}
U=\int u(\mathbf{r}) d^{3} r, \quad \text { with } u(\mathbf{r}) \equiv \frac{1}{2 \mu_{0}} \mathbf{B}^{2}(\mathbf{r}), \tag{5.57b}
\end{equation*}
$$

clearly similar to Eq. (1.67). ${ }^{26}$ Again, the conceptual choice between the spatial localization of magnetic energy - either at the location of electric currents only, as implied by Eqs. (54) and (55), or in all regions where the magnetic field exists, as apparent from Eq. (57b), cannot be done within the framework of magnetostatics, and only electrodynamics gives the decisive preference for the latter choice.

For the practically important case of currents flowing in several thin wires, Eq. (54) may be first integrated over the cross-section of each wire, just as was done at the derivation of Eq. (4). Again, since the integral of the current density over $k^{\text {th }}$ wire's cross-section is just the current $I_{k}$ in the wire, and cannot change along its length, it may be taken from the remaining integrals, giving

$$
\begin{equation*}
U=\frac{\mu_{0}}{4 \pi} \frac{1}{2} \sum_{k, k^{\prime}} I_{k} I_{k^{\prime}} \oint_{l_{k}} \oint_{l_{k^{\prime}}} \frac{d \mathbf{r}_{k} \cdot d \mathbf{r}_{k^{\prime}}}{\left|\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right|}, \tag{5.58}
\end{equation*}
$$

where $l$ is the full length of the wire loop. Note that Eq. (58) is valid if currents $I_{k}$ are independent of each other, because the double sum counts each current pair twice, compensating coefficient $1 / 2$ in front of the sum. It is useful to decompose this relation as

Mutual inductance coefficients

$$
\begin{equation*}
U=\frac{1}{2} \sum_{k, k^{\prime}} I_{k} I_{k^{\prime}} L_{k k^{\prime}} \tag{5.59}
\end{equation*}
$$

$$
\begin{equation*}
L_{k k^{\prime}} \equiv \frac{\mu_{0}}{4 \pi} \oint_{l_{k}} \oint_{l_{k^{\prime}}} \frac{d \mathbf{r}_{k} \cdot d \mathbf{r}_{k^{\prime}}}{\left|\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right|} \tag{5.60}
\end{equation*}
$$

Coefficient $L_{k k^{\prime}}$ in the quadratic form (59), with $k \neq k^{\prime}$, is called the mutual inductance between current loops $k$ and $k$, while the diagonal coefficient $L_{k} \equiv L_{k k}$ is called the self-inductance (or just inductance) of $k^{\text {th }}$ loop. ${ }^{27}$ From the symmetry of Eq. (60) with respect to the index swap, $k \leftrightarrow k^{\prime}$, it evident that the matrix of coefficients $L_{k k}$, is symmetric: ${ }^{28}$

[^260]\[

$$
\begin{equation*}
L_{k k^{\prime}}=L_{k^{\prime} k}, \tag{5.61}
\end{equation*}
$$

\]

so that for the practically important case of two interacting currents $I_{1}$ and $I_{2}$, Eq. (59) reads

$$
\begin{equation*}
U=\frac{1}{2} L_{1} I_{1}^{2}+M I_{1} I_{2}+\frac{1}{2} L_{2} I_{2}^{2}, \tag{5.62}
\end{equation*}
$$

where $M \equiv L_{12}=L_{21}$ is the mutual inductance coefficient.
These formulas clearly show the importance of self- and mutual inductances, so I will demonstrate their calculation for at least a few basic geometries. Before doing that, however, let me recast Eq. (58) into one more form that may facilitate such calculations. Namely, let us notice that for the magnetic field induced by current $I_{k}$ in a thin wire, Eq. (28) is reduced to

$$
\begin{equation*}
\mathbf{A}_{k}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} I_{k} \int_{l^{\prime}} \frac{d \mathbf{r}_{k}}{\left|\mathbf{r}-\mathbf{r}_{k}\right|} \tag{5.63}
\end{equation*}
$$

so that Eq. (58) may be rewritten as

$$
\begin{equation*}
U=\frac{1}{2} \sum_{k, k^{\prime}} I_{k} \oint_{l_{k}} \mathbf{A}_{k^{\prime}}\left(\mathbf{r}_{k}\right) \cdot d \mathbf{r}_{k^{\prime}} . \tag{5.64}
\end{equation*}
$$

But according to the same Stokes theorem that was used earlier in this chapter to derive the Ampère law, and Eq. (27), such integral is nothing more than the magnetic field flux (more frequently called just the magnetic flux) through a surface $S$ limited by the contour $l: 29$

$$
\begin{equation*}
\oint_{l} \mathbf{A}(\mathbf{r}) \cdot d \mathbf{r}=\int_{S}(\nabla \times A)_{n} d^{2} r=\int_{S} B_{n} d^{2} r \equiv \Phi . \tag{5.65}
\end{equation*}
$$

$$
\begin{equation*}
U=\frac{1}{2} \sum_{k, k^{\prime}} I_{k} \Phi_{k k^{\prime}} \tag{5.66}
\end{equation*}
$$

where $\Phi_{k k^{\prime}}$ is the flux of the field induced by $k^{\prime}$-th current through the loop of the $k$-th current. Comparing this expression with Eq. (59), we see that

$$
\begin{equation*}
\Phi_{k k^{\prime}} \equiv \int_{S_{k}}\left(\mathbf{B}_{k^{\prime}}\right)_{n} d^{2} r=L_{k k^{\prime}} I_{k^{\prime}}, \tag{5.67}
\end{equation*}
$$

This expression not only gives us one more means for calculating coefficients $L_{k k^{\prime}}$, but also shows their physical sense: the mutual inductance characterizes how much field (colloquially, "how many field lines") induced by current $I_{k^{\prime}}$ penetrate the loop of current $I_{k}$, and vice versa. Since due to the linear superposition principle, the total flux piercing $k$-th loop may be presented as

$$
\begin{equation*}
\Phi_{k} \equiv \sum_{k^{\prime}} \Phi_{k k^{\prime}}=\sum_{k^{\prime}} L_{k k^{\prime}} I_{k^{\prime}} . \tag{5.68}
\end{equation*}
$$

[^261]For example, for the system of two currents this expression is reduced to a clear analog of Eqs. (2.19):

$$
\begin{align*}
& \Phi_{1}=L_{1} I_{1}+M I_{2},  \tag{5.69}\\
& \Phi_{2}=M I_{1}+L_{2} I_{2} .
\end{align*}
$$

For the even simpler case of a single current,
$\Phi$ and $U$ of a
single current

$$
\begin{equation*}
\Phi=L I \tag{5.70}
\end{equation*}
$$

so that the magnetic energy of the current may be presented in several equivalent forms:

$$
\begin{equation*}
U=\frac{L}{2} I^{2}=\frac{1}{2} I \Phi=\frac{1}{2 L} \Phi^{2} \tag{5.71}
\end{equation*}
$$

These relations, similar to Eqs. (2.14)-(2.15) of electrostatics, show that the self-inductance $L$ of a current loop may be considered as a measure of system's magnetic energy at fixed current.

Now we are well equipped for the calculation of inductances, having three options. The first one is to use Eq. (60) directly. ${ }^{30}$ The second one is to calculate the magnetic field energy from Eq. (57) as the function of currents $I_{k}$ in the system, and then use Eq. (59) to find all coefficients $L_{k k^{\prime}}$. For example, for a system with just one current, Eq. (71) yields

$$
\begin{equation*}
L=\frac{U}{I^{2} / 2} . \tag{5.72}
\end{equation*}
$$

Finally, if the system consists of thin wires, so that the loop areas $S_{k}$ and hence fluxes $\Phi_{k k^{\prime}}$ are well defined, we may calculate them from Eq. (65), and then use Eq. (67) to find the inductances.

Actually, the first two options may have advantages over the third one even for such system of thin wires for whom the notion of magnetic flux is not quite clear. As an important example, let us find inductance of a long solenoid - see Fig. 6a. We have already calculated the magnetic field inside it - see Eq. (40) - so that, due to the field uniformity, the magnetic flux piercing each wire turn is just

$$
\begin{equation*}
\Phi_{1}=B A=\mu_{0} n I A \tag{5.73}
\end{equation*}
$$

where $A$ is the area of solenoid's cross-section - for example $\pi R^{2}$ for a round solenoid, though Eq. (40) is more general. Comparing Eqs. (73) and (67), one might wrongly conclude that $L=\Phi_{1} / I=\mu_{0} n A$ [WRONG!], i.e. that the solenoid's inductance is independent on its length. Actually, the magnetic flux $\Phi_{1}$ pierces each wire turn, so that the total flux through the whole current loop, consisting of $N$ turns, is

$$
\begin{equation*}
\Phi=N \Phi_{1}=\mu_{0} n^{2} l A I, \tag{5.74}
\end{equation*}
$$

and the correct expression for solenoid's inductance is

$$
\begin{equation*}
L=\frac{\Phi}{I}=\mu_{0} n^{2} l A \tag{5.75}
\end{equation*}
$$

i.e. the inductance per unit length is constant: $L / l=\mu_{0} n^{2} A$. Since this reasoning may seem a bit flimsy, it is prudent to verify it by using Eq. (72) to calculate the full magnetic energy inside the solenoid (neglecting minor fringe and external field contributions):

[^262]\[

$$
\begin{equation*}
U=\frac{1}{2 \mu_{0}} B^{2} A l=\frac{1}{2 \mu_{0}}\left(\mu_{0} n I\right)^{2} A l=\mu_{0} n^{2} l A \frac{I^{2}}{2} . \tag{5.76}
\end{equation*}
$$

\]

Plugging this result into Eq. (72) immediately confirms result (75).
The use of the first two options for inductance calculation becomes inevitable for continuously distributed currents. As an example, let us calculate self-inductance $L$ of a long coaxial cable with the cross-section shown in the Fig. 7. ${ }^{31}$


Fig. 5.7. Cross-section of a coaxial cable.

Let us assume that the current is uniformly distributed over the cross-sections of both conductors. (As we know from the previous chapter, such distribution indeed takes place if both the internal and external conductors are made of a uniform resistive material.) First, we should calculate the radial distribution of the magnetic field (that of course has only one, azimuthal component, because of the axial symmetry of the problem). This distribution may be immediately found from the application of the Ampère law to circles of radii $\rho$ within four different ranges:

$$
2 \pi \rho B=\left.\mu_{0} I\right|_{\text {piercing the circle area }}=\mu_{0} I \times\left\{\begin{array}{cc}
\frac{\rho^{2}}{a^{2}}, & \text { for } \rho<a  \tag{5.77}\\
1, & \text { for } a<\rho<b, \\
\frac{c^{2}-\rho^{2}}{c^{2}-b^{2}}, & \text { for } b<\rho<c \\
0, & \text { for } c<\rho
\end{array}\right.
$$

Now, an elementary integration yields the magnetic energy per unit length of the cable:

$$
\begin{align*}
\frac{U}{l} & =\frac{1}{2 \mu_{0}} \int B^{2} d^{2} r=\frac{\pi}{\mu_{0}} \int_{0}^{\infty} B^{2} \rho d \rho=\frac{\mu_{0} I^{2}}{4 \pi}\left[\int_{0}^{a}\left(\frac{\rho}{a^{2}}\right)^{2} \rho d \rho+\int_{a}^{b}\left(\frac{1}{\rho}\right)^{2} \rho d \rho+\int_{b}^{c}\left(\frac{c^{2}-\rho^{2}}{\rho\left(c^{2}-b^{2}\right)}\right)^{2} \rho d \rho\right]  \tag{5.78}\\
& =\frac{\mu_{0}}{2 \pi}\left[\ln \frac{b}{a}+\frac{c^{2}}{c^{2}-b^{2}}\left(\frac{c^{2}}{c^{2}-b^{2}} \ln \frac{c}{b}-\frac{1}{2}\right)\right] \frac{I^{2}}{2}
\end{align*}
$$

From here, and Eq. (72), we get the final answer:

$$
\begin{equation*}
\frac{L}{l}=\frac{\mu_{0}}{2 \pi}\left[\ln \frac{b}{a}+\frac{c^{2}}{c^{2}-b^{2}}\left(\frac{c^{2}}{c^{2}-b^{2}} \ln \frac{c}{b}-\frac{1}{2}\right)\right] . \tag{5.79}
\end{equation*}
$$

[^263]Note that for the particular case of a thin outer conductor, $c-b \ll b$, this expression reduces to

$$
\begin{equation*}
\frac{L}{l} \approx \frac{\mu_{0}}{2 \pi}\left(\ln \frac{b}{a}+\frac{1}{4}\right), \tag{5.80}
\end{equation*}
$$

where the first term in the parentheses may be traced back to the contribution of the magnetic field energy in the free space between the conductors. This distinction is important for some applications, because in superconductor cables, as well as resistive-metal cables as high frequencies (to be discussed in the next chapter), the field does not penetrate the conductor bulk, so that Eq. (80) is valid without the last term, $1 / 4$, in the parentheses, which is due to the magnetic field energy inside the wire.

As the last example, let us calculate the mutual inductance between a long straight wire and a round wire loop adjacent to it (Fig. 8), neglecting the thickness of both wires.


Fig. 5.8. Study case for the mutual inductance calculation.

Here there is no problem with using the last formalism, based on the magnetic flux calculation. Indeed, in the Cartesian coordinates shown in Fig. 8, Eq. (20) reads $B_{1}=\mu_{0} I_{1} / 2 \pi y$, giving the following magnetic flux through the round wire loop:

$$
\begin{equation*}
\Phi_{21}=\frac{\mu_{0} I_{1}}{2 \pi} \int_{-R}^{+R} d x \int_{R-\left(R^{2}-x^{2}\right)^{1 / 2}}^{R+\left(R^{2}-x^{2}\right)^{1 / 2}} d y \frac{1}{y}=\frac{\mu_{0} I_{1}}{\pi} \int_{0}^{R} \ln \frac{R+\left(R^{2}-x^{2}\right)^{1 / 2}}{R-\left(R^{2}-x^{2}\right)^{1 / 2}} d x=\frac{\mu_{0} I_{1} R}{\pi} \int_{0}^{1} \ln \frac{1+\left(1-\xi^{2}\right)^{1 / 2}}{1+\left(1-\xi^{2}\right)^{1 / 2}} d \xi \tag{5.81}
\end{equation*}
$$

This is a table integral equal to $\pi,{ }^{32}$ so that $\Phi_{21}=\mu_{0} I_{1} R$, and the final answer for the mutual inductance $M=L_{12}=L_{21}=\Phi_{21} / I_{1}$ is finite (and very simple):

$$
\begin{equation*}
M=\mu_{0} R, \tag{5.82}
\end{equation*}
$$

despite magnetic field's divergence at the lowest point of the loop $(y=0)$. Note that in contrast with the finite mutual inductance of this system, self-inductances of both wires are formally infinite in the thinwire limit - see, e.g., Eq. (80), that in the limit $b / a \gg 1$ describes a thin straight wire. However, since this divergence is very weak (logarithmic), it is quenched by any deviation from this perfect geometry. For example, a good estimate of the inductance of a wire of a large but finite length $l$ may be obtained from Eq. (81) via the replacement of $b$ with $l$ :

$$
\begin{equation*}
L \sim \frac{\mu_{0}}{2 \pi} l \ln \frac{l}{a} . \tag{5.83}
\end{equation*}
$$

[^264](Note, however, that the exact result depends on where from/to the current flows beyond that segment. ) A close estimate, with $l$ replaced with $2 \pi R$, and $b$ replaced with $R$, is valid for the self-inductance of the round loop. A more exact calculation of this inductance, which would be asymptotically correct in the limit $a \ll R$, is a very useful exercise, which is highly recommended to the reader. ${ }^{33}$

### 5.4. Magnetic dipole moment, and magnetic dipole media

The most natural way of description of magnetic media parallels that described in Chapter 3 for dielectrics, and is based on properties of magnetic dipoles. To introduce this notion quantitatively, let us consider, just as in Sec. 3.1, a spatially-localized system with current distribution $\mathbf{j}(\mathbf{r})$, whose magnetic field is measured at relatively large distances $r \gg r^{\prime}$ (Fig. 9).


Applying the truncated Taylor expansion (3.4) to definition (28) of the vector potential, we get

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}) \approx \frac{\mu_{0}}{4 \pi}\left[\frac{1}{r} \int_{V} \mathbf{j}\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime}+\frac{1}{r^{3}} \int_{V}\left(\mathbf{r} \cdot \mathbf{r}^{\prime}\right) \mathbf{j}\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime}\right] . \tag{5.84}
\end{equation*}
$$

Due to the vector character of this potential, we have to depart slightly from the approach of Sec. 3.1 and use the following vector algebra identity: ${ }^{34}$

$$
\begin{equation*}
\int_{V}[f(\mathbf{j} \cdot \nabla g)+g(\mathbf{j} \cdot \nabla f)] d^{3} r=0 \tag{5.85}
\end{equation*}
$$

that is valid for any pair of smooth (differentiable) scalar functions $f(\mathbf{r})$ and $g(\mathbf{r})$, and any vector function $\mathbf{j}(\mathbf{r})$ that, as the de current density, satisfies the continuity condition $\nabla \cdot \mathbf{j}=0$ and whose normal component vanishes on its surface.

First, let us use Eq. (85) with $f \equiv 1$ and $g$ equal to any component of the radius-vector $\mathbf{r}: g=r_{i}(i$ $=1,2,3)$. Then it yields

$$
\begin{equation*}
\int_{V}\left(\mathbf{j} \cdot \mathbf{n}_{i}\right) d^{3} r=\int_{V} j_{i} d^{3} r=0, \tag{5.86}
\end{equation*}
$$

so that for the vector as the whole

[^265]\[

$$
\begin{equation*}
\int_{V} \mathbf{j}(\mathbf{r}) d^{3} r=0 \tag{5.87}
\end{equation*}
$$

\]

showing that the first term in the right-hand part of Eq. (84) equals zero. Next, let us use Eq. (85) with $f$ $=r_{i}, g=r_{i^{\prime}}\left(i, i^{\prime}=1,2,3\right)$; then it yields

$$
\begin{equation*}
\int_{V}\left(r_{i} j_{i^{\prime}}+r_{i^{\prime}} j_{i}\right) d^{3} r=0, \tag{5.88}
\end{equation*}
$$

so that the $i^{\text {th }}$ Cartesian component of the second integral in Eq. (84) may be transformed as

$$
\begin{align*}
\int_{V}\left(\mathbf{r} \cdot \mathbf{r}^{\prime}\right) j_{i} d^{3} r^{\prime} & =\int_{V} \sum_{i^{\prime}=1}^{3} r_{i^{\prime}} r_{i^{\prime}}^{\prime} j_{i} d^{3} r^{\prime}=\frac{1}{2} \sum_{i^{\prime}=1}^{3} r_{i^{\prime}} \int_{V}\left(r_{i^{\prime}}^{\prime} j_{i}+r_{i^{\prime}}^{\prime} j_{i}\right) d^{3} r^{\prime} \\
& =\frac{1}{2} \sum_{i^{\prime}=1}^{3} r_{i^{\prime}} \int_{V}\left(r_{i^{\prime}}^{\prime} j_{i}-r_{i^{\prime}}^{\prime} j_{i^{\prime}}\right) d^{3} r^{\prime}=-\frac{1}{2}\left[\mathbf{r} \times \int_{V}\left(\mathbf{r}^{\prime} \times \mathbf{j}\right) d^{3} r^{\prime}\right]_{i} . \tag{5.89}
\end{align*}
$$

As a result, Eq. (85) may be rewritten as

$$
\begin{equation*}
\mathbf{A}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \frac{\mathbf{m} \times \mathbf{r}}{r^{3}}, \tag{5.90}
\end{equation*}
$$

Magnetic dipole and its potential
where vector $\mathbf{m}$, defined as ${ }^{35}$

$$
\begin{equation*}
\mathbf{m} \equiv \frac{1}{2} \int_{V} \mathbf{r} \times \mathbf{j}(\mathbf{r}) d^{3} r, \tag{5.91}
\end{equation*}
$$

is called the magnetic dipole moment of our system - that itself, within approximation (90), is called the magnetic dipole.

Note a close analogy between $\mathbf{m}$ and the angular momentum of a non-relativistic particle with mass $m_{k}$ :

$$
\begin{equation*}
\mathbf{L}_{k} \equiv \mathbf{r}_{k} \times \mathbf{p}_{k}=\mathbf{r}_{k} \times m_{k} \mathbf{v}_{k}, \tag{5.92}
\end{equation*}
$$

where $\mathbf{p}_{k}=m_{k} \mathbf{v}_{k}$ is its mechanical momentum. Indeed, for a continuum of such particles with the same electric charge $q$, with the spatial density $n, \mathbf{j}=q n \mathbf{v}$, and Eq. (91) yields

$$
\begin{equation*}
\mathbf{m}=\int_{V} \frac{1}{2} \mathbf{r} \times \mathbf{j} d^{3} r=\int_{V} \frac{n q}{2} \mathbf{r} \times \mathbf{v} d^{3} r \tag{5.93}
\end{equation*}
$$

while the total angular momentum of such continuous system of particles of the same mass $\left(m_{k}=m_{0}\right)$ is

$$
\mathbf{L}=\int_{V} n m_{0} \mathbf{r} \times \mathbf{v} d^{3} r
$$

so that we get a very straightforward relation
m vs. L

$$
\begin{equation*}
\mathbf{m}=\frac{q}{2 m_{0}} \mathbf{L} \tag{5.95}
\end{equation*}
$$

[^266]For the orbital motion, this classical relation survives in quantum mechanics for operators and hence for eigenvalues, in whom the angular momentum is quantized in the units of the Planck's constant $\hbar$, so that for an electron, the orbital magnetic moment is always a multiple of the so-called Bohr magneton

$$
\begin{equation*}
\mu_{\mathrm{B}} \equiv \frac{e \hbar}{2 m_{e}} \tag{5.96}
\end{equation*}
$$

where $m_{e}$ is the free electron mass. ${ }^{36}$ However, for particles with spin, such a universal relation between vectors $\mathbf{m}$ and $\mathbf{L}$ is no longer valid. For example, electron's spin $s=1 / 2$ gives contribution $\hbar / 2$ to the mechanical momentum, but its contribution to the magnetic moment it still very close to $\mu_{\mathrm{B}} .{ }^{37}$

The next important example of a magnetic dipole is a planar wire loop limiting area $A$ (of an arbitrary shape), carrying current $I$, for which $\mathbf{m}$ has a surprisingly simple form,

$$
\begin{equation*}
\mathbf{m}=I \mathbf{A}, \tag{5.97}
\end{equation*}
$$

where the modulus of vector A equals area $A$, and its direction is perpendicular to loop's plane. This formula may be readily proved by noticing that if we select the coordinate origin on the plane of the loop (Fig. 10), then the elementary component of the magnitude of integral (91),

$$
\begin{equation*}
d m=\frac{1}{2}\left|\oint_{C} \mathbf{r} \times I d \mathbf{r}\right|=I \oint_{C}\left|\frac{1}{2} \mathbf{r} \times d \mathbf{r}\right|=I \oint_{C} \frac{1}{2} r^{2} d \varphi, \tag{5.98}
\end{equation*}
$$

is just the elementary area $d A=(1 / 2) r d(r \varphi) \equiv r^{2} d \varphi / 2$.


Fig. 5.10. Calculating the magnetic dipole moment of a planar current loop.

The combination of Eqs. (96) and (97) allows a useful estimate of the scale of atomic currents, by finding what current $I$ should flow in a circular loop of atomic size scale (the Bohr radius) $r_{\mathrm{B}} \approx$ $0.5 \times 10^{-10} \mathrm{~m}$, i.e. of area $A \approx 10^{-20} \mathrm{~m}^{2}$, to produce a magnetic moment equal to $\mu_{\mathrm{B}} .{ }^{38}$ The result is surprisingly macroscopic: $I \sim 1 \mathrm{~mA}$ (quite comparable to the currents driving your earbuds :-). Though this estimate should not be taken too literally, due to the quantum-mechanical spread of electron's wavefunctions, it is very useful for getting a feeling how significant the atomic magnetism is and hence why ferromagnets may provide such a strong field.

[^267]After these illustrations, let us return to Eq. (90). Plugging it into the general formula (27), we may calculate the magnetic field of a magnetic dipole:

Magnetic dipole in external field

$$
\begin{equation*}
\mathbf{B}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \frac{3 \mathbf{r}(\mathbf{r} \cdot \mathbf{m})-\mathbf{m} r^{2}}{r^{5}} \tag{5.99}
\end{equation*}
$$

The structure of this formula exactly duplicates that of Eq. (3.15) for the electric dipole field. Because of this similarity, the energy of a dipole in an external field, and hence the torque and force exerted on it by the field, are also absolutely similar to the expressions for an electric dipole - see Eqs. (3.15)-(3.18):

$$
\begin{equation*}
U=-\mathbf{m} \cdot \mathbf{B}_{\mathrm{ext}}, \tag{5.100}
\end{equation*}
$$

and as a result,

$$
\begin{gather*}
\boldsymbol{\tau}=\mathbf{m} \times \mathbf{B}_{\mathrm{ext}},  \tag{5.101}\\
\mathbf{F}=\nabla\left(\mathbf{m} \cdot \mathbf{B}_{\mathrm{ext}}\right) . \tag{5.102}
\end{gather*}
$$

Now let us consider a system of many magnetic dipoles (e.g., atoms or molecules), distributed in space with density $n$. Then we can use Eq. (90) (generalized in the evident way for an arbitrary position, $\mathbf{r}$ ', of a dipole), and the linear superposition principle, to calculate the "macroscopic" component of the vector-potential A - in other words, dipole's potential averaged over short-scale variations on the interdipole distances:

$$
\begin{equation*}
\mathbf{A}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \int \frac{\mathbf{M}\left(\mathbf{r}^{\prime}\right) \times\left(\mathbf{r}-\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|^{3}} d^{3} r^{\prime} \tag{5.103}
\end{equation*}
$$

where $\mathbf{M} \equiv n \mathbf{m}$ is the macroscopic (average) magnetization, i.e. the magnetic moment per unit volume. Transforming this integral absolutely similarly to how Eq. (3.27) had been transformed into Eq. (3.29), we get:

$$
\begin{equation*}
\mathbf{A}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \int \frac{\nabla^{\prime} \times \mathbf{M}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} \tag{5.104}
\end{equation*}
$$

Comparing this result with Eq. (28), we see that $\nabla \times \mathbf{M}$ is equivalent, in its effect, to the density $\mathbf{j}_{\text {ef }}$ of a certain effective "magnetization current". Just as the electric-polarization "charge" $\rho_{\text {ef }}$ discussed in Sec. 3.2 (see Fig. 3.3), $\mathbf{j}_{\text {ef }}=\nabla \times \mathbf{M}$ may be interpreted the uncompensated part of vortex currents representing single magnetic dipoles (Fig. 11).


Fig. 5.11. Cartoon illustrating the physical nature of the "magnetization current" $\mathbf{j}_{\text {ef }}=\nabla \times \mathbf{M}$.

Now, using Eq. (28) to add the possible contribution from "stand-alone" currents j, not included into the currents of microscopic dipoles, we get the general equation for the vector-potential of the macroscopic field:

$$
\begin{equation*}
\mathbf{A}(\mathbf{r})=\frac{\mu_{0}}{4 \pi} \int \frac{\left[\mathbf{j}\left(\mathbf{r}^{\prime}\right)+\nabla^{\prime} \times \mathbf{M}\left(\mathbf{r}^{\prime}\right)\right]}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} d^{3} r^{\prime} . \tag{5.105}
\end{equation*}
$$

Repeating the calculations that have led us from Eq. (28) to the Maxwell equation (35), with the account of the magnetization current term, for the macroscopic magnetic field $\mathbf{B}$ we get ${ }^{39}$

$$
\begin{equation*}
\nabla \times \mathbf{B}=\mu_{0}(\mathbf{j}+\nabla \times \mathbf{M}) \tag{5.106}
\end{equation*}
$$

Following the same philosophy as in Sec. 3.2, we may recast this equation as

$$
\begin{equation*}
\nabla \times \mathbf{H}=\mathbf{j} \tag{5.107}
\end{equation*}
$$

where a new field defined as

$$
\begin{equation*}
\mathbf{H} \equiv \frac{\mathbf{B}}{\mu_{0}}-\mathbf{M}, \tag{5.108}
\end{equation*}
$$

by historic reasons (and very unfortunately) is also called the magnetic field. ${ }^{40}$ It is crucial to remember that the physical sense of field $\mathbf{H}$ is very much different from field $\mathbf{B}$. In order to understand the difference better, let us use Eq. (107) to complete a macroscopic analog of system (36), called the macroscopic Maxwell equations (again, so far for the stationary case $\partial / \partial t=0$ ):

$$
\begin{array}{ll}
\nabla \times \mathbf{E}=0, & \nabla \times \mathbf{H}=\mathbf{j}  \tag{5.109}\\
\nabla \cdot \mathbf{D}=\rho, & \nabla \cdot \mathbf{B}=0 .
\end{array}
$$

One can clearly see that the roles of vector fields $\mathbf{D}$ and $\mathbf{H}$ are very similar: they could be called "wouldbe" fields - which would be induced by stand-alone charges and currents, if the media had not modified them by its dielectric and/or magnetic polarization.

[^268]Despite this similarity, let me note an important difference of signs in the relation (3.33) between $\mathbf{E}, \mathbf{D}$, and $\mathbf{P}$, on one hand, and relation (108) between $\mathbf{B}, \mathbf{H}$, and $\mathbf{M}$, on the other hand. It is not just the matter of definition. Indeed, due to the similarity of Eqs. (3.15), and (100), including similar signs, the electric and magnetic fields both try to orient the corresponding dipole moments along the field. Hence, in the media that allow such orientation (and as we will see momentarily, for magnetic media it is not always the case), the induced polarizations $\mathbf{P}$ and $\mathbf{M}$ are directed along, respectively, vectors $\mathbf{E}$ and $\mathbf{B}$. According to Eq. (3.33), if the would-be field $\mathbf{D}$ is fixed - say, by a fixed stand-alone charge distribution $\rho(\mathbf{r})$ - such polarization reduces the genuine average electric field $\mathbf{E}=(\mathbf{D}-\mathbf{P}) / \varepsilon_{0}$. On the other hand, Eq. (108) shows that in a magnetic media with a fixed would-be field $\mathbf{H}$, magnetic polarization with $\mathbf{M} \Uparrow \mathbf{B}$ enhances the average magnetic field $\mathbf{B}=\mu_{0}(\mathbf{H}+\mathbf{M})$. This difference may be traced back to the sign difference in the initial relations (1.1) and (5.1), i.e. to the basic fact that charges of the same sign repulse, while currents of the same direction attract each other.

In order to form a complete system of differential equations, the macroscopic Maxwell equations (109) have to be complemented with "constitutive relations" $\mathbf{D} \leftrightarrow \mathbf{E}, \mathbf{j} \leftrightarrow \mathbf{E}$, and $\mathbf{B} \leftrightarrow \mathbf{H}$. In previous two chapters we already discussed, in brief, two of them; let us proceed to the last one.

### 5.5. Magnetic materials

A major difference between the dielectric and magnetic material equations $\mathbf{D}(\mathbf{E})$ and $\mathbf{B}(\mathbf{H})$ is that while a typical dielectric media reduces the external electric field, magnetic media may either reduce or enhance it. In order to quantify this fact, let us consider the so-called linear magnetics in which $\mathbf{M}$ (and hence $\mathbf{H}$ ) are proportional to $\mathbf{B}$. Just as in dielectrics, in material without spontaneous magnetization, such linearity at relatively low fields follows from the Taylor expansion of function $\mathbf{M}(\mathbf{B})$. For isotropic materials, this proportionality is characterized by a scalar - either the magnetic permeability $\mu$, defined by the following relation:

Magnetic permeability

$$
\begin{equation*}
\mathbf{B} \equiv \mu \mathbf{H} \tag{5.110}
\end{equation*}
$$

or the magnetic susceptibility ${ }^{41}$ defined as

Magnetic
susceptibility susceptibility

$$
\begin{equation*}
\mathbf{M}=\chi_{m} \mathbf{H} \tag{5.111}
\end{equation*}
$$

Plugging these relations into Eq. (108), we see that these two parameters are not independent, but are related as

$$
\begin{equation*}
\mu=\left(1+\chi_{m}\right) \mu_{0} . \tag{5.112}
\end{equation*}
$$

Note that despite the superficial similarity between Eqs. (110)-(111) and relations (3.35)-(3.38) for linear dielectrics:

[^269]\[

$$
\begin{equation*}
\mathbf{D}=\varepsilon \mathbf{E}, \quad \mathbf{P}=\chi_{e} \varepsilon_{0} \mathbf{E}, \quad \varepsilon=\left(1+\chi_{e}\right) \varepsilon_{0}, \tag{5.113}
\end{equation*}
$$

\]

there is an important conceptual difference between them. Namely, while vector $\mathbf{E}$ in the right-hand parts of Eqs. (113) is the real (average) electric field, vector $\mathbf{H}$ in the right-hand part of Eqs. (110)-(111) represents a "would-be" magnetic field, in all aspects similar to vector $\mathbf{D}$ rather than $\mathbf{E}$. For relatively dense media, whose polarization may affect the genuine fields substantially, this difference between parameters $\varepsilon$ and $\mu$ may make their properties (e.g., the Kramers-Kronig relations, to be discussed in Sec. 7.3) rather different.

Another difference between parameters $\varepsilon$ and $\mu$ (and hence between $\chi_{e}$ and $\chi_{m}$ ) is evident from Table 1 which lists the values of magnetic susceptibility for several materials. It shows that in contrast to linear dielectrics whose susceptibility $\chi_{e}$ is always positive, i.e. the dielectric constant $\varepsilon_{r}=\chi_{e}+1$ is always larger than 1 (see Table 3.1), linear magnetics may be either paramagnets ( $\chi_{m}>0$, i. e. $\mu>\mu_{0}$ ) or diamagnets ( $\chi_{m}<0, \mu<\mu_{0}$ ).

Table 5.1. Magnetic susceptibility $\left(\chi_{m}\right)_{\mathrm{SI}}$ of a few representative (and/or important) materials ${ }^{(\mathrm{a})}$

| "Mu-metal" (75\% Ni + 15\% Fe + a few \%\% of Cu and Mo) | $\sim 20,000^{(\mathrm{b})}$ |
| :---: | :---: |
| Permalloy ( $80 \% \mathrm{Ni}+20 \% \mathrm{Fe}$ ) | $\sim 8,000^{(\mathrm{b})}$ |
| "Soft" (or "transformer") steel (Fe +a few $\% \%$ of Si) | $\sim 4,000^{\text {(b) }}$ |
| Nickel | $\sim 100$ |
| Aluminum | $+2 \times 10^{-5}$ |
| Diamond | $-2 \times 10^{-5}$ |
| Copper | $-7 \times 10^{-5}$ |
| Water | $-9 \times 10^{-6}$ |
| Bismuth (the strongest non-superconducting diamagnet) | $-1.7 \times 10^{-4}$ |

${ }^{(2)}$ The table does not include bulk superconductors, which in a crude ("macroscopic") approximation may be described as perfect diamagnets (with $\mathbf{B}=0$, i.e. $\chi_{m}=-1$ and $\mu=0$ ), though the actual physics of this phenomenon is more complex - see Sec. 6.3 below.
${ }^{(b)}$ The exact values of $\chi_{m}$ for soft ferromagnetic materials depend not only on their exact composition, but also on their thermal processing ("annealing"). Moreover, due to unintentional vibrations, the extremely high $\chi_{m}$ of such materials may somewhat decay with time, though may be restored to approach the original value by new annealing.

The reason of this difference is that in dielectrics, two different polarization mechanisms (schematically illustrated by Fig. 12) lead to the same sign of the average polarization. The first of them takes place in atoms without their own spontaneous polarization. A crude classical image of such an atom is an isotropic cloud of negatively charged electrons surrounding a positively charged nucleus - see Fig. 12a. The external electric field shifts the positive charge in the direction of $\mathbf{E}$, and negative charges in the opposite direction, thus creating a dipole with aligned vectors $\mathbf{p}$ and $\mathbf{E}$, and hence positive
polarizability $\alpha_{\text {mol }}$ - see Eq. (3.39). As a result, the electric susceptibility is also positive - see Eqs. (3.41) or (3.71).

In the second case (Fig. 12b) of a gas or liquid consisting of polar molecules, each molecule has its own, spontaneous dipole moment $\mathbf{p}_{0}$ even in the absence of external electric field. (A typical example is a water molecule $\mathrm{H}_{2} \mathrm{O}$, with the positive oxygen ion positioned out of the line connecting two positive hydrogen atoms, thus producing a spontaneous dipole with moment's magnitude $p_{0} \approx e \times 0.38 \times 10^{-10} \mathrm{~m}$.) However, in the absence of the applied electric field, the orientation of such dipoles is random, so that the average polarization $\mathbf{P}=n\left\langle\mathbf{p}_{0}\right\rangle$ equals zero. A weak applied field does not change the magnitude of the dipole moments significantly, but creates their preferential orientation along the field (in order to decrease the potential energy $U=-\mathbf{p}_{0} \cdot \mathbf{E}$ ), thus creating a nonvanishing vector average $\left\langle\mathbf{p}_{0}\right\rangle$ directed along E. If the applied field is not two high $\left(p_{0} E \ll k_{\mathrm{B}} T\right)$, the induced polarization $\mathbf{P}=n\left\langle\mathbf{p}_{0}\right\rangle$ is proportional to $\mathbf{E}$, again giving a positive polarizability $\alpha_{\mathrm{mol}}{ }^{42}$


Fig. 5.12. Cartoons of two types of induced electrical polarization: (a) elementary dipole induction and (b) partial ordering of spontaneous elementary dipoles.

Returning to magnetics, the second of the above mechanisms, i.e. the ordering of spontaneous dipoles by the applied field, is responsible for the paramagnetism. Again, now according to Eq. (100), such field tends to align the dipoles along its direction, so that the average direction of spontaneous elementary moments $\mathbf{m}_{0}$, and hence the direction of $\mathbf{M}$, is the same as that of the average field $\mathbf{B}$ (i.e., for a diluted media, of $\mathbf{H} \approx \mathbf{B} / \mu_{0}$ ), resulting in a positive susceptibility $\chi_{m}$. However, in contrast to the electric polarization, there is a mechanism of magnetic polarization, called the orbital (or "Larmor"43) diamagnetism, which gives $\chi_{m}<0$. As its simplest model, let us consider the orbital motion of an atomic electron as classical particle of mass $m_{0}$, with electric charge $q$, about an immobile attractive center - modeling the atomic nucleus. As classical mechanics tells us, the central attractive force does

[^270]not change particle's angular momentum $\mathbf{L} \equiv m_{0} \mathbf{r} \times \mathbf{v}$, but the applied magnetic field $\mathbf{B}$ (that may be taken uniform on the atomic scale) does, due to the torque (101) it applies to magnetic moment (95):
\[

$$
\begin{equation*}
\frac{d \mathbf{L}}{d t}=\boldsymbol{\tau}=\mathbf{m} \times \mathbf{B}=\frac{q}{2 m_{0}} \mathbf{L} \times \mathbf{B} . \tag{5.114}
\end{equation*}
$$

\]

The vector diagram in Fig. 13 shows that in the limit of relatively weak field, when the magnitude of the angular momentum $\mathbf{L}$ may be considered constant, this equation describes the rotation (called the torque-induced precession ${ }^{44}$ ) of vector $\mathbf{L}$ about the direction of vector $\mathbf{B}$, with angular frequency $\boldsymbol{\Omega}=-q \mathbf{B} / 2 m_{0}$, independent on angle $\theta$. Let me leave for the reader to use Eq. (114) for checking that, irrespectively the sign of charge $q$, the resulting additional magnetic moment $\Delta \mathbf{m}$ has a direction opposite to that of vector $\mathbf{B}$, and hence $\chi_{m}$ is negative, leading to the Larmor diamagnetism. ${ }^{45}$


Fig. 5.13. Torque-induced precession of a charged particle in a magnetic field.

An important conceptual question is what exactly prevents the initial magnetic moment $\mathbf{m}$ that, according to Eq. (95), is associated with the angular momentum $\mathbf{L}$ of the electron, from turning along the magnetic field, just as in the second polarization mechanism illustrated by Fig. 12b - thus decreasing the potential energy (100) of the system. The answer is the same as for the usual mechanical top - it "wants" to fall due to the gravity field, but cannot do that due to the mechanical inertia. In classical physics, even a small friction (dissipation) eventually drains top's rotational kinetic energy, and it falls. However, in quantum mechanics the ground-state "motion" of electrons in an atom is not subjected to friction, because they cannot be brought to full rest due to Heisenberg's uncertainty principle. Somewhat counter-intuitively, the magnetic moments due to such fully-quantum effect as spin are much more susceptible to interaction with environment, so that in atoms with uncompensated spins, the magnetic dipole orientation mechanism prevails over the orbital diamagnetism, and the materials incorporating such atoms usually exhibit net paramagnetism - see Table 1.

Due to possible strong interactions between elementary dipoles, magnetism of materials is an extremely rich field of physics, with numerous interesting phenomena and elaborated theories.

[^271]Unfortunately, all this physics is well outside the framework of this course, and I have to refer the interested reader to special literature, ${ }^{46}$ but still need to mention its key notions.

Most importantly, a sufficiently strong dipole-dipole interaction may lead to their spontaneous ordering, even in the absence of the applied field. This ordering may correspond to either parallel alignment of the atomic dipoles (ferromagnetism) or anti-parallel alignment of the adjacent dipoles (antiferromagnetism). Evidently, the external effects of ferromagnetism are stronger, because such phase corresponds to a substantial spontaneous magnetization $\mathbf{M}$. (This value is frequently called the saturation magnetization, $\mathbf{M}_{s}$, while the corresponding magnitude of $\mathbf{B}=\mu_{0} \mathbf{M}$ is called either the saturation magnetic field, or the remanence field, $\mathbf{B}_{R}$ ). The direction of $\mathbf{B}_{R}$ may switched by the application an external magnetic field, with a magnitude above certain value $H_{C}$ called coercivity, ${ }^{47}$ leading to the well-known hysteretic loops on the $[B, H]$ plane - see Fig. 14 for a typical example.


Fig. 5.14. Experimental magnetization curves of specially processed (cold-rolled) transformer steel, i.e. a solid solution of $\sim 10 \% \mathrm{C}$ and $\sim 6 \% \mathrm{Si}$ in Fe. (Adapted from www.thefullwiki.org/Hysteresis.)

In relatively low fields, $H \ll H_{C}$, such materials may be described as hard (or "permanent") ferromagnets; at such approximate treatment, magnetization $\mathbf{M}$ is considered constant. On the other hand, the theory needed for a fair description phenomena at $H \sim H_{C}$ is rather complicated. Indeed, the direction of magnetization of crystals may be affected by the anisotropy of the crystal lattice. Because of that, typical non-crystalline ferromagnetic materials (like steel, permalloy, "mu-metal", etc.) consist of randomly oriented magnetic domains, each with certain spontaneous magnetization direction. The magnetic interaction of the domain with its neighbors and the external field determines the evolution of its magnetization and hence the average magnetic properties of the ferromagnet. In particular, such interaction explains why the hysteresis loop shape is dependent on the cycled field amplitude and cycling history - see Fig. 14. A very important class of multi-domain materials is the so-called soft ferromagnets, whose coercivity is relatively low. At low cycled field amplitude, the soft ferromagnets behave, on the average, as linear magnetics with very high values of $\chi_{m}$ and hence $\mu$ (see the top rows of Table 1, and Fig. 14) that are highly dependent on the material's fabrication technology and its postfabrication thermal and mechanical treatments.

[^272]High values of $\chi_{m}$ are is also pertinent to magnetics in which the molecular dipole interaction is relatively weak, so that their ferromagnetic ordering may be destroyed by thermal fluctuations, if temperature is increased above the so-called Curie temperature $T_{\mathrm{C}}$. At $T>T_{\mathrm{C}}$, such materials behave as paramagnets, with susceptibility obeying the Curie-Weiss law

$$
\begin{equation*}
\chi_{m} \propto \frac{1}{T-T_{\mathrm{C}}} . \tag{5.115}
\end{equation*}
$$

(At vanishing moment interaction, $T_{\mathrm{C}} \rightarrow 0$, and Eq. (115) is reduced to the Curie law $\chi_{m} \propto 1 / T$ typical for weak paramagnets.) The transition between the ferromagnetic and paramagnetic phase at $T=T_{\mathrm{C}}$ is the classical example of continuous phase transitions, similar to that between the paraelectric and ferroelectric phases of a dielectric. In both cases, the "macroscopic" (average) polarization - either $\mathbf{M}$ or $\mathbf{P}$ - plays the role of the so-called order parameter that (in the absence of external fields) appears at $T=$ $T_{\mathrm{C}}$ and increases gradually at the further reduction of temperature. ${ }^{48}$

Before returning to magnetostatics per se, I have to mention the large practical role played by hard ferromagnetic materials (well beyond refrigerator magnets :-). Indeed, despite the decades of the exponential (Moore's-law) progress of semiconductor electronics, most computer data storage systems are still based on the hard disk drives whose active medium is a submicron-thin ferromagnetic layer, with bits stored in the form of the direction of the spontaneous magnetization of small film spots. This technology has reached a fantastic sophistication, ${ }^{49}$ with recording data density approaching $10^{12}$ bits per square inch. Only recently it has started to be seriously challenged by the so-called solid state drives based on the flash semiconductor memories already mentioned in Chapter 3.

### 5.6. Systems with magnetics

Similarly to the electrostatics of linear dielectrics, magnetostatics of linear magnetics is very simple in the particular case when the stand-alone currents are deeply embedded into a medium with a constant permeability $\mu$. Indeed, in this case, boundary conditions on the distant surface of the media do not affect the solution of the boundary problem described by the magnetic equations of the macroscopic Maxwell system (109). Now let us assume that we know the solution $\mathbf{B}_{0}(\mathbf{r})$ of the magnetic pair of the genuine ("microscopic") Maxwell equations (36) in free space, i.e. when the genuine current density $\mathbf{j}$ coincides with that of stand-alone currents. Then the macroscopic equations and the material equation (110) are completely satisfied with the pair of functions

$$
\begin{equation*}
\mathbf{H}(\mathbf{r})=\frac{\mathbf{B}_{0}(\mathbf{r})}{\mu_{0}}, \quad \mathbf{B}(\mathbf{r})=\mu \mathbf{H}(\mathbf{r})=\frac{\mu}{\mu_{0}} \mathbf{B}_{0}(\mathbf{r}) . \tag{5.116}
\end{equation*}
$$

Hence the only effect of a complete filling a system of fixed currents with a uniform, linear magnetic is the increase of the magnetic field $\mathbf{B}$ at all points by the same constant factor $\mu / \mu_{0} \equiv 1+\chi_{m}$. (As a reminder, a similar filling of a system of fixed charges with a uniform, linear dielectric leads to a reduction of the electric field $\mathbf{E}$ by factor $\varepsilon / \varepsilon_{0}=\varepsilon_{\mathrm{r}}=1+\chi_{e}$.)

[^273]However, this simple result is generally invalid in the case of non-uniform (or piece-wise uniform) magnetic samples. Theoretical analyses of magnetic field distribution in such non-uniform systems may be facilitated by two additional tools. First, integrating the macroscopic Maxwell equation (107) along a closed contour $C$ limiting a smooth surface $S$, and using the Stokes theorem, we get the macroscopic version of the Ampère law (37):

$$
\begin{equation*}
\oint_{C} \mathbf{H} \cdot d \mathbf{r}=I \tag{5.117}
\end{equation*}
$$

This is exactly the replica of the "microscopic" equation Eq. (37), with the replacement $\mathbf{B} / \mu_{0} \rightarrow \mathbf{H}$.
Let us apply this relation to a boundary between two regions with constant, but different $\mu$, with no stand-alone currents on the border, similarly how this was done for field $\mathbf{E}$ in Sec. 3.4-see Fig. 3.5. The result is similar as well:

$$
\begin{equation*}
H_{\tau}=\text { const } . \tag{5.118}
\end{equation*}
$$

On the other hand, the integration of the Maxwell equation (29) over a Gaussian pillbox enclosing a border fragment (again similar to that shown in Fig. 3.5) yields the result similar to Eq. (3.46):

$$
\begin{equation*}
B_{n}=\text { const, i.e. } \mu H_{n}=\text { const } . \tag{5.119}
\end{equation*}
$$

Let us use these boundary conditions, first, to see what happens with a thin sheet of magnetic material (or any other strongly elongated sample) placed parallel to a uniform external field $\mathbf{H}_{0}$. Such sample cannot noticeably disturb the field in the free space outside it: $\mathbf{H}_{\text {ext }}=\mathbf{H}_{0}, \mathbf{B}_{\text {ext }}=\mathbf{H}_{\text {ext }} / \mu_{0}=\mathbf{H}_{0} / \mu_{0}$. Now applying Eq. (118) to the dominating, large-area interfaces, we get $\mathbf{H}_{\text {int }}=\mathbf{H}_{0}$, i.e., $\mathbf{B}_{\text {int }}=\left(\mu / \mu_{0}\right) \mathbf{B}_{0} .{ }^{50}$ The fact of constancy of field $\mathbf{H}$ in this geometry explains why this field is used as the horizontal axis in plots like Fig. 14: such measurements are typically carried out by placing an elongated sample of the material into the uniform field - say the one produced by a long solenoid.

Samples of other geometries may create strong perturbations of the external field, extended to distances of the order of the transversal dimensions of the sample. In order to analyze such problems, we may benefit from a simple, partial differential equation for a scalar function, e.g., the Laplace equation, because in Chapter 2 we have learned how to solve it for many simple geometries. In magnetostatics, the introduction of a scalar potential is generally impossible due to the vortex-like magnetic field lines, but if there are no stand-alone currents within the region we are interested in, then the Maxwell equation (32) for field $\mathbf{H}$ is reduced to $\nabla \times \mathbf{H}=0$, and we may introduce the scalar potential of the magnetic field, $\phi_{m}$, using the relation similar to Eq. (1.33):

$$
\begin{equation*}
\mathbf{H}=-\nabla \phi_{m} . \tag{5.120}
\end{equation*}
$$

Combining it with the homogenous Maxwell equation for magnetic field, $\nabla \cdot \mathbf{B}=0$, we arrive at the familiar differential equation,

$$
\begin{equation*}
\nabla \cdot\left(\mu \nabla \phi_{m}\right)=0 \tag{5.121}
\end{equation*}
$$

that, for a uniform media ( $\mu=$ const), is reduced to our beloved Laplace equation. Moreover, Eqs. (118) and (119) give the very familiar boundary conditions: first

[^274]\[

$$
\begin{equation*}
\frac{\partial \phi_{m}}{\partial \tau}=\mathrm{const} \tag{5.122a}
\end{equation*}
$$

\]

which is equivalent to

$$
\begin{equation*}
\phi_{m}=\text { const }, \tag{5.122b}
\end{equation*}
$$

and also

$$
\begin{equation*}
\mu \frac{\partial \phi_{m}}{\partial n}=\text { const } . \tag{5.123}
\end{equation*}
$$

Note that these boundary conditions are similar for (3.46) and (3.47) of electrostatics, with the replacement $\varepsilon \rightarrow \mu .{ }^{51}$

Let us analyze the geometric effects on magnetization, using the (too?) familiar structure: a sphere, made of a linear magnetic material, in a uniform external field. Since the differential equation and boundary conditions are similar to those of the similar electrostatics problem (see Fig. 3.8), we can use the above analogy to recycle the solution we already have got - see Eqs. (3.55)-(3.56). Just as in the electric case, the field outside the sphere, with potential

$$
\begin{equation*}
\left(\phi_{m}\right)_{r>R}=H_{0}\left(-r+\frac{\mu-\mu_{0}}{\mu+2 \mu_{0}} \frac{R^{3}}{r^{2}}\right) \cos \theta \tag{5.125a}
\end{equation*}
$$

is a sum of the uniform external field $\mathbf{H}_{0}$ and the dipole field (99) with the following induced magnetic dipole moment of the sphere: ${ }^{52}$

$$
\begin{equation*}
\mathbf{m}=4 \pi \frac{\mu-\mu_{0}}{\mu+2 \mu_{0}} R^{3} \mathbf{H}_{0} . \tag{5.125b}
\end{equation*}
$$

On the contrary, the internal field is perfectly uniform:

$$
\begin{equation*}
\left(\phi_{m}\right)_{r<R}=-H_{0} \frac{3 \mu_{0}}{\mu+2 \mu_{0}} r \cos \theta, \quad \frac{H_{\mathrm{int}}}{H_{0}}=\frac{3 \mu_{0}}{\mu+2 \mu_{0}}, \quad \frac{B_{\mathrm{int}}}{B_{0}}=\frac{\mu H_{\mathrm{int}}}{\mu_{0} H_{0}}=\frac{3 \mu}{\mu+2 \mu_{0}} . \tag{5.126}
\end{equation*}
$$

Note that though $\mathbf{H}$ inside the sphere is not equal to its value of the external field $\mathbf{H}_{0}$. This example shows that the interpretation of $\mathbf{H}$ as the "would-be" magnetic field generated by external

[^275]currents $\mathbf{j}$ should not be exaggerated into saying that its distribution is independent on the magnetic bodies in the system. ${ }^{53}$

In the limit $\mu \gg \mu_{0}$, Eqs. (126) yield $H_{\text {int }} / H_{0} \ll 1, B_{\text {int }} / H_{0}=3 \mu_{0}$, the factor 3 being specific for the particular geometry of the sphere. If a sample is stretched along the applied field, this limitation of the field concentration is gradually removed, and $B_{\text {int }}$ tends to its maximum value $\mu H_{0} \gg B_{\text {ext }}$, as was discussed above. This effect of "magnetic line concentration" in high $-\mu$ materials is used in such practically important devices as transformers, in which two multi-turn coils are wound on a ring-shaped (e.g., toroidal, see Fig. 6b) core made of a soft ferromagnetic material (such as the transformer steel, see Table 1) with $\mu \gg \mu_{0}$. This minimizes the number of "stray" field lines, and makes the magnetic flux $\Phi$ piercing each wire turn (of either coil) virtually the same - the equality important for secondary voltage induction - see the next chapter.

The second theoretical tool, frequently useful for problem solution, is a macroscopic expression for magnetic field energy $U$. For a system with linear magnetic materials, we may repeat the transformation of Eq. (55), made in Sec. 3, but with due respect to the magnetization, i.e. replacing $\mathbf{j}$ not from Eq. (56), but from Eq. (107). As a result, instead of Eq. (57) we get

energy in a
linear magnetic

General magnetic energy variation

$$
\begin{equation*}
U=\int_{V} u(\mathbf{r}) d^{3} r, \quad \text { with } u=\frac{\mathbf{B} \cdot \mathbf{H}}{2}=\frac{B^{2}}{2 \mu}=\frac{\mu H^{2}}{2}, \tag{5.127}
\end{equation*}
$$

This result is evidently similar to Eq. (3.79) of electrostatics.
For the general case of nonlinear magnetics, calculations similar to those resulting in Eq. (3.82) give the following analog of that relation:
for a linear magnetic yielding Eq. (127). Similarly to the electrostatics of dielectrics, we may argue that according to Eq. (128), in systems with magnetic media, $\mathbf{H}$ plays the role of the generalized force, and $\mathbf{B}$ of the generalized coordinate (per unit volume). ${ }^{54}$ As the result, the Gibbs potential energy, whose minimum corresponds to the stable equilibrium of the system in an external field $\mathbf{H}_{\text {ext }}$, is

$$
\begin{equation*}
g=\int_{V} g(\mathbf{r}) d^{3} r, \quad \text { with } g(\mathbf{r}) \equiv u(\mathbf{r})-\mathbf{H}_{\mathrm{ext}} \cdot \mathbf{B}, \tag{5.129}
\end{equation*}
$$

the expression to be compared with Eq. (3.84). Similarly, for a system with linear magnetics, the latter of these expressions may be integrated over the variations to give

[^276]\[

$$
\begin{equation*}
g(\mathbf{r})=\frac{1}{2 \mu} \mathbf{B} \cdot \mathbf{B}-\mathbf{H}_{\mathrm{ext}} \cdot \mathbf{B}=\frac{1}{2 \mu}\left(\mathbf{B}-\mu \mathbf{H}_{\mathrm{ext}}\right)^{2}+\text { const } \tag{5.130}
\end{equation*}
$$

\]

with similar consequences for the external magnetic field penetration into a system with magnetics. As a sanity check, for a uniform system with negligible fringe fields, such as a long solenoid filled with a uniform, linear magnetic material, Eq. (130) may be readily integrated over the sample volume to give

$$
\begin{equation*}
g(\mathbf{r})=\frac{1}{2 \mu}\left(\mathbf{B}-\mu \mathbf{H}_{\mathrm{ext}}\right)^{2} V+\mathrm{const} \tag{5.131}
\end{equation*}
$$

so that the minimum of the Gibbs potential energy, i.e. the stable equilibrium of the system, corresponds to the result that has already been derived in the beginning of this section: $\mathbf{B}=\mu \mathbf{H}_{\text {ext }}$, i.e. $\mathbf{H}=\mathbf{H}_{\text {ext }}$.

For the important particular case of a long solenoid (Fig. 6a) filled with a linear magnetic material, we hay find field $H$ from Eq. (117), just as we used Eq. (37) in Sec. 2 for finding $B$ for a similar empty solenoid, getting

$$
\begin{equation*}
H=I n, \text { and hence } B=\mu I n . \tag{5.132}
\end{equation*}
$$

Now we may plug this result into Eq. (127) to calculate the magnetic energy stored in the solenoid:

$$
\begin{equation*}
U=u V=\frac{\mu H^{2}}{2} l A=\frac{\mu(n I)^{2} l A}{2} \tag{5.132}
\end{equation*}
$$

and then use Eq. (72) to calculate its self-inductance:

$$
\begin{equation*}
L=\frac{U}{I^{2} / 2}=\mu n^{2} l A \tag{5.133}
\end{equation*}
$$

- as evident generalization of Eq. (75). This result explains why filling of solenoids with soft ferromagnets with $\mu \gg \mu_{0}$ is so popular in the electrical engineering practice, where large self- and mutual inductances are frequently needed in systems with size and/or weight restrictions.

Now, let us use these two tools to discuss a curious (and practically important) approach to systems with ferromagnetic cores. First, let us find the magnetic flux $\Phi$ in a system with a relatively thin, closed magnetic core made of sections of (possibly, different) soft ferromagnets, with the crosssection areas $A_{k}$ much smaller than the squared lengths $l_{k}$ of the sections - see Fig. 15.


Fig. 5.15. Deriving the "magnetic Ohm law" (135).

If all $\mu_{k} \gg \mu_{0}$, virtually all field lines are confined to the interior of the core. Then, applying the macroscopic Ampère law (117) to contour $C$, which follows a magnetic field line inside the core (see the
dashed line in Fig. 15), we get the following approximate expression (exactly valid only in the limit $\left.\mu_{k} / \mu_{0}, l_{k}^{2} / A_{k} \rightarrow \infty\right)$ :

$$
\begin{equation*}
\oint_{C} H_{l} d l \approx \sum_{k} l_{k} H_{k}=\sum_{k} l_{k} \frac{B_{k}}{\mu_{k}}=N I . \tag{5.134}
\end{equation*}
$$

However, since the magnetic field lines stay in the core, the magnetic flux $\Phi_{k} \approx B_{k} A_{k}$ should be the same $(\equiv \Phi)$ for each section, so that $B_{k}=\Phi / A_{k}$. Plugging this condition into Eq. (134), we get

$$
\begin{equation*}
\Phi=\frac{N I}{\sum_{k} R_{k}}, \quad \text { where } R_{k} \equiv \frac{l_{k}}{\mu_{k} A_{k}} \tag{5.135}
\end{equation*}
$$

Note a close analogy of the first of these equations with the Ohm law for several resistors connected in series, with the magnetic flux playing the role of electric current, while the product $N I$, of the voltage applied to the resistor chain. This analogy is fortified by the fact that the second of Eqs. (135) is similar to the expression for resistance $R=l / \sigma A$ of a long uniform conductor, with the magnetic permeability $\mu$ playing the role of the electric conductivity $\sigma$. (In order to sound similar, but still different from resistance $R$, parameter $\mathbb{R}$ is called the reluctance.) This is why Eq. (135) is called the magnetic Ohm law; it is very useful for approximate analyses of systems like ac transformers, magnetic energy storage systems, etc.

The role of the "magnetic e.m.f." NI may be also played by a permanent-magnet section of the core. Indeed, for relatively low fields we may use the Taylor expansion of the nonlinear function $B(H)$ near $H=0$ to write

$$
\begin{equation*}
B \approx \mp \mu_{0} M_{s}+\mu_{d} H,\left.\quad \mu_{d} \equiv \frac{d B}{d H}\right|_{H=0}, \tag{5.136}
\end{equation*}
$$

where $M_{s}$ is the spontaneous magnetization magnitude at $H=0$, the $\mp$ sign corresponds to two possible directions of the magnetization, and parameter $\mu_{d}$ is called the differential (or "dynamic") permeability. Expressing $H$ from this relation, and using it in one of components of the sum (134), we again get a result similar to Eq. (135)

$$
\begin{equation*}
\Phi=\mp \frac{(N I)_{\mathrm{ef}}}{R_{H}+\sum_{k} R_{k}}, \quad \text { with } R_{H} \equiv \frac{l_{H}}{A_{H} \mu_{d}} \tag{5.137}
\end{equation*}
$$

where $l_{H}$ and $A_{H}$ are geometric dimensions of the hard-ferromagnet section, and product $N I$ is replaced with its effective value

$$
\begin{equation*}
(N I)_{\mathrm{ef}}=\mp \frac{\mu_{0}}{\mu_{d}} M_{s} l_{H} . \tag{5.138}
\end{equation*}
$$

This result may be used for a semi-quantitative explanation of the well-known short-range forces acting between permanent magnets (or between them and soft ferromagnets) at their mechanical contact (Fig. 16).


Fig. 5.16. Short-range interaction between magnets.

Indeed, considering the free-space gaps between them as sections of the core (which is approximately correct, because due to the small gap thickness $d$ the magnetic field lines cannot stray far from the contact area), and neglecting the reluctance $\mathbb{P}$ of the bulk material (due to its larger crosssection), we get

$$
\begin{equation*}
|\Phi| \propto\left(\frac{2 d}{\mu_{0}}+\frac{l}{\mu_{d}}\right)^{-1} \tag{5.139}
\end{equation*}
$$

so that, according to Eq. (127), the magnetic energy of the system (disregarding the constant energy of the permanent magnetization) is

$$
\begin{equation*}
U \propto\left(\frac{2 d}{\mu_{0}}+\frac{l}{\mu_{d}}\right) B^{2} \propto\left(\frac{2 d}{\mu_{0}}+\frac{l}{\mu_{d}}\right)^{-1} \propto \frac{1}{d+d_{0}}, \quad d_{0} \equiv \frac{1}{2} \frac{\mu_{0}}{\mu_{d}} l \ll l . \tag{5.140}
\end{equation*}
$$

Hence the magnet attraction force,

$$
\begin{equation*}
F=\left|\frac{\partial U}{\partial d}\right| \propto \frac{1}{\left(d+d_{0}\right)^{2}}, \tag{5.141}
\end{equation*}
$$

behaves almost as the divergence $1 / d^{2}$ truncated at a short distance $d_{0} \ll l$. Due to that truncation, the force is finite at $d=0$; this exactly the force you need to apply to detach two magnets.

Finally, let us discuss in brief a related effect in experiments with thin and long hard ferromagnetic samples - "needles", like those used in magnetic compasses. Using the definition (108) of field $\mathbf{H}$, the Maxwell equation (29) takes the form

$$
\begin{equation*}
\nabla \cdot \mathbf{B} \equiv \mu_{0} \nabla \cdot(\mathbf{H}+\mathbf{M})=0 \tag{5.142}
\end{equation*}
$$

and may be rewritten as

$$
\begin{equation*}
\nabla \cdot \mathbf{H}=-\nabla \cdot \mathbf{M} . \tag{5.143}
\end{equation*}
$$

While this relation is general, it is especially convenient in hard ferromagnets, where $\mathbf{M}$ is virtually fixed by the saturation. Comparing this equation with Eq. (1.27) for the electrostatic field, we see that the right-hand part of Eq. (143) may be considered as a fixed source of a Coulomb-like magnetic field.

For example, let us apply Eq. (143) to a thin, long needle made of a hard ferromagnet (Fig. 17a). Inside the needle, $\mathbf{M}=\mathbf{M}_{s}=$ const, while outside it $\mathbf{M}=0$, so that the right-hand part of Eq. (143) is substantially different from zero only in two small areas at the needle's ends, and on much larger distances we can use the following approximation:

$$
\begin{equation*}
\nabla \cdot \mathbf{H}=-q_{m} \delta\left(\mathbf{r}-\mathbf{r}_{1}\right)+q_{m} \delta\left(\mathbf{r}-\mathbf{r}_{2}\right), \tag{5.155}
\end{equation*}
$$

where $\mathbf{r}_{1,2}$ are ends' positions, and $q_{m} \equiv M_{s} A$, with $A$ being the needle's cross-section area. This equation is completely similar to Eq. (1.27) for the electric field created by two equal and opposite point charges. In particular, if two ends of two needles are hold at an intermediate distance $r$ ( $A^{1 / 2} \ll r \ll l$, where $l$ is the needle length, see Fig. 17b), the ends interact in accordance with the magnetic Coulomb law

$$
\begin{equation*}
F \propto \frac{q_{m}^{2}}{r^{2}}=\frac{M_{s}^{2} A^{2}}{r^{2}} \tag{5.156}
\end{equation*}
$$



Fig. 5.17. (a) "Magnetic charges" at the ends of a thin ferromagnetic needle and (b) the result of its breaking into two parts (schematically).

The "only" (but conceptually, very significant!) difference with electrostatics is that the "magnetic charges" $\pm q_{m}$ cannot be fully separated. For example, if we break a magnetic needle in the middle in at attempt to bring its two ends further apart, two new "charges" appear - see Fig. 17b. There are several solid state systems where more flexible structures, similar to the magnetic needles, may be implemented. First of all, certain ("type-II") superconductors may sustain so-called Abrikosov vortices crudely, flexible tubes with field-suppressed superconductivity inside, each carrying one magnetic flux quantum $\Phi_{0}=\pi \hbar / e \approx 2 \times 10^{-15} \mathrm{~Wb}$ - see Sec. 6.3. Ending on superconductor's surface, these tubes let the magnetic field lines to spread into the surrounding space, essentially forming a magnetic monopole analog (of course, with an equal and opposite "monopole" on another end of the line). Such flux tubes are not only flexible but readily stretchable, resulting in several peculiar effects. ${ }^{55}$ Another, recently found, examples of paired "monopoles" include spin chains in so-called spin ices - crystals with paramagnetic ions arranged into a specific (pyrochlore) lattice - such as dysprosium titanate $\mathrm{Dy}_{2} \mathrm{Ti}_{2} \mathrm{O}_{7} .{ }^{56}$

### 5.7. Exercise problems

5.1. Two straight, parallel, long, plane, thin strips of width $d$, separated by distance $d$, are used to form a current loop - see Fig. on the right. Calculate the magnetic field in the plane located at the middle between the planes of the strips, assuming that current $I$ is uniformly distributed across strip width.

${ }^{55}$ A detailed discussion of the Abrikosov vortices may be found, for example, in Chapter 5 of M. Tinkham, Introduction to Superconductivity, $2^{\text {nd }}$ ed., McGraw-Hill, 1996.
${ }^{56}$ See, e.g., L. Jaubert and P. Holdworth, J. Phys. - Cond. Matt. 23, 164222 (2011) and references therein.
5.2. For the system studied in the previous problem, but now only in the limit $d \ll w$, calculate:
(i) the distribution of the magnetic field (in the simplest possible way),
(ii) the vector-potential of the field,
(iii) the force (per unit length) acting on each strip, and
(iv) the magnetic energy and self-inductance of the system (per unit length).
5.3. Calculate the magnetic field distribution near the center of the system of two similar, plane, round, coaxial wire coils, fed by equal but oppositely directed currents - see Fig. on the right.

5.4. The two-coil-system, similar to that considered in the previous problem, carries equal and similarly directed currents - see Fig. on the right. Calculate what should be the ratio $d / R$ for the second derivative $\partial^{2} B_{z} / \partial z^{2}$ at $z=0$ to vanish. ${ }^{57}$
5.5. Calculate the magnetic field distribution along the axis of a straight solenoid (see Fig. 6a, partly reproduced on the right) with a finite length $l$, and round cross-section of radius $R$. Assume that the solenoid has many wire turns ( $N \gg 1$ ) that are uniformly distributed along its length.

5.6. A thin spherical shell of radius $R$, with charge $Q$ uniformly distributed over its surface, rotates about its axis with angular velocity $\omega$. Calculate the distribution of the magnetic field everywhere in space.
5.7. A sphere of radius $R$, made of an insulating material with a uniform electric charge density $\rho$, rotates about its diameter with angular velocity $\omega$. Calculate the magnetic field distribution inside the sphere and outside it.
5.8. The reader is (hopefully :-) familiar with the classical Hall effect when it takes place in the usual rectangular Hall bar geometry - see the left panel of the Fig. below. However, the effect takes a different form in the so-called Corbino disk - see the right panel below. (Dark shading shows electrodes, with no appreciable resistance.) Analyze the effect in both geometries, assuming that in both cases the conductors are thin, planar, have a constant Ohmic conductivity $\sigma$ and charge carrier density $n$, and that the applied magnetic field $\mathbf{B}$ is uniform and normal to conductors' planes.

[^277]
5.9. ${ }^{*}$ The simplest model of the famous homopolar motor ${ }^{58}$ is a thin, round conducting disk, placed into a uniform magnetic field normal to its plane, and fed by dc current flowing from disk's center to a sliding electrode ("brush") - see Fig. on the right.
(i) Express the torque, rotating the disk, via its radius $R$, magnetic field $\mathbf{B}$, and current $I$.

(ii) If the disk is allowed to rotate about its axis, and the motor is driven by a battery with e.m.f. $V$, calculate its angular velocity $\omega$, neglecting electric circuit's resistance and friction.
(iii) Now assuming that the current circuit (battery + wires + contacts + disk itself) has full resistance $R$, derive and solve the equation for the time evolution of $\omega$, and analyze the solution.
5.10. ${ }^{*}$ Estimate the values of magnetic susceptibility due to
(i) orbital diamagnetism, and
(ii) spin paramagnetism,
for a dilute medium with negligible interaction between molecular dipoles.
Hints: For task (i), you may use the classical model described by Eq. (114) (see Fig. 13), while for task (ii), assume the mechanism of ordering of spontaneous magnetic dipoles $\mathbf{m}_{0}$, similar to the one sketched for electric dipoles in Fig. 12b, with the magnitude of the order of the Bohr magneton $\mu_{\mathrm{B}}-$ see Eq. (96).
5.11.* Use the classical picture of the orbital ("Larmor") diamagnetism, discussed in Sec. 5.5 of the lecture notes, to calculate its (small) correction $\Delta \mathbf{B}(0)$ to the magnetic field $\mathbf{B}$, as felt by the atomic nucleus, modeling atomic electrons by a spherically-symmetric cloud with electric charge density $\rho(r)$. Express the result via the value $\phi(0)$ of the electrostatic potential of electrons' cloud, and use this expression for a crude numerical estimate of the relative correction, $\Delta B(0) / B$, for the hydrogen atom.
5.12. Current $I$ is flows in a thin wire bent into a plane, round loop of radius $R$. Calculate the net magnetic flux through the whole plane in which the loop is located.

[^278]5.13. Calculate the (self-) inductance of a toroidal solenoid (Fig. 6b) with the round cross-section of radius $r \sim R$ (see Fig. on the right), filled with a material of magnetic permeability $\mu$, with many ( $N \gg 1, R / r$ ) wire turns uniformly distributed along the perimeter. Check your results by analyzing the limit $r \ll R$.


Hint : You may like to use the following table integral:59

$$
\int_{0}^{1} \ln \frac{a+\left(1-\xi^{2}\right)^{1 / 2}}{a-\left(1-\xi^{2}\right)^{1 / 2}} d \xi=\pi\left[a-\left(a^{2}-1\right)^{1 / 2}\right], \quad \text { for } a \geq 1
$$

5.14. Prove that:
(i) the self-inductance $L$ of a current loop cannot be negative, and
(ii) each mutual inductance coefficient $L_{k k}$, defined by Eq. (60), cannot be larger than $\left(L_{k k} L_{k^{\prime} k^{\prime}}\right)^{1 / 2}$.
5.15. A round cylindrical shell, made of a soft ferromagnet, is placed into a uniform external field $\mathbf{H}_{0}$ perpendicular to its axis - see Fig. on the right. Find the distribution of the magnetic field everywhere in the system, and discuss its efficiency as a "magnetic shield".
5.16. A straight thin wire, carrying current $I$, passes parallel to the plane boundary between two uniform, linear magnetics - see Fig. on the right. Calculate the magnetic field everywhere in the system, and the force (per unit length) exerted on the wire.

5.17. Calculate the distribution of magnetic field around a sphere made of a hard ferromagnet with a permanent, uniform magnetization $\mathbf{M}=$ const.
5.18.* A limited volume $V$ is filled with a magnetic material with magnetization $\mathbf{M}(\mathbf{r})$.
(i) Use Eq. (5.143) to write explicit expressions for the magnetic field and its potential, induced by the magnetization.
(ii) Recast these expressions in forms convenient when $\mathbf{M}(\mathbf{r})=\mathbf{M}_{0}=$ const inside volume $V$.
5.19. Use the results of the previous problem to calculate the distribution of the magnetic field along the axis of a straight


[^279]permanent magnet of length $2 l$, with round cross-section of radius $R$, and uniform magnetization $\mathbf{M}_{0}$ parallel to the axis - see Fig. on the right.
5.20. A very broad film of thickness $2 t$ is magnetized normally to its plane, with a periodic checkerboard pattern with square side $a$ :
\[

\left.\mathbf{M}\right|_{|z|<t}=\mathbf{n}_{z} M(x, y), \quad with M(x, y)=M_{0} \times $$
\begin{cases}(+1), & \text { if } \cos \frac{\pi x}{a} \cos \frac{\pi y}{a}>0 \\ (-1), & \text { if } \cos \frac{\pi x}{a} \cos \frac{\pi y}{a}<0 .\end{cases}
$$
\]

Calculate the magnetic field distribution in space. ${ }^{60}$
5.21. A flat end of a rod magnet, with cross-section area $A$, with saturated magnetization $\boldsymbol{M}_{s}$ directed along rod's length, is let to stuck to a plane surface of a large sample made of a soft ferromagnetic material with $\mu \gg \mu_{0}$. Calculate the force necessary to detach the rod from the surface, if it is applied strictly perpendicular to the contact surface - see Fig. on the right.

5.22.* Based on the discussion of the quadrupole electrostatic lens in Sec. 2.4 of the lecture notes, suggest permanent-magnet systems which may similarly focus particles moving close to system's axis, and carrying:
(i) an electric charge,
(ii) no net electric charge, but a nonvanishing spontaneous magnetic dipole moment $\mathbf{m}$.
5.23. A circular wire loop, carrying a fixed dc current, has been placed inside a similar but larger loop, carrying a fixed current in the same direction - see Fig. on the right. Use semi-quantitative arguments to analyze the mechanical stability of the coaxial, coplanar position of the inner loop
 with respect to its possible angular, axial, and lateral displacements, if the position of the outer loop is fixed.

[^280]

## Chapter 6. Time-Dependent Electromagnetism

This chapter discusses two major new effects that appear if the electric and magnetic fields are changing in time: the "electromagnetic induction" of electric field by changing magnetic field, and the reciprocal effect of "displacement currents" - the induction of magnetic field by changing electric field. These two phenomena, which make the time-dependent electric and magnetic fields inseparable, contribute to the system of four Maxwell equations, and make it valid for arbitrary electromagnetic processes. On the way, I will pause for a brief review of the electrodynamics of superconductivity, which (besides its own significance), provides a perfect platform for a discussion of the gauge invariance.

### 6.1. Electromagnetic induction

As Eqs. (5.36) and (5.109) show, in static situations $(\partial / \partial t=0)$ the Maxwell equations describing the electric and magnetic fields are independent, and are coupled only implicitly, via the continuity equation (4.5) relating their right-hand parts $\rho$ and $\mathbf{j}$. (In statics this relation imposes a restriction only on vector $\mathbf{j}$.) In dynamics, when the fields change in time, the situation in different.

Historically, the first discovered explicit coupling between the electric and magnetic fields was the effect of electromagnetic induction. ${ }^{1}$ The summary of Faraday's numerous experiments has turned out to be very simple: if the magnetic flux, defined by Eq. (5.65),

$$
\begin{equation*}
\Phi \equiv \int_{S} B_{n} d^{2} r \tag{6.1}
\end{equation*}
$$

through a surface $S$ limited by contour $C$, changes in time by whatever reason (e.g., either due to a change of the magnetic field $\mathbf{B}$, or contour's motion, or its deformation), it induces an additional, vortexlike electric field $\mathbf{E}_{\text {ind }}$, similar in its topology to the magnetic field induced by a current. The exact distribution of $\mathbf{E}_{\text {ind }}$ in space depends on system geometry details and may be rather complex, but its integral along the contour $C$, called the inductive electromotive force (e.m.f.), obeys a very simple Faraday induction law: ${ }^{2}$
 induction

$$
\begin{equation*}
V_{\text {ind }} \equiv \oint_{C} \mathbf{E}_{\text {ind }} \cdot d \mathbf{r}=-\frac{d \Phi}{d t} . \tag{6.2}
\end{equation*}
$$

In is straightforward (and hence left for the reader's exercise :-) to show that the e.m.f. may be measured, for example, either inserting a voltmeter into a conducting loop following contour $C$, or by measuring current $I=V_{\text {ind }} / R$ it induces in a thin wire with Ohmic resistance $R$, whose shape follows that contour. The minus sign in Eq. (2) corresponds to the so-called Lenz rule: the magnetic field of the induced Ohmic current provides a partial compensation of the change of the original $\Phi$ in time.

In order to recast Eq. (2) in a differential form, let us apply, to the above definition of $V_{\text {ind }}$, the same Stokes theorem that was repeatedly used in Chapter 5. ${ }^{3}$ The result is

[^281]\[

$$
\begin{equation*}
V_{\text {ind }}=\int_{S}\left(\nabla \times \mathbf{E}_{\text {ind }}\right)_{n} d^{2} r . \tag{6.3}
\end{equation*}
$$

\]

Now combining Eqs. (1)-(3), for a contour $C$ whose shape does not change in time (so that the integration along it is interchangeable with the time derivative), ${ }^{4}$ we get

$$
\begin{equation*}
\int_{S}\left(\nabla \times \mathbf{E}_{\mathrm{ind}}+\frac{\partial \mathbf{B}}{\partial t}\right)_{n} d^{2} r=0 . \tag{6.4}
\end{equation*}
$$

Since the induced electric field is additional to the field (1.33) created by electric charges, for the net field we should write $\mathbf{E}=\mathbf{E}_{\text {ind }}-\nabla \phi$. However, since curl of any gradient field is zero, ${ }^{5} \nabla \times(\nabla \phi)=0$, Eq. (4) is valid for the net field $\mathbf{E}$. Since this equation should be correct for any closed area $S$, we may conclude that

$$
\begin{equation*}
\nabla \times \mathbf{E}+\frac{\partial \mathbf{B}}{\partial t}=0 \tag{6.5}
\end{equation*}
$$

at any point. This is the final (time-dependent) form of this Maxwell equation. Superficially, it may look that Eq. (5) is less general than Eq. (2); for example that it does not describe any electric field, and hence any e.m.f. in a moving loop, if field $\mathbf{B}$ is constant in time, so that flux (1) does change in time. However, this is not true; in Chapter 9 we will see that in the reference frame moving with the loop such e.m.f. does appear.

Now let us re-formulate Eq. (5) in terms of the vector-potential. Since the induction effect does not alter the fundamental relation $\nabla \cdot \mathbf{B}=0$, we still may present the magnetic field as prescribed by Eq. (5.27), i.e. as $\mathbf{B}=\nabla \times \mathbf{A}$. Plugging this expression into Eq. (6), we get

$$
\begin{equation*}
\nabla \times\left(\mathbf{E}+\frac{\partial \mathbf{A}}{\partial t}\right)=0 \tag{6.6}
\end{equation*}
$$

Hence we can use the argumentation of Sec. 1.3 (there applied to vector $\mathbf{E}$ alone) to present the expression in parentheses as $-\nabla \phi$, so that

$$
\begin{equation*}
\mathbf{E}=-\frac{\partial \mathbf{A}}{\partial t}-\nabla \phi \tag{6.7}
\end{equation*}
$$

Differential form of the
Faraday law

Electric field vs. potentials

It is tempting to interpret the first term of the right-hand part as describing the electromagnetic induction alone, and the second term representing a purely electric field induced by electric charges. However, the separation of these two terms is, to a certain extent, conditional. Indeed, let us consider the gauge transformation already mentioned in Sec. 5.2,

$$
\begin{equation*}
\mathbf{A} \rightarrow \mathbf{A}+\nabla \chi \tag{6.8}
\end{equation*}
$$

[^282]that, as we already know, does not change the magnetic field. According to Eq. (8), in order to keep the full electric field intact (gauge-invariant) as well, the scalar electric potential has to be transformed simultaneously, as
\[

$$
\begin{equation*}
\phi \rightarrow \phi-\frac{\partial \chi}{\partial t} \tag{6.9}
\end{equation*}
$$

\]

leaving the choice of a time-independent addition to $\phi$ restricted only by the Laplace equation - since the full $\phi$ should satisfy the Poisson equation (1.41) with a gauge-invariant right-hand part. We will return to the discussion of gauge invariance in Sec. 3.

Now let us discuss whether Eqs. (2) or (5) describing the electromagnetic induction represent some completely new facts, on top of all the equations of electrostatics and magnetostatics, discussed in previous five chapters. The answer is not. To demonstrate that, let us consider a thin wire loop with current $I$, placed in a magnetic field (Fig. 1). According to Eq. (5.21), the magnetic force exerted by the field upon a small fragment of the wire is

$$
\begin{equation*}
d \mathbf{F}=I(d \mathbf{r} \times \mathbf{B})=-I(\mathbf{B} \times d \mathbf{r}), \tag{6.10}
\end{equation*}
$$

where $\mathrm{d} \mathbf{r}$ is a small vector, tangential to loop's contour and directed along current $I$. Now let the wire be slightly (and slowly) deformed so that this particular fragment is displaced by a small distance $\delta \mathbf{r}$. (Let me hope that Fig. 1 makes the difference between the elementary vectors $d \mathbf{r}$ and $\delta \mathbf{r}$ absolutely clear.)


Fig. 6.1. Thin wire with current in a magnetic field, and its small deformation.

Since the wire's acceleration (if any) is negligibly small, external (non-magnetic) forces should balance force (10), i.e. provide an equal and opposite force. This is why the work of these external forces at the displacement $\delta \mathbf{r}$, i.e. the change of the magnetic field energy $U$, is,

$$
\begin{equation*}
\delta(d U)=-d \mathbf{F} \cdot \delta \mathbf{r}=I \delta \mathbf{r} \cdot(\mathbf{B} \times d \mathbf{r}) \tag{6.11}
\end{equation*}
$$

Let us apply to this mixed product the general operand rotation rule of the vector algebra, ${ }^{6}$ so that vector B comes out of the vector product:

$$
\begin{equation*}
\delta(d U)=I \mathbf{B} \cdot(d \mathbf{r} \times \delta \mathbf{r}) \tag{6.12}
\end{equation*}
$$

But the magnitude of this vector product is nothing more than the area $\delta\left(d^{2} r\right) \equiv \delta(d S)$ swept by the wire's fragment at the deformation (Fig. 1), while its direction is perpendicular to this elementary area $d S$, along the "proper" normal vector $\mathbf{n}=(d \mathbf{r} / d r) \times(\delta \mathbf{r} / \delta r)$. The scalar multiplication of $\mathbf{B}$ by this vector is

[^283]equivalent to taking its normal component. Hence, integrating Eq. (12) over all the wire length, we get the following result for the total variation of the magnetic energy:
\[

$$
\begin{equation*}
\delta U=I \oint_{C} B_{n} \delta\left(d^{2} r\right) . \tag{6.13}
\end{equation*}
$$

\]

If $\mathbf{B}$ does not change at the wire deformation, the variation sign may be moved out from the integral, and Eq. (13) yields ${ }^{7}$

$$
\begin{equation*}
\delta U=I \delta \Phi \tag{6.14}
\end{equation*}
$$

where $\Phi$ is the magnetic flux through the loop.
Now let the work $\delta \mathcal{W}=\delta U$, necessary for this energy change, to come from a generator of voltage $V_{\text {ext }}$, inserted somewhere in the loop. In order for the system to be in quasi-equilibrium, this voltage should counter-balance the electromagnetic induction's e.m.f. $V_{\text {ind }}$. Work of the voltage at transfer of charge $\delta Q=I \delta t$, during elementary deformation's duration $\delta t$, is

$$
\begin{equation*}
\delta w=V_{\text {ext }} \delta Q=-V_{\text {ind }} \delta Q=-V_{\text {ind }} I \delta t . \tag{6.15}
\end{equation*}
$$

Comparing Eqs. (14) and (15), we arrive at the Faraday induction law (2).
Moreover, some authors derive Eq. (2) in this way, implying that there is no new information in the induction law at all. Note, however, that the simple derivation given above has used the assumption of magnetic field's independence on the deformation. A removal of this limitation would require using the Lorentz field transform (which will be only discussed in Chapter 9), and a very careful argumentation to exclude a faulty logic loop, because the transform itself is typically derived from Maxwell equations - including Eq. (5) that we are trying to prove. Personally I am happy that Dr. Faraday did his thorough work so early, placing the electromagnetic induction law on a firm experimental basis.

### 6.2. Quasistatic approximation and skin effect

As we will see later in this chapter, the interplay of the electromagnetic induction with one more time-dependent effect (the so-called displacement currents), enables electromagnetic waves propagating with speed $c=1 /\left(\varepsilon_{0} \mu_{0}\right)^{1 / 2}$ in free space, and with a comparable speed $v=1 /(\varepsilon \mu)^{1 / 2}$ in dielectric and/or magnetic materials. For the phenomena whose spatial scale is much smaller than the wavelength $\lambda=$ $2 \pi v / \omega$, the displacement current effects are negligible, and time-dependent phenomena may be described by using Eq. (6) together with three other macroscopic Maxwell equations in their unmodified form: ${ }^{8}$

$$
\begin{array}{ll}
\nabla \times \mathbf{E}+\frac{\partial \mathbf{B}}{\partial t}=0, & \nabla \times \mathbf{H}=\mathbf{j}  \tag{6.16}\\
\nabla \cdot \mathbf{D}=\rho, & \nabla \cdot \mathbf{B}=0
\end{array}
$$

These equations define the so-called quasistatic approximation of electromagnetism, and are sufficient to describe many important phenomena. Let us use them first of all for an analysis of the so-

[^284]called skin effect, the phenomenon of self-shielding of the alternating (ac) magnetic fields by currents flowing in a conductor.

In order to form a complete system of equations, Eqs. (16) should be augmented by material equations describing the medium. Let us take them, for a conductor, in the simplest (and simultaneously, most common) linear and isotropic form:

$$
\begin{equation*}
\mathbf{j}=\sigma \mathbf{E}, \quad \mathbf{B}=\mu \mathbf{H} \tag{6.17}
\end{equation*}
$$

If the conductor is uniform, i.e. coefficients $\sigma$ and $\mu$ are constant inside it, the whole system of equations (16)-(17) may be reduced to a single equation. Indeed, a sequential substitution of these equations into each other yields:

$$
\begin{align*}
\frac{\partial \mathbf{B}}{\partial t} & =-\nabla \times \mathbf{E}=-\frac{1}{\sigma} \nabla \times \mathbf{j}=-\frac{1}{\sigma} \nabla \times(\nabla \times \mathbf{H})=-\frac{1}{\sigma \mu} \nabla \times(\nabla \times \mathbf{B})=-\frac{1}{\sigma \mu}\left[\nabla(\nabla \cdot \mathbf{B})-\nabla^{2} \mathbf{B}\right]  \tag{6.18}\\
& =\frac{1}{\sigma \mu} \nabla^{2} \mathbf{B} .
\end{align*}
$$

Thus we have arrived, without any further assumptions, at a very simple partial differential equation. Let us use it to analyze the skin effect in the simplest geometry (Fig. 2a) when an external source (which, at this point, does not need to be specified) produces, near a plane surface of a bulk conductor, a spatially-uniform ac magnetic field $\mathbf{H}^{(0)}(t)$ parallel to the surface.

(a)

(b)

Fig. 6.2. (a) Skin effect in the simplest, planar geometry, and (b) two Ampère contours for deriving the "microscopic" (contour $C_{1}$ ) and the "macroscopic" (contour $C_{2}$ ) boundary conditions for $\mathbf{H}$.

Selecting the coordinate system as shown in Fig. 2, we may express this condition as

$$
\begin{equation*}
\left.\mathbf{H}\right|_{x=-0}=H^{(0)}(t) \mathbf{n}_{y} . \tag{6.19}
\end{equation*}
$$

The translational symmetry of our simple problem within the surface plane $[y, z]$ implies that inside the conductor $\partial / \partial y=\partial / \partial z=0$ as well, and $\mathbf{H}=H(x, t) \mathbf{n}_{y}$ even at $x \geq 0$, so that Eq. (18) for conductor's interior is reduced to a differential equation for just one scalar function $H(x, t)=B(x, t) / \mu:{ }^{9}$

$$
\begin{equation*}
\frac{\partial H}{\partial t}=\frac{1}{\sigma \mu} \frac{\partial^{2} H}{\partial x^{2}}, \quad \text { for } x \geq 0 \tag{6.20}
\end{equation*}
$$

[^285]This equation may be further simplified by noticing that due to its linearity, we may use the linear superposition principle for the time dependence of the field, ${ }^{10}$ via expanding it, as well as the external field (19), into the Fourier series,

$$
\begin{array}{ll}
H(x, t)=\sum_{\omega} H_{\omega}(x) e^{-i \omega t}, & \text { for } x . \geq 0,  \tag{6.21}\\
H^{(0)}(t)=\sum_{\omega} H_{\omega}^{(0)} e^{-i \omega t}, & \text { for } x=0,
\end{array}
$$

and arguing that if we know the solution for each frequency component, the whole field may be found through the elementary summation (17) of these solutions. For each single-frequency component, Eq. (21) is immediately reduced to an ordinary differential equation for the complex amplitude $H_{\omega}(x)$ :

$$
\begin{equation*}
-i \omega H_{\omega}=\frac{1}{\sigma \mu} \frac{d^{2}}{d x^{2}} H_{\omega} \tag{6.22}
\end{equation*}
$$

From the theory of linear differential equations we know that Eq. (22) has the following general solution:

$$
\begin{equation*}
H_{\omega}(x)=H_{+} e^{\kappa_{+} x}+H_{-} e^{\kappa_{-} x}, \tag{6.23}
\end{equation*}
$$

where constants $\kappa_{ \pm}$are roots of the characteristic equation that may be obtained by substitution of any of these two exponents into the initial differential equation. For our particular case, the characteristic equation, following from Eq. (22), is

$$
\begin{equation*}
-i \omega=\frac{\kappa^{2}}{\sigma \mu} \tag{6.24}
\end{equation*}
$$

and its roots are complex constants

$$
\begin{equation*}
\kappa_{ \pm}=(-i \mu \omega \sigma)^{1 / 2}= \pm \frac{1-i}{\sqrt{2}}(\mu \omega \sigma)^{1 / 2} \tag{6.25}
\end{equation*}
$$

For our problem, the field cannot grow exponentially at $x \rightarrow+\infty$, so that only one of the coefficients, namely $H$. corresponding to the decaying exponent, with $\operatorname{Re} \kappa<0$ (i.e. $\kappa=\kappa$ ), may be nonvanishing, so that $H_{\omega}(x)=H_{\omega}(0) \exp \left\{\kappa_{X} x\right\}$. In order to find the constant factor $\mathrm{H}_{\omega}(0)$, we can integrate the Maxwell equation $\nabla \times \mathbf{H}=\mathbf{j}$ along a pre-surface contour - say, contour $C_{1}$ shown in Fig. 2b. The right-hand part's integral is negligible, because $\mathbf{j}$ does not contain any "genuinely surface" currents, localized at a depth much smaller than $1 / \operatorname{Re}[-\mathcal{K}]$. As a result, we get the "microscopic" ${ }^{11}$ boundary condition similar to Eq. (5.118) for the stationary magnetic field, $H_{\tau}=$ const at $x=0$, we get

$$
\begin{equation*}
H(0, t)=H^{(0)}(t), \quad \text { i.e. } H_{\omega}(0)=H_{\omega}^{(0)} \tag{6.26}
\end{equation*}
$$

[^286]so that the final solution of the problem may be presented as
\[

$$
\begin{equation*}
H_{\omega}(x)=H_{\omega}^{(0)} \exp \left\{-\frac{x}{\delta_{s}}\right\} \exp \left\{-i\left(\omega t-\frac{x}{\delta_{s}}\right)\right\}, \tag{6.27a}
\end{equation*}
$$

\]

where constant $\delta_{s}$ is called the skin depth:

$$
\begin{equation*}
\delta_{s} \equiv-\frac{1}{\operatorname{Re} \kappa_{-}}=\left(\frac{2}{\mu \sigma \omega}\right)^{1 / 2} \tag{6.27b}
\end{equation*}
$$

This solution describes the skin effect: the penetration of the ac magnetic field of frequency $\omega$ into a conductor only to a depth of the order of $\delta_{s}$. A couple of examples of the skin depth: for copper at room temperature, $\delta_{s} \approx 1 \mathrm{~cm}$ at the ac power distribution frequency of 60 Hz , and is of the order of just $1 \mu \mathrm{~m}$ at a few GHz , i.e. at typical frequencies of cell phone signals and kitchen microwave magnetrons. For a modestly salted water, $\delta_{s}$ is close to 250 m at 1 Hz (with big implications for radio communications with submarines), and is of the order of 1 cm at a few GHz (explaining a nonuniform heating of a soup bowl in a microwave oven).

In order to complete the skin effect discussion, let us consider what happens with the induced ac currents ${ }^{12}$ and the electric field at this effect. When deriving our basic equation (18), we have used, in particular, relations $\mathbf{j}=\nabla \times \mathbf{H}=\mu^{-1} \nabla \times \mathbf{B}$, and $\mathbf{E}=\mathbf{j} / \sigma$. Since a spatial differentiation of an exponent yield a similar exponents, the electric field and current density have the same spatial dependence as the magnetic field, i.e. penetrate inside the conductor by distances of the order of $\delta_{s}(\omega)$, but their vectors are directed perpendicularly to $\mathbf{B}$, while still being parallel to the conductor surface: ${ }^{13}$

$$
\begin{equation*}
\mathbf{j}_{\omega}(x)=\kappa_{-} H_{\omega}(x) \mathbf{n}_{z}, \quad \mathbf{E}_{\omega}(x)=\frac{\kappa_{-}}{\sigma} H_{\omega}(x) \mathbf{n}_{z} . \tag{6.28}
\end{equation*}
$$

By the way, integrating the first of these relations with the help of Eq. (26a), we may find that the linear density $\mathbf{J}$ of the surface currents (measured in $\mathrm{A} / \mathrm{m}$ ), is simply and fundamentally related to the applied magnetic field:

$$
\begin{equation*}
\mathbf{J}_{\omega} \equiv \int_{0}^{\infty} \mathbf{j}_{\omega}(x) d x=H_{\omega}^{(0)} \mathbf{n}_{z} \tag{6.29}
\end{equation*}
$$

Since this relation does not have frequency-dependent factors, we may sum it up for all frequencies and get a universal relation

$$
\begin{equation*}
\mathbf{J}(t)=H^{(0)}(t) \mathbf{n}_{z} \equiv H^{(0)}(t)\left(-\mathbf{n}_{y} \times \mathbf{n}_{x}\right)=\mathbf{H}^{(0)}(t) \times\left(-\mathbf{n}_{x}\right)=\mathbf{H}^{(0)}(t) \times \mathbf{n} \tag{6.30}
\end{equation*}
$$

where $\mathbf{n}=-\mathbf{n}_{X}$ is the outer normal to the surface - see Fig. 2b. This simple relation (whose last form is independent of the reference frame choice) is not occasional. Indeed, Eq. (30) may be readily obtained from the Ampère law (5.37) applied to a contour drawn around a fragment of the surface, but extending under it much deeper than the skin depth - see contour $C_{2}$ in Fig. 2b, regardless of the exact law of the

[^287]field penetration. Relation (30) is frequently called the "macroscopic" boundary condition for the magnetic field near conductor's surface, to distinguish it from the "microscopic" boundary condition (26).

For the skin effect, the fundamental relation between the surface current density and the external magnetic field means that the effect implementation does not require a dedicated ac magnetic field source. For example, it takes place in any wire that carries ac current, and leads to current concentration in a surface sheet of thickness $\sim \delta_{s}$. (Of course the quantitative analysis of this problem in a wire with an arbitrary cross-section may be technically complicated, because it requires to solve Eq. (18) for a 2D geometry; even for the round cross-section, the solution involves the Bessel functions.) In this case, the ac magnetic field outside the conductor, that still obeys Eq. (30), is better understood as the effect, rather than the reason, of the ac current flow.

Finally, the reader should mind the validity limits of these results - besides the universal Eq. (30). First, in order for the quasistatic approximation to be valid, frequency $\omega$ should not be too high, so that the skin depth (27) remains much smaller than the corresponding wavelength,

$$
\begin{equation*}
\lambda=\frac{2 \pi v}{\omega}=\left(\frac{4 \pi^{2}}{\varepsilon \mu \omega^{2}}\right)^{1 / 2} \tag{6.31}
\end{equation*}
$$

which decreases with $\omega$ faster than $\delta_{s}(27 \mathrm{~b})$. Note that the crossover frequency (at which $\delta_{s}=\lambda$ ),

$$
\begin{equation*}
\omega_{r}=\frac{\sigma}{\varepsilon}=\frac{\sigma}{\varepsilon_{r} \varepsilon_{0}} \tag{6.32}
\end{equation*}
$$

is nothing else than the reciprocal charge relaxation time (4.10). As was discussed in Sec. 4.2, for good metals this frequency is extremely high (about $10^{18} \mathrm{~s}^{-1}$ ).

A more practical upper limit on $\omega$ is that the skin depth $\delta_{s}$ should stay much larger than the mean free path $l$ of charge carriers. ${ }^{14}$ Beyond this point, a non-local relation between vectors $\mathbf{j}(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$ becomes essential. Both theory and experiment show that at $\delta_{s}<l$, the skin effect still persists, but acquires a slightly different frequency dependence, $\delta_{s} \propto \omega^{-1 / 3}$. Such anomalous skin effect has useful applications, for example, for experimental measurements of the Fermi surface in metals. ${ }^{15}$

### 6.3. Electrodynamics of superconductivity and gauge invariance

The effect of superconductivity ${ }^{16}$ takes place when temperature $T$ is reduced below a certain critical temperature $\left(T_{c}\right)$, specific for each material. For most metallic superconductors, $T_{c}$ is of the order of typically a few kelvins, though several exotic compounds (the so-called high-temperature superconductors) with $T_{c}$ above 100 K have been found since 1987 . The most notable property of superconductors is the absence, at $T<T_{c}$, of measurable resistance to not very high dc currents.

[^288]However, electromagnetic properties of superconductors cannot be described by just taking $\sigma=$ $\infty$ in our previous results. Indeed, for this case, Eq. (27b) would give $\delta_{s}=0$, i.e., no ac magnetic field penetration at all, while for the dc field we would have the uncertainty $\sigma \omega=$ ? Experiment shows something substantially different: weak magnetic fields do penetrate into superconductors by a materialspecific London penetration depth $\delta_{\mathrm{L}} \sim 10^{-7}-10^{-6} \mathrm{~m},{ }^{17}$ which is virtually frequency-independent until the skin depth $\delta_{s}$, measured in the same material in its "normal" state, i.e. the absence of superconductivity, becomes less than $\delta_{\mathrm{L}}$. (This crossover happens typically at frequencies $\sim 10^{13} \mathrm{~s}^{-1}$.) The smallness of $\delta_{\mathrm{L}}$ means that the magnetic field is pushed out of macroscopic samples at their transition into the superconducting state.

This Meissner-Ochsenfeld effect, discovered experimentally in 1933, ${ }^{18}$ may be partly understood using the following classical reasoning. When we discussed the physics of conductivity in Sec. 4.2, we implied that the current (and electric field) frequency $\omega$ is either zero or sufficiently low. In the classical Drude reasoning (see Sec. 4.2), this is acceptable while $\omega \tau \ll 1$, where $\tau$ is the effective carrier scattering time participating in Eqs. (4.12)-(4.13). If this condition is not satisfied, we should take into account the charge carrier inertia; moreover, in the opposite limit $\omega \tau \gg 1$ we may neglect the scattering at all. Classically, we can describe the charge carriers in such a "perfect conductor" as particles that are accelerated by the electric field in accordance with the $2^{\text {nd }}$ Newton law (4.11) at all times,

$$
\begin{equation*}
\dot{\mathbf{v}}=\frac{1}{m} \mathbf{F}=\frac{q}{m} \mathbf{E}, \tag{6.33}
\end{equation*}
$$

so that the current density $\mathbf{j}=q n \mathbf{v}$ they create changes in time as

$$
\begin{equation*}
\dot{\mathbf{j}}=\frac{q^{2} n}{m} \mathbf{E} \tag{6.34}
\end{equation*}
$$

In terms of the Fourier amplitudes (see the previous section), this means

$$
\begin{equation*}
-i \omega \mathbf{j}_{\omega}=\frac{q^{2} n}{m} \mathbf{E}_{\omega} \tag{6.35}
\end{equation*}
$$

Comparing this formula with the relation $\mathbf{j}_{\omega}=\sigma \mathbf{E}_{\omega}$ implied in the last section, we see that we can use all its results with the following replacement:

$$
\begin{equation*}
\sigma \rightarrow i \frac{q^{2} n}{m \omega} \tag{6.36}
\end{equation*}
$$

This change replaces the characteristic equation (24) with

$$
\begin{equation*}
-i \omega=\frac{\kappa^{2} m \omega}{i q^{2} n \mu} \tag{6.37}
\end{equation*}
$$

i.e. replaces the skin effect with the field penetration by the following frequency-independent depth:

[^289]\[

$$
\begin{equation*}
\delta=\left(\frac{m}{\mu q^{2} n}\right)^{1 / 2} \tag{6.38}
\end{equation*}
$$

\]

Superficially, this means that the field decay into the superconductor does not depend on frequency:

$$
\begin{equation*}
H(x, t)=H(0, t) \exp \left\{-\frac{x}{\delta}\right\} \tag{6.39}
\end{equation*}
$$

explaining the Meissner-Ochsenfeld effect.
However, there are two problems with this result. First, for the parameters typical for good metals ( $q=-e, n \sim 10^{29} \mathrm{~m}^{-3}, m \sim m_{e}, \mu \approx \mu_{0}$ ), Eq. (38) gives $\delta \sim 10^{-8} \mathrm{~m}$, a factor of $10-10^{2}$ lower than the typical experimental values of $\delta_{\mathrm{L}}$. Experiment also shows that the penetration depth diverges at $T \rightarrow T_{c}$, which is not predicted by Eq. (38). Another, much more fundamental problem with Eq. (38) is that it has been derived for $\omega \tau \gg 1$. Even is we assume that somehow there are no collisions at all, i.e. $\tau=\infty$, at $\omega \rightarrow 0$ both parts of the characteristic equation (37) vanish, and we cannot make any conclusion about $k$. This is not just a mathematical artifact we could ignore. For example, let us place a non-magnetic metal at $T>T_{c}$ into a static external magnetic field. The field will completely penetrate into the sample. Now let us cool it. As soon as the temperature drops below $T_{c}$, our calculations become valid, forbidding the penetration into the superconductor of any change of the field, so that the initial field would be "frozen" inside the sample. The experiment shows something completely different: as $T$ is lowered below $T_{c}$, the initial field is being pushed out of the sample.

The resolution of these contradictions has been provided by quantum mechanics. As was explained in 1957 in a seminal work by J. Bardeen, L. Cooper, and J. Schrieffer (commonly referred to the BSC theory), superconductivity is due to the correlated motion of electron pairs, with opposite spins and nearly opposite momenta. Such Cooper pairs, each with the electric charge $q=-2 e$ and zero spin, may form only in a narrow energy layer near the Fermi surface, of certain thickness $\Delta(T)$. Parameter $\Delta(T)$, which may be also considered as the binding energy of the pair, tends to zero at $T \rightarrow T_{\mathrm{c}}$, while at $T$ $\ll T_{c}$ it has a virtually constant value $\Delta(0) \approx 3.5 k_{\mathrm{B}} T_{c}$, of the order of a few meV for most superconductors. This fact readily explains the relatively low spatial density of the Cooper pairs: $n_{p}(T) \sim$ $n \Delta(T) / \varepsilon_{\mathrm{F}} \sim 10^{26} \mathrm{~m}^{-3}$. With the correction $n \rightarrow n_{p}$, our Eq. (38) for the penetration depth becomes

$$
\begin{equation*}
\delta \rightarrow \delta_{\mathrm{L}}=\left(\frac{m}{\mu q^{2} n_{p}(T)}\right)^{1 / 2} \tag{6.40}
\end{equation*}
$$

London penetration depth

This expression diverges at $T \rightarrow T_{c}$, and generally fits the experimental data reasonably well, at least for the so-called "clean" superconductors (with the mean free path $l \equiv v \tau$ much longer that the Cooper pair size $\xi$ - see below).

The smallness of the coupling energy $\Delta(T)$ is also a key factor in the explanation of the Meissner-Ochsenfeld effect, as well as several macroscopic quantum phenomena in superconductors. Because of Heisenberg's quantum uncertainty relation $\delta r \delta p \sim \hbar$, the Cooper-pair size (the so-called coherence length) is relatively large: $\xi \sim \delta r \sim \hbar / \delta p \sim \hbar \nu_{\mathrm{F}} / \Delta(T) \sim 10^{-6} \mathrm{~m}$. As a result, $n_{p} \xi^{3} \gg 1$, meaning that Cooper pairs are strongly overlapped in space. Now, due to their integer spin, Cooper pairs behave like bosons, which means in particular that at low temperature they exhibit the so-called Bose-Einstein
condensation onto the same energy level. ${ }^{19}$ This means that the frequency $\omega=E / \hbar$ of the time evolution of each pair's wavefunction $\Psi=\psi \exp \{-i \omega t\}$ is the same, i.e. that the phases $\varphi$ of the wavefunctions, defined by equation

$$
\begin{equation*}
\psi=|\psi| e^{i \varphi} \tag{6.41}
\end{equation*}
$$

become equal, so that the current is carried not by individual Cooper pairs but rather their Bose-Einstein condensate described by a single wavefunction. Due to this coherence, the quantum effects (which are, in usual Fermi-liquids of single electrons, masked by the statistical spread of phases $\varphi$ ), become very explicit - "macroscopic".

To illustrate this, let us write the well-known quantum-mechanical formula for the probability current of a free, non-relativistic particle, ${ }^{20}$

$$
\begin{equation*}
\mathbf{j}_{p}=\frac{i \hbar}{2 m}\left(\psi \nabla \psi^{*}-\text { c.c. }\right)=\frac{1}{2 m}\left[\psi^{*}(-i \hbar \nabla) \psi-\text { c.c. }\right] . \tag{6.42}
\end{equation*}
$$

Now let me borrow one result that will be proved later in the course (in Sec. 9.7) when we discuss the analytical mechanics of a charged particle moving in an electromagnetic field. Namely, in order to account for the magnetic field effects, particle's kinetic momentum $\mathbf{p}$, equal to $m \mathbf{v}$ (where $\mathbf{v} \equiv d \mathbf{r} / d t$ is particle's velocity) has to be distinguished from its canonical momentum, ${ }^{21}$

$$
\begin{equation*}
\mathbf{P} \equiv \mathbf{p}+q \mathbf{A} . \tag{6.43}
\end{equation*}
$$

where $\mathbf{A}$ is the vector-potential of the field - see Eq. (5.27). In contrast with Cartesian components $p_{j}=$ $m u_{j}$ of momentum $\mathbf{p}$, the canonical momentum components are the generalized momenta corresponding to components $r_{j}$ of the radius-vector $\mathbf{r}$, considered as generalized coordinates of the particle: $P_{j}=$ $\partial \mathcal{L} / \partial v_{j}$, where $\mathcal{L}$ is the particle's Lagrangian function. According to the general rules of transfer from classical to quantum mechanics, ${ }^{22}$ it is vector $\mathbf{P}$ whose operator (in the Schrödinger picture) equals $-i \hbar \nabla$, so that the operator of kinetic momentum $\mathbf{p}=\mathbf{P}-q \mathbf{A}$ is equal to $-i \hbar \nabla-q \mathbf{A}$. Hence, the in order to account for the magnetic field effects, we should make the following replacement:

$$
\begin{equation*}
-i \hbar \nabla \rightarrow-i \hbar \nabla-q \mathbf{A} . \tag{6.44}
\end{equation*}
$$

In particular, Eq. (42) has to be replaced with

$$
\begin{equation*}
\mathbf{j}_{p}=\frac{1}{2 m}\left[\psi^{*}(-i \hbar \nabla-q \mathbf{A}) \psi-\text { c.c. }\right] . \tag{6.45}
\end{equation*}
$$

This expression becomes more transparent if we take the wavefunction in form (41):

[^290]\[

$$
\begin{equation*}
\mathbf{j}_{p}=\frac{\hbar}{m}|\psi|^{2}\left(\nabla \varphi-\frac{q}{\hbar} \mathbf{A}\right) . \tag{6.46}
\end{equation*}
$$

\]

This relation means, in particular, that in order to keep $\mathbf{j}$ invariant, the gauge transformation (8)-(9) has to be accompanied by a simultaneous transformation of the wavefunction phase:

$$
\begin{equation*}
\varphi \rightarrow \varphi+\frac{q}{\hbar} \chi \tag{6.47}
\end{equation*}
$$

It is fascinating that the quantum-mechanical wavefunction (more exactly, its phase) is not gaugeinvariant - meaning that you may change it in your mind - at will! Again, this does not change any observable (such as $\mathbf{j}$ or the probability density $\psi \psi^{*}$ ), i.e. any experimental results.

For the electric current density of the whole superconducting condensate, Eq. (46) yields

$$
\begin{equation*}
\mathbf{j}=\frac{\hbar q n_{p}(T)}{m}\left(\nabla \varphi-\frac{q}{\hbar} \mathbf{A}\right) . \tag{6.48}
\end{equation*}
$$

This equation shows that this supercurrent may be induced by dc magnetic field alone and does not require any electric field. Indeed, for the simplest, 1D geometry shown in Fig. 2a, $\mathbf{j}(\mathbf{r})=j(x) \mathbf{n}_{z}, \mathbf{A}(\mathbf{r})=$ $A(x) \mathbf{n}_{z}$, and $\partial / \partial z=0$, so that the Coulomb gauge condition (5.48) is satisfied for any choice of the gauge function $\chi(x)$, and for the sake of simplicity we can choose it to provide $\varphi(\mathbf{r}) \equiv$ const, ${ }^{23}$ so that

$$
\begin{equation*}
\mathbf{j}=-\frac{q^{2} n_{p}(T)}{m} \mathbf{A} . \tag{6.49}
\end{equation*}
$$

This is the so-called London equation, proposed (in a different form) by brothers F. and H. London in 1935 for a phenomenological description of the Meissner-Ochsenfeld effect. Combining it with Eq. (5.47), generalized for an arbitrary uniform media by the replacement $\mu_{0} \rightarrow \mu$, we get

$$
\begin{equation*}
\nabla^{2} \mathbf{A}=\frac{\mu q^{2} n_{p}(T)}{m} \mathbf{A} \tag{6.50}
\end{equation*}
$$

This simple differential equation, similar in structure to Eq. (18), has a similar exponential solution,

$$
\begin{equation*}
A(x)=A(0) \exp \left\{-\frac{x}{\delta_{L}}\right\}, \quad B(x)=B(0) \exp \left\{-\frac{x}{\delta_{L}}\right\}, \quad j(x)=j(0) \exp \left\{-\frac{x}{\delta_{L}}\right\}, \tag{6.51}
\end{equation*}
$$

that shows that the magnetic field and supercurrent penetrate into a superconductor only by the London's penetration depth $\delta_{\mathrm{L}}$, given by Eq. (40), regardless of frequency. ${ }^{24}$ By the way, integrating the last result through the penetration layer, and using Eqs. (34), (43) and the vector-potential definition, B $=\nabla \times \mathbf{A}$ (for our geometry, giving $B(x)=d A(x) / d x=-\delta_{\mathrm{L}} A(x)$ ) we may check that the linear density $\mathbf{J}$ of the surface supercurrent still satisfies the universal relation (30).

[^291]Let me hope that the physical intuition of the reader enables him or her to make the following semi-quantitative generalization of the quantitative solution (51) to superconductor sample of arbitrary shape: B and $\mathbf{j}$ may only penetrate into the sample by distances of the order of $\delta_{\mathrm{L}}(0)$. In particular, for samples much larger than $\delta_{\mathrm{L}}$, the London theory gives the following "macroscopic" description of the Meissner-Ochsenfeld effect: $\mathbf{j}=0$ and $\mathbf{B}=0$ everywhere inside a superconductor. In this coarse description, the bulk superconductor sample behaves as an ideal diamagnet, with $\mu=0 .{ }^{25}$ In particular, we can use this analogy and the first of Eqs. (5.125) to immediately obtain the magnetic field distribution outside a superconducting sphere:

$$
\begin{equation*}
\mathbf{B}=\mu_{0} \mathbf{H}=-\mu_{0} \nabla \phi_{m}, \quad \phi_{m}=H_{0}\left(-r-\frac{R^{3}}{2 r^{2}}\right) \cos \theta \tag{6.52}
\end{equation*}
$$

Figure 3 shows the corresponding surfaces of equal potential $\phi_{m}$. It is evident that the magnetic field lines (normal to the equipotential surfaces) bend to become parallel to the superconductor's surface. By the way, this pattern illustrates the answer to the question that might arise at making assumption (19): what happens to superconductors in a normal magnetic field? The answer is: the field is deformed outside the superconductor to provide $B_{n}=0$ at the surface - otherwise, due to the continuity of $B_{n}$, the magnetic field would penetrate the superconductor, which is impossible. Of course this answer should be taken with a grain of salt: strong magnetic fields do penetrate into superconductors, destroying superconductivity (completely or partly), thus violating the Meissner-Ochsenfeld effect. Such a penetration by itself features several interesting electrodynamic effects, for whose discussion we unfortunately do not have time. ${ }^{26}$


Fig. 6.3. Surfaces of constant scalar potential $\phi_{m}$ of magnetic field around a superconducting sphere of radius $R \gg \delta_{\mathrm{L}}$, placed into a weak uniform, vertical magnetic field.

### 6.4. Electrodynamics of macroscopic quantum phenomena

We have seen that for the ac magnetic field penetration, the quantum theory of superconductivity gives essentially the same result as the classical theory of a perfect conductor - cf. Eqs. (39) and (51) with the "only" conceptual exception that the former theory extends the effect to dc fields. However, the

[^292]quantum theory of superconductors is much more rich. For example, let us use Eq. (48) to derive the fascinating effect of magnetic flux quantization. Consider a closed ring made of a superconducting "wire" with a cross-section much larger than $\delta_{\mathrm{L}}{ }^{2}$ (Fig. 4a).


Fig. 6.4. (a) Closed, flux-quantizing superconducting ring, (b) a ring cut with a narrow slit, and (c) a Superconducting QUantum Interference Device (SQUID).

From the last section's analysis, we know that deep inside the wire the supercurrent is exponentially small. Integrating Eq. (48) along any closed contour $C$ that does not approach the surface closer than a few $\delta_{\mathrm{L}}$ at any point, we get

$$
\begin{equation*}
\oint_{C} \nabla \varphi \cdot d \mathbf{r}-\frac{q}{\hbar} \oint_{C} \mathbf{A} \cdot d \mathbf{r}=0 . \tag{6.53}
\end{equation*}
$$

The first integral, i.e. the difference of $\varphi$ in the initial and final points, has to be equal to either zero or an integer number of $2 \pi$, because the change $\varphi \rightarrow \varphi+2 \pi n$ does not change condensate's wavefunction:

$$
\begin{equation*}
\psi^{\prime}=|\psi| e^{i(\varphi+2 \pi n)}=|\psi| e^{i \varphi}=\psi \tag{6.54}
\end{equation*}
$$

On the other hand, the second integral in Eq. (53) is just the magnetic flux $\Phi$ (1) through the contour and, due to the Meissner-Ochsenfeld effect, through the superconducting ring as a whole. As a result, we get

$$
\begin{equation*}
\Phi=n \Phi_{0}, \quad \Phi_{0} \equiv \frac{2 \pi \hbar}{q}=\frac{h}{q}, \quad n=0, \pm 1, \pm 2, \ldots \tag{6.55}
\end{equation*}
$$

i.e. the magnetic flux can only take values multiple of the flux quantum $\Phi_{0}$. This effect, predicted in 1950 by the same Fritz London (who expected $q$ to be equal to the electron charge $-e$ ), was confirmed experimentally in $1961,{ }^{27}$ with $|q|=2 e$ (so that in superconductors $\Phi_{0}=h / 2 e \approx 2.07 \times 10^{-15} \mathrm{~Wb}$ ). Historically, this observation gave a decisive support to the BSC theory of the Cooper pairs as the basis of superconductivity, which had been put forward just 4 years before. ${ }^{28}$

[^293]The flux quantization is just one of the so-called macroscopic quantum effects in superconductivity. Consider, for example, a superconducting ring interrupted with a very narrow slit (Fig. 4b). Integrating Eq. (48) along the current-free path from point 1 to point 2, along the dashed line in Fig. 4 (again, deeper than $\delta_{\mathrm{L}}(T)$ from the surface), we get

$$
\begin{equation*}
0=\int_{1}^{2}\left(\nabla \varphi-\frac{q}{\hbar} \mathbf{A}\right) \cdot d \mathbf{r}=\varphi_{2}-\varphi_{1}-\frac{q}{\hbar} \Phi . \tag{6.56}
\end{equation*}
$$

Using the flux quantum definition (55), this result may be rewritten as

phase difference

$$
\begin{equation*}
\varphi \equiv \varphi_{1}-\varphi_{2}=\frac{2 \pi}{\Phi_{0}} \Phi \tag{6.57}
\end{equation*}
$$

where $\varphi$ is called the Josephson phase difference. In contrast to each of the phases $\varphi_{1,2}$, their difference $\varphi$ is gauge-invariant, because it is directly related to the gauge-invariant magnetic flux.

Can this $\varphi$ be measured? Yes, using the Josephson effect. ${ }^{29}$ In order to understand his prediction, let us take two (for the argument simplicity, similar) superconductors, connected with some sort of weak link, for example a tunnel barrier or a short normal-metal bridge, through that a small Cooper pair current can flow. (Such system of two coupled superconductors is now called a Josephson junction.) Let us think what this supercurrent I may be a function of. For that, the reverse thinking is helpful: let us imagine we can change current from outside; what parameter of the superconducting condensate can it affect?

If the current is weak, it cannot perturb the superconducting condensate density, proportional to $|\psi|^{2}$; hence it may only change the Cooper condensate phases $\varphi_{1,2}$. However, according to Eq. (41), the phases are not gauge-invariant, while the current should be, hence I may affect - or should be a function of - the phase difference $\varphi$ defined by Eq. (57). Moreover, just has already been argued during the flux quantization discussion, a change of any of $\varphi_{1,2}$ (and hence of $\varphi$ ) by $2 \pi$ or any of its multiples should not change the current. In addition, if the wavefunction is the same in both superconductors $(\varphi=0)$, supercurrent should vanish due to the system symmetry. Hence function $I(\varphi)$ should satisfy conditions

$$
\begin{equation*}
I(0)=0, \quad I(\varphi+2 \pi)=I(\varphi) \tag{6.58}
\end{equation*}
$$

With this understanding, we should not be terribly surprised by the following Josephson's result that for the weak link provided by weak tunneling, ${ }^{30}$

$$
\begin{equation*}
I(\varphi)=I_{c} \sin \varphi, \tag{6.59}
\end{equation*}
$$

superconductors, whose coherence length $\xi$ is smaller than the London's penetration depth $\delta_{\mathrm{L}}(T)$, in the form of self-formed tubes surrounded by vortex-shaped supercurrents - the so-called Abrikosov vortices, with the superconductivity suppressed near the middle of each tube. This suppression makes each flux tube topologically equivalent to a superconducting ring, with the magnetic flux through it equal to one flux quantum, and its ends being magnetically similar to magnetic monopoles - see Sec. 5.6 above.
${ }^{29}$ It was predicted in 1961 by B. Josephson (then a PhD student!), and observed experimentally by several groups soon after that.
${ }^{30}$ For some other types of weak links, function $I(\varphi)$ may deviate from the sine form (59) rather considerably, still satisfying the general requirements (58).
where constant $I_{c}$, which depends on of the strength of the weak link and temperature, is called the critical current.

Let me show how such expression may be derived, for a narrow and short weak link made of a normal metal or a superconductor. ${ }^{31}$ Microscopic theory of superconductivity shows that, within certain limits, the Bose-Einstein condensate of Cooper pairs may be described by the following nonlinear Schrödinger equation ${ }^{32}$

$$
\begin{equation*}
\frac{1}{2 m}(-i \hbar \nabla-q \mathbf{A})^{2} \psi+U(r) \psi=\varepsilon \psi+\psi \times\left(\text { a nonlinear function of }|\psi|^{2}\right) . \tag{6.60}
\end{equation*}
$$

The first three terms of this equation are similar to those of the usual Schrödinger equation (which conserves the number of particles), while the nonlinear function in the last term describes the formation and dissolution of Cooper pairs, and in particular gives the equilibrium value of $n_{s}$ as a function of temperature. Now let the weak link size scale $a$ be much smaller than both the Cooper pair size $\xi$ and the London's penetration depth $\delta_{\mathrm{L}}$. The first of these relations ( $a \ll \xi$ ) makes the first term in Eq. (60), that scales as $1 / a^{2}$, much larger than all other terms, while the latter relation ( $a \ll \delta_{\mathrm{L}}$ ) allows one to neglect magnetic field effects, and hence drop term ( $-q \mathbf{A}$ ) from the parenthesis in Eq. (60), reducing it to just our familiar Laplace equation for the wavefunction:

$$
\begin{equation*}
\nabla^{2} \psi=0 \tag{6.61}
\end{equation*}
$$

Since the weak coupling cannot change $|\psi|$ in bulk superconducting electrodes, Eq. (61) may be solved with the following simple boundary conditions:

$$
\psi(r) \rightarrow \begin{cases}|\psi| e^{i \varphi_{1}}, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{1}  \tag{6.62}\\ |\psi| e^{i \varphi_{2}}, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{2}\end{cases}
$$

where $\mathbf{r}_{1}$ and $\mathbf{r}_{2}$ are some points well inside the corresponding superconductors, i.e. at distances much larger than $a$ from the weak link center. It is straightforward to verify that the solution of this boundary problem for complex function $\psi$ may be expressed as follows,

$$
\begin{equation*}
\psi(\mathbf{r})=|\psi| e^{i \varphi_{1}} f(\mathbf{r})+|\psi| e^{i \varphi_{1}}(1-f(\mathbf{r})) \tag{6.63}
\end{equation*}
$$

via the real function $f(\mathbf{r})$ that satisfies the Laplace equation and the following boundary conditions:

$$
f(\mathbf{r}) \rightarrow \begin{cases}1, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{1}  \tag{6.64}\\ 0, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{2}\end{cases}
$$

Function $f(\mathbf{r})$ depends on the weak link geometry and may be rather complicated, but we do not

[^294]need to know it to get the most important result. Indeed, plugging this solution into Eq. (48) (with term $q \mathbf{A}$ ignored as being negligibly small), we get
\[

$$
\begin{equation*}
\mathbf{j}_{p}=-\frac{\hbar}{m}|\psi|^{2} \nabla f \sin \varphi, \quad \text { so that } \mathbf{j}=-\frac{\hbar q n_{p}(T)}{m} \nabla f \sin \varphi . \tag{6.65}
\end{equation*}
$$

\]

Integrating this relation over any cross-section $S$ of the weak link, we arrive at Josephson's result (59), with the following critical current:

$$
\begin{equation*}
I_{c}=-\frac{\hbar q n_{p}(T)}{m} \int_{S}(\nabla f)_{n} d^{2} r . \tag{6.66}
\end{equation*}
$$

This expression may be readily evaluated via the resistance of the same weak link in the "normal" (non-superconducting) state, say at $T>T_{c}$. Indeed, as we know from Sec. 4.3, the distribution of the electrostatic potential $\phi$ at normal conduction also obeys the Laplace equation, with boundary conditions that may be taken in the form

$$
\phi(\mathbf{r}) \rightarrow \begin{cases}V, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{1}  \tag{6.67}\\ 0, & \text { for } \mathbf{r} \rightarrow \mathbf{r}_{2}\end{cases}
$$

Comparing the boundary problem for $\phi(\mathbf{r})$ with that for function $f(\mathbf{r})$, we get $\phi=V f$. This means that the gradient $\nabla f$, which participates in Eq. (66), is just $(-E / V)=(-\mathbf{j} / \sigma V)$. Hence the integral in that formula is just $-I / \sigma V=-1 / \sigma R_{n}$, where $R_{n}$ is the resistance of the Josephson junction in its normal state. As a result, Eq. (66) yields

$$
\begin{equation*}
I_{c}=\frac{\hbar q n_{p}(T)}{m \sigma} \frac{1}{R_{n}}, \tag{6.68}
\end{equation*}
$$

showing that the $I_{c} R_{n}$ product does not depend on the junction geometry, though it does depend on temperature, vanishing, together with $n_{p}(T)$, at $T \rightarrow T_{\mathrm{c}}$. (Well below the critical temperature, $I_{c} R_{n}$ of a sufficiently short weak links is of the order of $\Delta(0) / e$, i.e. of the order of a few mV .)

Now let us see what happens if a Josephson junction is placed into the gap in a superconductor ring - see Fig. 4c. In this case, we can combine Eqs. (57) and (59), getting

Macroscopic quantum interference

$$
\begin{equation*}
I=I_{c} \sin 2 \pi \frac{\Phi}{\Phi_{0}} \tag{6.69}
\end{equation*}
$$

This effect of periodic dependence of the current on flux is called the macroscopic quantum interference, ${ }^{33}$ while the system shown in Fig. 4b, a superconducting quantum interference device, abbreviated as SQUID (with all letters capital, please :-). The low value of the magnetic flux quantum $\Phi_{0}$, and hence the high sensitivity of $\varphi$ to the magnetic field, allows using SQUIDs as ultrasensitive magnetometers. Indeed, for a superconducting ring of area $\sim 1 \mathrm{~cm}^{2}$, one period of the change of supercurrent (69) is produced by magnetic filed change of the order of $10^{-11} \mathrm{~T}\left(10^{-7} \mathrm{Gs}\right)$, while sensitive electronics allows to measure a tiny fraction of this period - limited by thermal noise at a level of the

[^295]order of a few pT . This sensitivity allows measurements, for example, of the magnetic fields induced by the beating human heart, and even by brain activity, outside of the body.

An important aspect of the quantum interference is the so-called Aharonov-Bohm (AB) effect. ${ }^{34}$ Let the magnetic field lines be limited to the central part of the SQUID ring, so that no appreciable magnetic field ever touches the superconducting ring material. (This may be done experimentally with very good accuracy, for example using high- $\mu$ magnetic cores - see their discussion in Sec. 5.6.) As predicted by Eq. (69), and confirmed by several careful experiments carried out in the mid-1960s, ${ }^{35}$ this restriction does not matter - the interference is observed anyway. This means that not only the magnetic field $\mathbf{B}$, but also the vector-potential $\mathbf{A}$ represents physical reality, albeit quite a peculiar one remember the gauge transformation?

Actually, the magnetic flux quantization (55) and the macroscopic quantum interference (69) are not completely different effects, but just two manifestations of the whole group of inter-related macroscopic quantum phenomena. In order to show that, one should note that if critical current $I_{c}$ (or rather its product by loop's self-inductance $L$ ) is high enough, flux $\Phi$ in the SQUID loop is due not only to the external magnetic field flux $\Phi_{e}$, but also has a self-field component - cf. Eq. (5.61):36

$$
\begin{equation*}
\Phi=\Phi_{\mathrm{ext}}-L I, \quad \text { where } \Phi_{\mathrm{ext}} \equiv \int_{S}\left(B_{\mathrm{ext}}\right)_{n} d^{2} r . \tag{6.70}
\end{equation*}
$$

Now the relation between $\Phi$ and $\Phi_{\text {ext }}$ may be found by solving this equation together with Eq. (69). Figure 5 shows this relation for several values of the dimensionless parameter $\lambda \equiv 2 \pi L I_{c} / \Phi_{0}$.


Fig. 6.5. Function $\Phi\left(\Phi_{\text {ext }}\right)$ for SQUIDs with various values of the normalized $L I_{c}$ product. Dashed arrows show the flux leaps as the external field is changed. (The branches with $d \Phi / d \Phi_{\text {ext }}<0$ are unstable.)

[^296]These plots show that if the critical current or (or the inductance) is low, $\lambda \ll 1$, the self-effects are negligible, and the total flux follows the external field (i.e., $\Phi_{\text {ext }}$ ) quite faithfully. However, at $\lambda>1$, the dependence $\Phi\left(\Phi_{\mathrm{ext}}\right)$ becomes hysteretic, and at $\lambda \gg 1$ the positive-slope (stable) branches of this function are nearly flat, with the total flux values corresponding to Eq. (55). Thus, a superconducting ring closed by a high- $I_{c}$ Josephson junction exhibits a nearly-perfect flux quantization.

The self-field effects described by Eq. (70) create certain technical problems for SQUID magnetometry, but they are the basis for one more application of these devices: ultrafast computing. Indeed, Fig. 5 shows that at the values of $\lambda$ modestly above 1 (e.g., $\lambda \approx 3$ ), and within a certain range of applied field, the SQUID has two stable flux states that differ by $\Delta \Phi \approx \Phi_{0}$ and may be used for coding binary 0 and 1 . For practical superconductors (like Nb ), the time of switching between these states (see dashed arrows in Fig. 4) are of the order of a picosecond, while the energy dissipated at such event may be as low as $\sim 10^{-19} \mathrm{~J}$. (This bound is determined not by device's physics, by the fundamental requirement for the energy barrier between the two states to be much higher than the thermal fluctuation energy scale $k_{\mathrm{B}} T$, ensuring a sufficiently long information retention time.) While the picosecond switching speed may be also achieved with some semiconductor devices, the power consumption of the SQUID-based digital devices may be 5 to 6 orders of magnitude lower, enabling VLSI circuits with $100-\mathrm{GHz}$-scale clock frequencies and manageable power dissipation. Unfortunately, the range of practical application of these Rapid Single-Flux-Quantum (RSFQ) logic circuits is still narrow, due to the inconvenience of their deep refrigeration to temperatures below $T_{c} .{ }^{37}$

Since we have already got the basic relations (57) and (59) describing the macroscopic quantum phenomena in superconductivity, let me mention in brief two other members of this group, called the Josephson effects. Differentiating Eq. (57) over time, and using the Faraday induction law (2), we get ${ }^{38}$

$$
\begin{equation*}
\frac{d \varphi}{d t}=\frac{2 e}{\hbar} V . \tag{6.71}
\end{equation*}
$$

This famous phase-to-voltage relation should be valid regardless of the way how voltage $V$ has been created, ${ }^{39}$ so let us apply Eqs. (59) and (71) to the simplest circuit with a non-superconducting source of dc voltage - see Fig. 6.


Fig. 6.6. DC-voltage-biased Josephson junction.

[^297]If current $I$ is below the critical value,

$$
\begin{equation*}
-I_{c}<I<+I_{c}, \tag{6.72}
\end{equation*}
$$

Eq. (59) allows phase $\varphi$ to have a time-independent value

$$
\begin{equation*}
\varphi=\sin ^{-1} \frac{I}{I_{c}} \tag{6.73}
\end{equation*}
$$

and hence, according to Eq. (71), a vanishing voltage drop across the junction: $V=0$. This dc Josephson effect is not quite surprising - indeed, we have postulated from the very beginning that the Josephson junction may pass a certain supercurrent. Much more fascinating is the so-called ac Josephson effect that takes place if voltage across the junction has a nonvanishing average (dc) component $V_{0}$. For simplicity, let us assume that this is the only voltage component: $V(t)=V_{0}=$ const, ${ }^{40}$ then Eq. (71) may be readily integrated to give $\varphi=\omega_{\mathrm{J}} t+\varphi_{0}$, where

$$
\begin{equation*}
\omega_{\mathrm{J}} \equiv \frac{2 e}{\hbar} V_{0} . \tag{6.74}
\end{equation*}
$$

This result, plugged into Eq. (59), shows that supercurrent oscillates,

$$
\begin{equation*}
I(\varphi)=I_{c} \sin \left(\omega_{\mathrm{J}} t+\varphi_{0}\right) \tag{6.75}
\end{equation*}
$$

with the Josephson frequency $\omega_{\mathrm{J}}$ (74), which is proportional to the applied dc voltage. For practicable voltages, frequency $f_{\mathrm{J}}=\omega_{\mathrm{J}} / 2 \pi$ corresponds to the GHz or even THz ranges, because the proportionality coefficient in Eq. (74) is very high: $f_{\mathrm{J}} / V_{0}=2 e / h \approx 483 \mathrm{MHz} / \mu \mathrm{V} .41$ An important experimental fact is the universality of this coefficient. For example, in the mid-1980s, the group led by Prof. J. Lukens of our department proved that this factor is material-independent with the relative accuracy of at least $10^{-15}$. Very few experiments, especially in solid state physics, have ever reached such precision.

This fundamental nature of the Josephson voltage-to-frequency relation (74) allows an important application of the ac Josephson effect in metrology. Namely, phase locking the Josephson oscillations with an external microwave signal derived from an atomic frequency standards one can get the most precise dc voltage than from any other source. In NIST and other metrological institutions around the globe, this effect is used for the calibration of simpler "secondary" voltage standards that can operate at room temperature. ${ }^{42}$

### 6.5. Inductors, transformers, and ac Kirchhoff laws

Let a wire coil (meaning either a single loop illustrated in Fig. 5.4b, or a series of such loops, such as one of the solenoids shown in Fig. 5.6) have size $a$ that satisfies, at frequencies of our interest, the quasistatic limit condition $a \ll \lambda$. Moreover, let the coil's self-inductance $L$ be much larger than that of the wires connecting it to other components of our system: ac voltage sources, voltmeters, etc. (Since,

[^298]according to Eq. (5.75), (5.113), $L$ scales as the number $N$ of wire turns squared, this is easier to achieve at $N \gg 1$.) Then in a system consisting of such lumped induction coils and external wires (and other circuit elements such as resistors, capacitances, etc.), we may neglect the electromagnetic induction effects everywhere outside the coil, so that the electric field in those external regions is potential. Then the voltage $V$ between coil's terminals may be defined (as in electrostatics) as the difference of values of scalar potential $\phi$ between the terminals, i.e. as integral
\[

$$
\begin{equation*}
V=\int \mathbf{E} \cdot d \mathbf{r} \tag{6.76}
\end{equation*}
$$

\]

between the coil terminals along any path outside the coil. This voltage has to be balanced by the induction e.m.f. (2) in the coil, so that if the Ohmic resistance of the coil is negligible, ${ }^{43}$ we may write

$$
\begin{equation*}
V=\frac{d \Phi}{d t} \tag{6.77}
\end{equation*}
$$

where $\Phi$ is the magnetic flux in the coil. If the flux is due to the current $I$ in the same coil only (i.e. if it is magnetically uncoupled from other coils), we may use Eq. (5.70) to get the well-known relation

$$
\begin{equation*}
V=L \frac{d I}{d t} \tag{6.78}
\end{equation*}
$$

where the compliance with the Lenz sign rule is achieved by selecting the relations between the assumed voltage polarity and current direction as shown in Fig. 7a.


Fig. 6.7. (a) Induction coil, (b) two inductively coupled coils, and (c) an ac transformer.

If similar conditions are satisfied for two magnetically coupled coils (Fig. 7b), then, in Eq. (77), we need to use Eqs. (5.69) instead, getting

$$
\begin{equation*}
V_{1}=L_{1} \frac{d I_{1}}{d t}+M \frac{d I_{2}}{d t}, \quad V_{2}=L_{2} \frac{d I_{2}}{d t}+M \frac{d I_{1}}{d t} \tag{6.79}
\end{equation*}
$$

where the repeating index is dropped for notation simplicity. Such systems of inductively coupled coils have numerous applications in electrical engineering and physical experiment. ${ }^{44}$ Probably the most important is the ac transformer (Fig. 7c) where both coils share a common soft-ferromagnetic core. As we already know, such material (with $\mu \gg \mu_{0}$ ) tries to not let any magnetic field lines out, so that the magnetic flux $\Phi(t)$ in the core is nearly the same in each of its cross-sections. This gives

$$
\begin{equation*}
V_{1} \approx N_{1} \frac{d \Phi}{d t}, \quad V_{2} \approx N_{2} \frac{d \Phi}{d t} \tag{6.80}
\end{equation*}
$$

[^299]where $N_{1,2}$ is the number of wire turns in each coil, so that the voltage ratio is completely determined by the $N_{1} / N_{2}$ ratio.

Now we may generalize, to the ac current case, the notion of an electric circuit, already discussed in Chapter 4 - see Fig. 4.3 reproduced in Fig. 8a below. Let not only wire inductances but also wire capacitances be negligible in comparison with those of compact (lumped) capacitances. Then we may present the circuit as the connection of lumped circuit elements with ideal (voltage- and charge-free wires), with the list of its circuit elements now including not only resistors and current sources (as in the dc case), but also induction coils (including magnetically coupled ones) and capacitors - see Fig. 8b.


(b)

Fig. 6.8. (a) Typical ac system obeying ac Kirchhoff laws in the quasistatic approximation, and (b) the simplest circuit elements.

In the quasi-static limit, current through each wire is conserved, so that the "node rule", i.e. the $1^{\text {st }}$ Kirchhoff law (4.7),

$$
\begin{equation*}
\sum_{j} I_{j}=0 . \tag{6.81}
\end{equation*}
$$

remains valid. Also, if the electromagnetic induction effect is restricted to the interiors of lumped induction coils as discussed above, voltage drops $V_{k}$ across each circuit element may be still presented, just as in dc circuits, as differences of potentials of the adjacent nodes, so that the "loop rule", i.e. $2^{\text {nd }}$ Kirchhoff law given by Eq. (4.8),

$$
\begin{equation*}
\sum_{k} V_{k}=0 \tag{6.82}
\end{equation*}
$$

is also valid.
In contrast to the dc case, Eqs. (81) and (82) are now the (ordinary) differential equations. However, if all circuit elements are linear (as in the examples presented in Fig. 8b), these equations may be readily reduced to linear algebraic equations using the Fourier expansion. (In the most common case of sinusoidal ac sources, the final stage of Fourier series summation is unnecessary.) I do not have time to discuss even the simplest examples of such circuits, such as $L C, L R, R C$, and $L R C$ loops and periodic structures, ${ }^{45}$ but my experience shows that the potential readers of these notes are well familiar with these problems from their undergraduate studies. Let me only emphasize again that the standard ac

[^300]circuit theory is only valid within the quasistatic limit $a \ll \lambda$, and only under the condition of the electric and magnetic field confinement inside lumped circuit elements.

### 6.6. Displacement currents

The electromagnetic induction is not the only new effect arising in non-stationary electrodynamics. Indeed, though Eqs. (16) are adequate for the description of quasistatic phenomena, a deeper analysis shows that one of these equations, namely $\nabla \times \mathbf{H}=\mathbf{j}$, cannot be exact. To see that, let us take the divergence of its both sides of this equation:

$$
\begin{equation*}
\nabla \cdot(\nabla \times \mathbf{H})=\nabla \cdot \mathbf{j} . \tag{6.83}
\end{equation*}
$$

But, as the divergence of any curl, ${ }^{46}$ the left hand part should equal zero. Hence we get

$$
\begin{equation*}
\nabla \cdot \mathbf{j}=0 \tag{6.84}
\end{equation*}
$$

This is fine in statics, but in dynamics this equation forbids any charge accumulation, because according to the continuity relation (4.5),

$$
\begin{equation*}
\nabla \cdot \mathbf{j}=-\frac{\partial \rho}{\partial t} \tag{6.85}
\end{equation*}
$$

This discrepancy had been recognized by James Clerk Maxwell who suggested, in 1864, a way out of this contradiction. If we generalize the equation for $\boldsymbol{\nabla} \times \mathbf{H}$ by adding to term $\mathbf{j}$ (that describes real currents) the so-called displacement current term,

$$
\begin{equation*}
\mathbf{j}_{d} \equiv \frac{\partial \mathbf{D}}{\partial t} \tag{6.86}
\end{equation*}
$$

(that of course vanishes in statics), then the equation takes the form

$$
\begin{equation*}
\nabla \times \mathbf{H}=\mathbf{j}+\mathbf{j}_{d}=\mathbf{j}+\frac{\partial \mathbf{D}}{\partial t} . \tag{6.87}
\end{equation*}
$$

In this case, due to equation $\nabla \cdot \mathbf{D}=\rho$, the divergence of the right hand part equals zero due to the continuity relation (4.5), and the discrepancy is removed.

This conclusion, and equation (87), are so important that it is worthwhile to have one more look at its derivation, using a particular "electrical engineering" model shown in Fig. 9.47 Neglecting the fringe field effects, we may use Eq. (4.1) to describe the relation between current $I$ flowing through a wire and the electric charge $Q$ of the capacitor: ${ }^{48}$

[^301]\[

$$
\begin{equation*}
\frac{d Q}{d t}=I . \tag{6.88}
\end{equation*}
$$

\]

Now let us consider a closed contour $C$ drawn around the wire. (Solid points in Fig. 9 show the places where the contour intercepts the plane of drawing.) This contour may be seen as either the line limiting surface $S_{1}$ (crossed by the wire) or the line limiting surface $S_{2}$ (avoiding such crossing by passing through capacitor's gap). Applying the macroscopic Ampère law (5.117) to the former surface, we get

$$
\begin{equation*}
\oint_{C} \mathbf{H} \cdot d \mathbf{r}=\int_{S_{1}} j_{n} d^{2} r=I, \tag{6.89}
\end{equation*}
$$

while for the latter surface the same law gives a different result,

$$
\begin{equation*}
\oint_{C} \mathbf{H} \cdot d \mathbf{r}=\int_{S_{2}} j_{n} d^{2} r=0, \quad[\mathrm{WRONG}!] \tag{6.90}
\end{equation*}
$$

for the same integral. This is just an integral-form manifestation of the discrepancy outlined above, but it shows clearly how serious the problem is (or rather it was - before Maxwell).


Now let us see how the introduction of the displacement currents saves the day, considering for the sake of simplicity a plane capacitor of area $A$, with a constant electrode spacing. In this case, as we already know, the field inside it is uniform, with $D=\sigma$, so that the total capacitor's charge $Q=A \sigma=$ $A D$, and current (88) may represented as

$$
\begin{equation*}
I=\frac{d Q}{d t}=A \frac{d D}{d t} . \tag{6.91}
\end{equation*}
$$

So, instead of Eq. (90), the modified Ampère law gives

$$
\begin{equation*}
\oint_{C} \mathbf{H} \cdot d \mathbf{r}=\int_{S_{2}}\left(j_{d}\right)_{n} d^{2} r=\int_{S_{2}} \frac{\partial D_{n}}{\partial t} d^{2} r=\frac{d D}{d t} A=I, \tag{6.92}
\end{equation*}
$$

i.e. the Ampère integral becomes independent of the choice of the (imaginary!) surface limited by contour $C$ - as it should.

### 6.7. Finally, the full Maxwell equation system

This is a very special moment in the course: with the displacement current introduction, we have finally arrived at the full set of macroscopic Maxwell equations for time-dependent fields, ${ }^{49}$

$$
\begin{array}{ll}
\nabla \times \mathbf{E}+\frac{\partial \mathbf{B}}{\partial t}=0, & \nabla \times \mathbf{H}-\frac{\partial \mathbf{D}}{\partial t}=\mathbf{j} \\
\nabla \cdot \mathbf{D}=\rho, & \nabla \cdot \mathbf{B}=0 \tag{6.93b}
\end{array}
$$

whose validity has been confirmed in by an enormous body of experimental data. ${ }^{50}$ The most striking feature of these equations is that, even in the absence of (local) charges and currents, when all the equations become homogeneous,

$$
\begin{array}{ll}
\nabla \times \mathbf{E}=-\frac{\partial \mathbf{B}}{\partial t}, & \nabla \times \mathbf{H}=\frac{\partial \mathbf{D}}{\partial t}, \\
\nabla \cdot \mathbf{D}=0, & \nabla \cdot \mathbf{B}=0 \tag{6.94b}
\end{array}
$$

they still describe something very non-trivial: electromagnetic waves, including light. ${ }^{51}$ Indeed, one can interpret Eqs. (94a) in the following way: the change of magnetic field creates, via the Faraday induction effect, a vortex (divergence-free) electric field, while the dynamics of the electric field, in turn, creates a vortex magnetic field via the Maxwell's displacement currents.

We will carry out a detailed quantitative analysis of the waves in the next chapter, but it is easy (and very instructive) to use the Maxwell equations to estimate their velocity $v$ and the field amplitude ratio $E / H$ in a medium with $\mathbf{D}=\varepsilon \mathbf{E}, \mathbf{B}=\mu \mathbf{H}$, and $\mathbf{j}=0$. Indeed, let the solution of these equations, in a uniform, linear medium have a time period $T$, and hence the wavelength $\lambda=v T$. Then the magnitude of the left-hand part of the first of Eqs. (94a) is of the order of $E / \lambda \sim E / v T$, while that of its right-hand part may be estimated as $B / T=\mu H / T$. Using similar estimates for the second of Eqs. (94a), we arrive at the following two requirements for the $E / H$ ratio: ${ }^{52}$

$$
\begin{equation*}
\frac{E}{H} \sim \mu v \sim \frac{1}{\varepsilon v} . \tag{6.95}
\end{equation*}
$$

In order to insure the compatibility of these two relations, the wave speed should satisfy the estimate

$$
\begin{equation*}
v \sim \frac{1}{(\varepsilon \mu)^{1 / 2}} \tag{6.96}
\end{equation*}
$$

reduced to $v \sim 1 /\left(\varepsilon_{0} \mu_{0}\right)^{1 / 2} \equiv c$ in free space, while the ratio of the electric and magnetic field amplitudes should be of the following order:

[^302]\[

$$
\begin{equation*}
\frac{E}{H} \sim \mu v \sim \mu \frac{1}{(\varepsilon \mu)^{1 / 2}}=\left(\frac{\mu}{\varepsilon}\right)^{1 / 2} \tag{6.97}
\end{equation*}
$$

\]

In the next chapter we will see that these are indeed the exact results for a plane electromagnetic wave.
Now let me fulfill the promise given in Sec. 2 and establish the validity limits of the quasistatic approximation (16). For that, let the spatial scale of our system be $a$, generally unrelated to wavelength $\lambda=v T$, and carry real currents $\mathbf{j}$ producing certain magnetic field $H$. Then, according to Eqs. (94a), this magnetic field Faraday-induces electric field $E \sim \mu H a / T$, whose displacement currents, in turn, produce an additional magnetic field with magnitude

$$
\begin{equation*}
H^{\prime} \sim \frac{a \varepsilon}{T} E \sim \frac{a \varepsilon}{T} \frac{\mu a}{T} H \sim\left(\frac{a \lambda}{v T \lambda}\right)^{2} H=\left(\frac{a}{\lambda}\right)^{2} H \tag{6.98}
\end{equation*}
$$

Hence, at $a \ll \lambda$, the displacement current effect is indeed negligible.
Before going after the analysis of the full Maxwell equations in particular situations (that will be the main goal of all the next chapters of this course), let us have a look at the energy balance they yield for a certain volume $V$ - that may include both charged particles and the electromagnetic field. Since, according to Eq. (5.10), the magnetic field does no work on charged particles even if they move, the total power $\mathcal{P}$ being transferred from the field to the particles inside the volume is due to the electric field alone:

$$
\begin{equation*}
\mathcal{P}=\int_{V} p d^{3} r, \quad p=\mathbf{j} \cdot \mathbf{E}, \tag{6.99}
\end{equation*}
$$

where I have used Eq. (4.38). Expressing $\mathbf{j}$ from the corresponding Maxwell equation of system (93), and plugging it into Eq. (99), we get

$$
\begin{equation*}
\mathcal{P}=\int_{V}\left[\mathbf{E} \cdot(\nabla \times \mathbf{H})-\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t}\right] d^{3} r \tag{6.100}
\end{equation*}
$$

Let us pause here for a second, and transform the divergence of vector $\mathbf{E} \times \mathbf{H}$ using the wellknown vector algebra identity: ${ }^{53}$

$$
\begin{equation*}
\nabla \cdot(\mathbf{E} \times \mathbf{H})=\mathbf{H} \cdot(\nabla \times \mathbf{E})-\mathbf{E} \cdot(\nabla \times \mathbf{H}) \tag{6.101}
\end{equation*}
$$

The last term in the right-hand part of this equation is exactly the first term in the square brackets of Eq. (100), so that we can rewrite that formula as

$$
\begin{equation*}
\mathcal{P}=\int_{V}\left[-\nabla \cdot(\mathbf{E} \times \mathbf{H})+\mathbf{H} \cdot(\nabla \times \mathbf{E})-\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t}\right] d^{3} r . \tag{6.102}
\end{equation*}
$$

However, according to the Maxwell equation for $\nabla \times \mathbf{E}$, it is equal to $-\partial \mathbf{B} / \partial t$, so that the second term in the square brackets of Eq. (102) equals $-\mathbf{H} \cdot \partial \mathbf{B} / \partial t$ and, according to Eq. (5.128), is just the (minus) time derivative of the magnetic energy per unit volume. Similarly, according to Eq. (3.82), the third term under the integral is the minus time derivative of the electric energy per unit volume. Finally, we can use the divergence theorem to transform the integral of the first term to a 2D integral over the surface $S$

[^303]limiting volume $V$. As the result, we get the so-called Poynting theorem ${ }^{54}$ for the power balance in the system:

Poynting theorem

Electromagnetic energy density
so that for an isotropic, linear, and dispersion-free medium, with $\mathbf{D}(t)=\varepsilon \mathbf{E}(t), \mathbf{B}(t)=\mu \mathbf{H}(t)$,

$$
\begin{equation*}
u=\frac{\mathbf{E} \cdot \mathbf{D}}{2}+\frac{\mathbf{H} \cdot \mathbf{B}}{2}=\frac{\varepsilon E^{2}}{2}+\frac{B^{2}}{2 \mu} \tag{6.104b}
\end{equation*}
$$

and $\mathbf{S}$ is the Poynting vector defined as ${ }^{55}$

$$
\begin{equation*}
\int_{V}\left(p+\frac{\partial u}{\partial t}\right) d^{3} r+\oint_{S} S_{n} d^{2} r=0 \tag{6.103}
\end{equation*}
$$

Here $u$ is the density of the total (electric plus magnetic) energy of the electromagnetic field, with

$$
\begin{equation*}
\delta u \equiv \mathbf{E} \cdot \delta \mathbf{D}+\mathbf{H} \cdot \delta \mathbf{B} \tag{6.104a}
\end{equation*}
$$

The first integral in Eq. (103) is evidently the net change of the energy of the system (particles + field) in unit time, so that the second (surface) integral is certainly the power flowing out from the system through the surface, and it is tempting to interpret the Poynting vector $\mathbf{S}$ locally, as the power flow density at the given point. ${ }^{56}$ In many cases such a local interpretation of vector $\mathbf{S}$ is legitimate; however, in some cases it may lead to wrong conclusions. Indeed, let us consider a simple system shown in Fig. 10: a planar capacitor placed into a static and uniform external magnetic field so that the electric and magnetic fields are mutually perpendicular. In this static situation, no charges are moving, both $\boldsymbol{p}$ and $\partial / \partial t$ equal to zero, and there should be no power flow in the system. However, Eq. (105) shows that the Poynting vector is not equal to zero inside the capacitor, being directed as shown in Fig. 10.


Fig. 6.10. The Poynting vector paradox.

From the point of view of our only unambiguous corollary of the Maxwell equations, Eq. (103), there is no contradiction here, because the fluxes of vector $\mathbf{S}$ through the walls of any volume $V$, for example the side walls of the volume shown with dashed lines in Fig. 10, are equal and opposite (and they are zero for other faces of this rectilinear volume), so that the total flux of the Poynting vector

[^304]equals zero, as it should. It is, however, useful to recall this example each time before giving the local interpretation to vector $\mathbf{S}$.

Finally, to complete the initial discussion of the Maxwell equations, ${ }^{57}$ let us rewrite them in terms of potentials $\mathbf{A}$ and $\phi$, because this is more convenient for the solution of some (though not all!) problems. Even when dealing with a more general system (93) of Maxwell equations than before, Eqs. (7) and (5.27),

$$
\begin{equation*}
\mathbf{E}=-\nabla \phi-\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B}=\nabla \times \mathbf{A} \tag{6.106}
\end{equation*}
$$

are still used as potential definitions. It is straightforward to verify that with these definitions, two homogeneous Maxwell equations (93b) are satisfied automatically. Plugging Eqs. (106) into the inhomogeneous equations (93a), and considering, for simplicity, a linear, uniform medium with frequency-independent $\varepsilon$ and $\mu$, we get

$$
\begin{align*}
& \nabla^{2} \phi+\frac{\partial}{\partial t}(\nabla \cdot \mathbf{A})=-\frac{\rho}{\varepsilon} \\
& \nabla^{2} \mathbf{A}-\varepsilon \mu \frac{\partial^{2} \mathbf{A}}{\partial t^{2}}-\nabla\left(\nabla \cdot \mathbf{A}+\varepsilon \mu \frac{\partial \phi}{\partial t}\right)=-\mu \mathbf{j} . \tag{6.107}
\end{align*}
$$

This is a more complex result than what we would like to get. However, let us select a special gauge that is frequently called (especially for the free space case, when $v=c$ ) the Lorenz gauge condition ${ }^{58}$

$$
\begin{equation*}
\nabla \cdot \mathbf{A}+\varepsilon \mu \frac{\partial \phi}{\partial t}=0 \tag{6.108}
\end{equation*}
$$

which is a natural generalization of the Coulomb gauge (5.48) for time-dependent phenomena. With this condition, Eqs. (107) are reduced to a simpler, beautifully symmetric form: ${ }^{59}$

$$
\begin{align*}
& \nabla^{2} \phi-\frac{1}{v^{2}} \frac{\partial^{2} \phi}{\partial t^{2}}=-\frac{\rho}{\varepsilon}  \tag{6.109}\\
& \nabla^{2} \mathbf{A}-\frac{1}{v^{2}} \frac{\partial^{2} \mathbf{A}}{\partial t^{2}}=-\mu \mathbf{j}
\end{align*}
$$

where $v^{2} \equiv 1 / \varepsilon \mu .{ }^{60}$
${ }^{57}$ We will return to their general discussion (in particular, to the analytical mechanics of the electromagnetic field, and its stress tensor) in Sec. 9.8, after we have got equipped with the special relativity theory.
${ }^{58}$ This condition, named after L. Lorenz, should not be confused with the Lorentz invariance condition of the relativity theory, due to H. Lorentz (note the names' spelling) - see Sec. 9.4.
${ }^{59}$ Note that Eqs. (109) are essentially a set of 4 similar equations for 4 scalar functions (namely, $\phi$ and three Cartesian components of vector $\mathbf{A}$ ) and thus clearly invite the 4 -component vector formalism of the relativity theory - which will be discussed in Chapter 9.
${ }^{60}$ Here I have to mention in passing the so-called Hertz vector potentials $\Pi_{e}$ and $\Pi_{m}$ (whose introduction may be traced to at least the 1904 work by E. Whittaker). They may be defined by the following relations:

$$
\mathbf{A}=\mu \frac{\partial \boldsymbol{\Pi}_{e}}{\partial t}+\mu \nabla \boldsymbol{\Pi}_{m}, \quad \phi=-\frac{1}{\varepsilon} \nabla \cdot \boldsymbol{\Pi}_{e},
$$

Electromagnetic field potentials

If $\phi$ and $\mathbf{A}$ depend on just one spatial coordinate, say $z$, in a region without field sources: $\rho=0, \mathbf{j}$ $=0$, Eqs. (109) are reduced to the well-known 1D wave equations

$$
\begin{align*}
& \frac{\partial^{2} \phi}{\partial^{2} z}-\frac{1}{v^{2}} \frac{\partial^{2} \phi}{\partial t^{2}}=0 \\
& \frac{\partial^{2} \mathbf{A}}{\partial^{2} z}-\frac{1}{v^{2}} \frac{\partial^{2} \mathbf{A}}{\partial t^{2}}=0 \tag{6.110}
\end{align*}
$$

describing waves propagating with velocity $v$. Note that due to the definitions of constants $\varepsilon_{0}$ and $\mu_{0}$, in free space $v$ is just the speed of light:

$$
\begin{equation*}
v=\frac{1}{\left(\varepsilon_{0} \mu_{0}\right)^{1 / 2}} \equiv c . \tag{6.110}
\end{equation*}
$$

Historically, the experimental observation of relatively low-frequency ( GHz -scale) electromagnetic waves and the proof that their speed in free space is equal to that of light, was the decisive proof of Maxwell's theory. ${ }^{61}$ A detailed study of this most important physical phenomenon is the main goal of the next chapters of this course.

### 6.8 Exercise problems

6.1. Prove that the electromagnetic induction e.m.f. $V_{\text {ind }}$ in a conducting loop may be measured:
(i) by measuring the current $I=V_{\text {ind }} / R$ induced in the closed loop with Ohmic resistance $R$, or
(ii) using a voltmeter inserted into the loop - see Fig. on the right.

6.2. The magnetic flux $\Phi$ that pierces a plane, round, uniform, resistive ring is being changed in time, while the magnetic field outside of the ring is negligibly low. A voltmeter is connected to a part the ring as shown in Fig. on the right. What would the voltmeter show?

6.3. A weak, uniform magnetic field $\mathbf{B}$ is applied to an axially-symmetric permanent magnet, with a dipole magnetic moment $\mathbf{m}$ directed along its symmetry axis, rapidly rotating about the same axis, with an angular momentum $\mathbf{L}$. Calculate the electric field resulting from field's application, and formulate the conditions of your result's validity.
which make the Lorenz gauge condition (108) automatically satisfied. These potentials are especially convenient for the solution of problems in which the electromagnetic field is excited by external sources characterized by externally fixed electric and magnetic polarizations $\mathbf{P}_{\text {ext }}$ and $\mathbf{M}_{\text {ext }}$ - rather than fixed charge and current densities $\rho$ and $\mathbf{j}$. Indeed, it is straightforward to check that both $\Pi_{e}$ and $\Pi_{m}$ satisfy equations similar to Eqs. (109), but with the right-hand parts equal to, respectively, $-\mathbf{P}_{\text {ext }}$ and $-\mathbf{M}_{\text {ext }}$.
${ }^{61}$ This was first accomplished in 1886 by H. Hertz, using specially designed electronic circuits and antennas.
6.4. Use the electromagnetic induction law (5) to derive Eq. (5.128) for the magnetic field energy variation.
6.5. A uniform, static magnetic field $\mathbf{B}$ is applied along the axis of a long round pipe of a radius $R$, and a very small thickness $\tau$, made of a material with Ohmic conductance $\sigma$. A sphere of mass $M$ and radius $R^{\prime}<R$, made of a linear magnetic with permeability $\mu \gg \mu_{0}$, is launched, with an initial velocity $v_{0}$, to fly ballistically along pipe's axis - see Fig. on the right. Use the quasistatic approximation to calculate the distance the sphere
 would pass before it stops. Formulate conditions of validity of your result.
6.6. AC current of frequency $\omega$ is being passed through a long uniform wire with a round crosssection of radius $R$ that is comparable with the skin depth $\delta_{s}$. In the quasistatic approximation, find the current density distribution across the wire. Analyze the limits $R \ll \delta_{s}$ and $R \gg \delta_{s}$.
6.7. A very long, round cylinder of radius $R$, made of a uniform Ohmic conductor with conductivity $\sigma$ and magnetic permittivity $\mu$, has been placed into a uniform ac magnetic field $\mathbf{H}_{\mathrm{ext}}=\mathbf{H}_{0} \cos \omega t$, directed along its symmetry axis see Fig. on the right. Calculate the spatial distribution of the magnetic field's amplitude, and in particular its value on cylinder's axis. Spell out the last result in the limits of relatively small and large $R$.

Hint: As shortcuts, you are welcome to reuse parts of the solution of the previous problem.

6.8. ${ }^{*}$ Define and calculate an appropriate spatial-temporal Green's function for Eq. (20), and use this function to analyze the dynamics of propagation of the external magnetic field, suddenly turned on at $t=0$ and then left constant:

$$
H(x=0, t)= \begin{cases}0, & \text { at } t<0 \\ H_{0}, & \text { at } t>0\end{cases}
$$

into an Ohmic conductor occupying half-space $x>0-$ see Fig. 6.2.
Hint: Try to use a function proportional to $\exp \left\{-\left(x-x^{\prime}\right)^{2} / 2(\delta x)^{2}\right\}$, with a suitable time dependence of parameter $\delta x$, and a properly selected pre-exponential factor.
6.9. Solve the previous problem using the variable separation method, and compare the results.
6.10. A small, planar wire loop, carrying current $I$, is located far from a plane surface of a superconductor. Within the "macroscopic" description of superconductivity $(\mathbf{B}=0)$, find:
(i) the energy of the loop-superconductor interaction,
(ii) the force and torque acting on the loop,
(iii) the distribution of supercurrents on the superconductor surface.
6.11. A straight, uniform magnet of length 21 , cross-section area $A$ $\ll l^{2}$, and mass $m$, with a permanent longitudinal magnetization $M_{0}$, is placed over a horizontal surface of a superconductor - see Fig. on the right. Within the macroscopic model of the Meissner-Ochsenfeld effect, find the stable equilibrium position of the magnet.
6.12. A plane superconducting wire loop, of area $A$ and inductance $L$, may rotate, without friction, about a horizontal axis 0 (in Fig. on the right, perpendicular to the plane of drawing) passing through its center of mass. Initially the loop was horizontal (with $\theta=0$ ), and carried supercurrent $I_{0}$ in such direction that its magnetic dipole vector was directed down. Then a uniform magnetic field $\mathbf{B}$, directed
 vertically up, was applied. Find all possible equilibrium positions (angles $\theta$ ) of the loop, analyze their stability, and give a physical interpretation of the results.
6.13. Use the London equation to analyze the penetration of external magnetic field into a thin $(t$ $\sim \delta_{\mathrm{L}}$ ), planar superconductor film whose plane is parallel to the field.
6.14. Use the London equation to calculate the distribution of supercurrent density $\mathbf{j}$ across the circular cross-section (with radius $R \sim \delta_{\mathrm{L}}$ ) of a long, straight superconducting wire carrying dc current $I$.
6.15.* Use the London equation to calculate the inductance (per unit length) of a long, uniform superconducting strip placed close to the surface of a similar superconductor see Fig. on the right, which shows the structure's cross-section.

Hint: Start from thinking how is the supercurrent
 distributed along the surfaces of the strip and the bulk superconductor.
6.16. Analyze the magnetic field shielding by a superconducting film of small thickness $t \ll \delta_{\mathrm{L}}$, by calculating the penetration of the field induced by current $I$ flowing in a thin wire which runs parallel to a wide, plane thin film, at distance $d \gg t$ from it, into the half-space behind the film.
6.17. Calculate the self-inductance of a superconducting cable with a round cross-section (see Fig. on the right) in the following limits:
(i) $\delta_{\mathrm{L}} \ll a, b, c-b$, and
(ii) $a \ll \delta_{\mathrm{L}} \ll b, c-b$.

6.18. Use Eqs. (59) and (71) to calculate the energy of a Josephson junction, and the full energy of the SQUID shown in Fig. 4c.
6.19. Analyze the possibility of wave propagation in a long, uniform chain of lumped inductances and capacitances - see Fig. on the right.

Hint: Readers without prior experience with electromagnetic
 wave analysis may like to use a substantial analogy between this effect and mechanical waves in a 1D chain of elastically coupled particles. ${ }^{62}$
6.20. A sinusoidal e.m.f. of amplitude $V_{0}$ and frequency $\omega$ is applied to an end of a long chain of similar, lumped resistors and capacitors (see Fig. on the right). Calculate the law of decay of the rf oscillation amplitude in the chain.

6.21. Calculate the pressure exerted by the magnetic field $\mathbf{B}$ inside a magnetic-free solenoid of length $l$, cross-section area $A \ll l^{2}$ and $N$ turns, on its "walls" (windings), and the force exerted by the field on solenoid's ends. Give a physical interpretation of the direction of these forces.
6.22. In Sec. 6 we have seen that the displacement current concept allows one to generalize the Ampère law to time-dependent processes as

$$
\oint_{C} \mathbf{H} \cdot d \mathbf{r}=I_{S}+\frac{\partial}{\partial t} \int_{S} D_{n} d^{2} r .
$$

We also have seen that such generalization makes $\int \mathbf{H} \cdot d \mathbf{r}$ over the contour C, which was shown in Fig. 9 (see also Fig. on the right), independent of the choice of surface $S$ limited by the contour. However, it may look like the situation is different for contour a $C^{\prime}$ drawn inside the capacitor. Indeed, if contour's radius $\rho$ is much larger than the capacitor's thickness $d$, the magnetic field $\mathbf{H}$, created by the linear current $I$ of the contour line is virtually the same as that of a continuous wire, and hence integral $\int \mathbf{H} \cdot d \mathbf{r}$ along contour $C^{\prime}$ is apparently the same as that along contour $C$, while the magnetic flux $\int D_{n} d^{2} r$ through the surface $S$ ' limited by contour $C^{\prime}$ is evidently smaller, while $I_{S^{\prime}}=I_{S}=0$, so that the above equation seems invalid. Resolve the paradox, for simplicity considering an axially-
 symmetric system.

[^305]
## Chapter 7. Electromagnetic Wave Propagation

This (long!) chapter focuses on the most important effect that follows from the time-dependent Maxwell equations, namely the electromagnetic waves, at this stage avoiding a discussion of their origin, i.e. radiation. I start from the simplest, plane waves in a uniform and isotropic media. The next step is a discussion non-uniform systems, in particular those with sharp boundaries between different materials, which bring in such new effects as wave reflection and refraction. Then I will proceed to the structure of electromagnetic waves propagating along various long, cylindrical structures, called transmission lines - such as coaxial cables, waveguides, and optical fibers. In the end of the chapter, electromagnetic oscillations in final-length fragments of such lines, serving as resonators, are also discussed.

### 7.1. Plane waves

Let us start from considering a spatial region that does not contain field sources $(\rho=0, \mathbf{j}=0)$, and is filled with a linear, uniform, isotropic medium, which obeys Eqs. (3.38) and (5.110):

$$
\begin{equation*}
\mathbf{D}=\varepsilon \mathbf{E}, \quad \mathbf{B}=\mu \mathbf{H} . \tag{7.1}
\end{equation*}
$$

Moreover, let us assume for a minute that these material equations hold for all frequencies of interest. As was already shown in Sec. 6.7, in this case the Lorenz gauge condition (6.108) allows the Maxwell equations to be recast into wave equations (6.110) for the vector and scalar potentials. However, for most our purposes it is more convenient to use directly the homogeneous Maxwell equations (6.94) for the electric and magnetic fields - which are independent of the gauge choice. After the elementary elimination of $\mathbf{D}$ and $\mathbf{B}$ using Eq. (1), ${ }^{1}$ these equations take a simple, symmetric form

equations for uniform linear media

$$
\begin{array}{ll}
\nabla \times \mathbf{E}+\mu \frac{\partial \mathbf{H}}{\partial t}=0, & \nabla \times \mathbf{H}-\varepsilon \frac{\partial \mathbf{E}}{\partial t}=0, \\
\nabla \cdot \mathbf{E}=0, & \nabla \cdot \mathbf{H}=0 . \tag{7.2b}
\end{array}
$$

Now, taking the curl $(\nabla \times)$ of each of Eqs. (2a), and using the vector algebra identity (5.31), whose first term, for both $\mathbf{E}$ and $\mathbf{H}$, vanishes due to Eqs. (2b), we get similar wave equations for the electric and magnetic fields:

$$
\begin{equation*}
\left(\nabla^{2}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) \mathbf{E}=0, \quad\left(\nabla^{2}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) \mathbf{H}=0, \tag{7.3}
\end{equation*}
$$

where parameter $v$ is defined by relation

EM wave velocity

$$
\begin{equation*}
v^{2} \equiv \frac{1}{\varepsilon \mu} \tag{7.4}
\end{equation*}
$$

with $v^{2}=1 / \varepsilon_{0} \mu_{0} \equiv c^{2}$ in free space.

[^306]Two vector equations (3) are of course six similar equations for three Cartesian components of two vectors $\mathbf{E}$ and $\mathbf{H}$. Each of these equations allows, in particular, the following solution,

$$
\begin{equation*}
f=f(z-v t) \tag{7.5}
\end{equation*}
$$

Plane wave
where $z$ is the Cartesian coordinate along a certain (arbitrary) direction $\mathbf{n}$. This solution describes a specific type of a wave, i.e. a certain field pattern moving, without deformation, along axis $z$, with velocity $v$. According to Eq. (5), each variable $f$ has the same value in each plane perpendicular to the direction $\mathbf{n}$ of wave propagation, hence the name - plane wave.

According to Eqs. (2), the independence of the wave equations (3) for vectors $\mathbf{E}$ and $\mathbf{H}$ does not mean that their plane-wave solutions are independent. Indeed, plugging solution (5) into Eqs. (2a), we get

$$
\begin{equation*}
\mathbf{H}=\frac{\mathbf{n} \times \mathbf{E}}{Z}, \quad \text { i.e. } \mathbf{E}=Z \mathbf{H} \times \mathbf{n}, \tag{7.6}
\end{equation*}
$$

Relation between the fields

$$
\begin{equation*}
Z \equiv \frac{E}{H}=\left(\frac{\mu}{\varepsilon}\right)^{1 / 2} \tag{7.7}
\end{equation*}
$$

The vector relation (6) means, first of all, that vectors $\mathbf{E}$ and $\mathbf{H}$ are perpendicular not only to vector $\mathbf{n}$ (such waves are called transverse), but also to each other (Fig. 1) - at any point of space and at any time instant.


Fig. 7.1. Field vectors in a plane electromagnetic wave propagating along direction $\mathbf{n}$.

Second, the field magnitudes are related by constant $Z$, called the wave impedance of the medium. Very soon we will see that the wave impedance plays a pivotal role in many problems, in particular at the wave reflection from the interface between two media. Since the dimensionality of $E$, in SI units, is $\mathrm{V} / \mathrm{m}$, and that of $H$ is $\mathrm{A} / \mathrm{m}$, Eq. (7) shows that $Z$ has the dimensionality of V/A, i.e. ohms $(\Omega) .{ }^{2}$ In particular, in free space,

$$
\begin{equation*}
Z=Z_{0} \equiv\left(\frac{\mu_{0}}{\varepsilon_{0}}\right)^{1 / 2}=4 \pi \times 10^{-7} c \approx 377 \Omega \tag{7.8}
\end{equation*}
$$

Now plugging Eq. (6) into Eqs. (6.104b) and (6.105), we get:

$$
u=\varepsilon E^{2}=\mu H^{2}
$$

Wave
impedance of free
space

Wave's
energy
per unit volume

[^307]Wave's power per unit area

$$
\begin{equation*}
\mathbf{S} \equiv \mathbf{E} \times \mathbf{H}=\mathbf{n} \frac{E^{2}}{Z}=\mathbf{n} Z H^{2}, \tag{7.9b}
\end{equation*}
$$

so that, according to Eqs. (4) and (7), wave's energy and power densities are universally related as

$$
\begin{equation*}
\mathbf{S}=\mathbf{n} u v . \tag{7.9c}
\end{equation*}
$$

In the view of the Poynting vector paradox discussed in Sec. 6.7 (see Fig. 6.10), one may wonder whether this expression may be interpreted as the actual density of power flow. In contrast to the static situation shown in Fig. 6.7, that limits the electric and magnetic fields to a vicinity of their sources, waves may travel far from them. As a result, they can form wave packets of finite length in free space see Fig. 2.


Fig. 7.2. Interpreting the Poynting vector in an electromagnetic wave.

Let us apply the Poynting theorem (6.103) to the cylinder shown by dashed lines in Fig. 2, with one lid inside the wave packet, and another lid in the region already passed by the wave. Then, according to Eq. (6.103), the rate of change of the full energy $\varepsilon$ inside the volume is $d \varepsilon / d t=-S A$ (where $A$ is the lid area), so that $S$ may be indeed interpreted as the power flow (per unit area) from the volume. Making a reasonable assumption that the finite length of a sufficiently long wave packet does not affect the physics inside it, we may indeed interpret the $\mathbf{S}$ given by Eq. (9) as the power flow density inside a plane electromagnetic wave.

As we will see later in this chapter, the free-space value $\mathrm{Z}_{0}$ of the wave impedance, given by Eq. (8), establishes the scale of wave impedances of virtually all wave transmission lines, so we may use is and Eq. (9) to get some sense of how different are the electric and magnetic field amplitudes in the waves, on the scale of typical electrostatics and magnetostatics experiments. For example, according to Eqs. (9), a wave of a modest intensity $S=1 \mathrm{~W} / \mathrm{m}^{2}$ (the power density we get from a usual electric bulb a few meters away from it) has $E \sim\left(S Z_{0}\right)^{1 / 2} \sim 20 \mathrm{~V} / \mathrm{m}$, quite comparable with the dc field created by an AA battery right outside it. On the other hand, the wave's magnetic field $H=\left(S / Z_{0}\right)^{1 / 2} \approx 0.05 \mathrm{~A} / \mathrm{m}$. For this particular case, the relation following from Eqs. (1), (4), and (7),

$$
\begin{equation*}
B=\mu H=\mu \frac{E}{Z}=\mu \frac{E}{(\mu / \varepsilon)^{1 / 2}}=(\varepsilon \mu)^{1 / 2} E=\frac{E}{v} \tag{7.10}
\end{equation*}
$$

gives $B=\mu_{0} H=E / c \sim 7 \times 10^{-8} \mathrm{~T}$, i.e. a magnetic field thousand times less than the Earth field, and about 8 orders of magnitude lower than the field of a typical permanent magnet. A possible interpretation of this huge difference is that the scale of magnetic fields $B \sim E / c$ in the waves is "normal" for
electromagnetism, while that of permanent magnet fields is abnormally high, because they are due to the ferromagnetic alignment of electron spins, essentially quantum objects - see the discussion in Sec. 5.5.

As soon as $\varepsilon$ and $\mu$ are simple constants, wave speed $v$ is also constant, and Eq. (5) is valid for an arbitrary function $f$ - defined by either initial or boundary conditions. In plain English, a medium with frequency-independent $\varepsilon$ and $\mu$ supports propagation of plane waves with an arbitrary waveform without either decay (attenuation) or deformation (dispersion). However, for any real medium but pure vacuum, this approximation is valid only within limited frequency intervals. We will discuss the effects of attenuation and dispersion in the next section and see that all our prior results remain valid even in that general case, provided that we limit them to single-frequency (i.e. sinusoidal, or monochromatic) waves. Such waves may be most conveniently presented as ${ }^{3}$

$$
\begin{equation*}
f=\operatorname{Re}\left[f_{\omega} e^{i(k z-\omega t)}\right] \tag{7.11}
\end{equation*}
$$

Monochromatic wave
where $f_{\omega}$ is the complex amplitude of the wave, and $k$ is its wave number (the magnitude of wave vector $\mathbf{k} \equiv \mathbf{n} k$ ), sometimes also called the spatial frequency. The last term is justified by the fact, evident from Eq. (11), that $k$ is related to the wavelength $\lambda$ exactly as the usual ("temporal") frequency $\omega$ is related to the time period $T$ :

$$
\begin{equation*}
k=\frac{2 \pi}{\lambda}, \quad \omega=\frac{2 \pi}{T} \tag{7.12}
\end{equation*}
$$

Spatial and temporal frequencies

Requiring Eq. (11) to be a particular form of Eq. (5), i.e. the argument $(k z-\omega t) \equiv k[z-(\omega / k) t]$ to be proportional to $(z-v t)$, so that $\omega / k=v$, we see that the wave number should equal

$$
\begin{equation*}
k=\frac{\omega}{v}=(\varepsilon \mu)^{1 / 2} \omega \tag{7.13}
\end{equation*}
$$

showing that in this "dispersion-free" case the dispersion relation $\omega(k)$ is linear.
Now note that Eq. (6) does not claim mean vectors $\mathbf{E}$ and $\mathbf{H}$ retain their direction in space. (The simple case when they do is called the linear polarization of the wave.) Indeed, nothing in the Maxwell equations prevents, for example, joint rotation of this pair of vectors around the fixed vector $\mathbf{n}$, while still keeping all these three vectors perpendicular to each other at all times. An arbitrary rotation law, or even an arbitrary constant frequency of such rotation, however, would violate the single-frequency (monochromatic) character of the elementary sinusoidal wave (11). In order to understand what is the most general type of polarization the wave may have without violating that condition, let us present two Cartesian components of one of these vectors (say, E) along any two fixed axes $x$ and $y$, perpendicular to each other and axis $z$ (i.e. vector $\mathbf{n}$ ), in the same form as used in Eq. (11):

$$
\begin{equation*}
E_{x}=\operatorname{Re}\left[E_{\omega x} e^{i(k z-\omega t)}\right], \quad E_{y}=\operatorname{Re}\left[E_{\omega y} e^{i(k z-\omega t)}\right] \tag{7.14}
\end{equation*}
$$

In order to keep the wave monochromatic, complex amplitudes $E_{\omega x}$ and $E_{\omega y}$ must be constant; however, they may have different magnitudes and an arbitrary phase shift between them.

[^308]In the simplest case when the arguments of the complex amplitudes are equal,

$$
\begin{equation*}
E_{\omega x, y}=\left|E_{\omega x, y}\right| e^{i \varphi} . \tag{7.15}
\end{equation*}
$$

the real field components have the same phase:

$$
\begin{equation*}
E_{x, y}=\left|E_{\omega x, y}\right| \cos (k z-\omega t+\varphi), \tag{7.16}
\end{equation*}
$$

so that their ratio is constant in time - see Fig. 3a. This means that the wave is linearly polarized, within the plane defined by relation

$$
\begin{equation*}
\tan \theta=\frac{\left|E_{\omega y}\right|}{\left|E_{\omega x}\right|} . \tag{7.17}
\end{equation*}
$$



Fig. 7.3. Time evolution of the electric field vector in (a) linearly-polarized, (b) circularly-polarized, and (c) elliptically-polarized waves.

Another simple case is when the moduli of the complex amplitudes $E_{\omega x}$ and $E_{\omega y}$ are equal, but their phases are shifted by $+\pi / 2$ or $-\pi / 2$ :

$$
\begin{equation*}
E_{\omega x}=\left|E_{\omega}\right| e^{i \varphi}, \quad E_{\omega y}=\left|E_{\omega}\right| e^{i(\varphi \pm \pi / 2)} . \tag{7.18}
\end{equation*}
$$

In this case

$$
\begin{equation*}
E_{x}=\left|E_{\omega}\right| \cos (k z-\omega t+\varphi), \quad E_{y}=\left|E_{\omega}\right| \cos \left(k z-\omega t+\varphi \pm \frac{\pi}{2}\right)=\mp\left|E_{\omega}\right| \sin (k z-\omega t+\varphi) \tag{7.19}
\end{equation*}
$$

This means that on the $[x, y]$ plane, the end of vector $\mathbf{E}$ moves, with wave's frequency $\omega$, either clockwise or counterclockwise around a circle - see Fig. 3b:

$$
\begin{equation*}
\theta(t)=\mp(\omega t-\varphi) . \tag{7.20}
\end{equation*}
$$

Such waves are called circularly-polarized. ${ }^{4}$ These particular solutions of the Maxwell equations are very convenient for quantum electrodynamics, because single electromagnetic field quanta with a

[^309]certain (positive or negative) spin direction may be considered as elementary excitations of the corresponding circularly-polarized wave. (This fact does not exclude, from the quantization scheme, waves of other polarizations, because any monochromatic wave may be presented as a linear combination of two circularly-polarized waves with opposite helicities, just as Eqs. (14) present it as a linear combination of two linearly-polarized waves.)

Finally, in the general case of arbitrary complex amplitudes $E_{\omega x}$ and $E_{\omega y}$, the electric field vector end moves along an ellipse on the $[x, y]$ plane (Fig. 3c), such wave is called elliptically polarized. The eccentricity and orientation of the ellipse are completely described by one complex number, the ratio $E_{\omega x} / E_{\omega y}$, i.e. two real numbers: $\left|E_{\omega x} / E_{\omega y}\right|$ and $\varphi=\arg \left(E_{\omega x} / E_{\omega y}\right)$.

The same information may be expressed via four so-called Stokes parameters $s_{0}, s_{1}, s_{2}, s_{3}$, which are popular in optics because they may be used for the description of not only completely coherent waves that are discussed here, but also of party coherent or even fully incoherent waves - including the natural light emitted by thermal sources like our Sun. In contrast to the notion of coherent waves whose complex amplitudes are considered deterministic numbers, the instant amplitudes of incoherent waves should be treated as stochastic variables. ${ }^{5}$

### 7.2. Attenuation and dispersion

Now let me show that any linear, isotropic medium may be characterized, by complex, frequency-dependent electric permittivity $\delta(\omega)$ and magnetic permeability $\mu(\omega)$. Indeed, starting from electric effects, the electric polarization of realistic elementary dipoles of the medium cannot follow the applied electric field instantly, if the field frequency $\omega$ is comparable with those of the internal processes - say, transitions between atomic energy levels. Let us consider the most general law of time evolution of polarization $P(t)$ for the case of arbitrary applied electric field $E(t),{ }^{6}$ but for a sufficiently dilute medium, so that the local electric field $\mathbf{E}_{\text {ef }}$ (3.63), acting on each elementary dipole, is essentially the microscopically-averaged field E. ${ }^{7}$ Then, due to the linear superposition principle, $P(t)$ should be a linear sum (integral) of the values of $E\left(t^{\prime}\right)$ at all previous moments of time, $t^{\prime}<t$, weighed by some function of $t$ and $t^{\prime}$ :

$$
\begin{equation*}
P(t)=\int_{-\infty}^{t} E\left(t^{\prime}\right) G\left(t, t^{\prime}\right) d t^{\prime} \tag{7.21}
\end{equation*}
$$

The condition $t^{\prime}<t$, which is implied by this relation, expresses a key principle of physics, the causal relation between a cause (in our case, the electric field applied to each dipole) and its effect (the

[^310]polarization it creates). Function $G(t, t$ ') is called the temporal Green's function for the electric polarization. ${ }^{8}$ In order to understand its physical sense, let us consider the case when the applied field $E(t)$ is a very short pulse at $t=t_{0}$, that may be approximated with the Dirac's delta-function:
\[

$$
\begin{equation*}
E(t)=\delta\left(t-t_{0}\right) . \tag{7.22}
\end{equation*}
$$

\]

Then Eq. (21) yields just $P(t)=G\left(t, t_{0}\right)$, showing that the Green's function is just the polarization at moment $t$, created by a unit $\delta$-functional pulse of the applied field at moment $t^{\prime}$ (Fig. 4). Thus, the temporal $G$ is the exact time analog of the spatial Green's functions $G(\mathbf{r}, \mathbf{r}$ ') we have already studied in the electrostatics - see Sec. 2.7.


Fig. 7.4. Temporal Green's function for electric polarization (schematically).

What are the general properties of the temporal Green's function? First, the function is evidently real, since the dipole moment $\mathbf{p}$ and hence polarization $\mathbf{P}=n \mathbf{p}$ are real by the definition - see Eq. (3.6). Next, for systems without infinite internal memory, $G$ should tend to zero at $t-t^{\prime} \rightarrow \infty$, although the type of this approach (e.g., whether function $G$ oscillates approaching zero) depends on the medium. Finally, if parameters of the medium do not change in time, the polarization response to an electric field pulse should depend not on its absolute timing, but only on the time difference $\theta \equiv t-t$ ' between the pulse and observation instants:

$$
\begin{equation*}
P(t)=\int_{-\infty}^{t} E\left(t^{\prime}\right) G\left(t-t^{\prime}\right) d t^{\prime}=\int_{0}^{\infty} E(t-\theta) G(\theta) d \theta \tag{7.23}
\end{equation*}
$$

For a sinusoidal waveform, $E(t)=\operatorname{Re}\left[E_{\omega} e^{-i \omega t}\right]$, this equation yields

$$
\begin{equation*}
P(t)=\operatorname{Re} \int_{0}^{\infty} E_{\omega} e^{-i \omega(t-\theta)} G(\theta) d \theta=\operatorname{Re}\left\{\left[E_{\omega} \int_{0}^{\infty} G(\theta) e^{i \omega \theta} d \theta\right] e^{-i \omega t}\right\} . \tag{7.24}
\end{equation*}
$$

The expression in square brackets is of course nothing more that the complex amplitude $P_{\omega}$ of the polarization. This means that though even if the static relation (3.35) $P=\chi_{e} \varepsilon_{0} E$ is invalid for an arbitrary time-dependent process, we may still keep its Fourier analog,

$$
\begin{equation*}
P_{\omega}=\chi_{e}(\omega) \varepsilon_{0} E_{\omega}, \quad \text { with } \quad \chi_{e}(\omega) \equiv \frac{1}{\varepsilon_{0}} \int_{0}^{\infty} G(\theta) e^{i \omega \theta} d \theta \tag{7.25}
\end{equation*}
$$

[^311]for each sinusoidal component of the process, using it as the definition of the frequency-dependent electric susceptibility $\chi_{e}(\omega)$. Similarly, the frequency-dependent electric permittivity may be defined using the Fourier analog of Eq. (3.38):
\[

$$
\begin{equation*}
D_{\omega} \equiv \varepsilon(\omega) E_{\omega} . \tag{7.26}
\end{equation*}
$$

\]

Then, according to Eq. (3.36), the permittivity is related to the temporal Green's function by the usual Fourier transform:

$$
\begin{equation*}
\varepsilon(\omega) \equiv \varepsilon_{0}+\frac{P_{\omega}}{E_{\omega}}=\varepsilon_{0}+\int_{0}^{\infty} G(\theta) e^{i \omega \theta} d \theta \tag{7.27}
\end{equation*}
$$

It is evident from this expression that $\varepsilon(\omega)$ may be complex,

$$
\begin{equation*}
\varepsilon(\omega)=\varepsilon^{\prime}(\omega)+i \varepsilon^{\prime \prime}(\omega), \quad \varepsilon^{\prime}(\omega)=\varepsilon_{0}+\int_{0}^{\infty} G(\theta) \cos \omega \theta d \theta, \quad \varepsilon^{\prime \prime}(\omega)=\int_{0}^{\infty} G(\theta) \sin \omega \theta d \theta \tag{7.28}
\end{equation*}
$$

and that its real part $\varepsilon^{\prime}(\omega)$ is always an even function of frequency, while the imaginary part $\varepsilon^{\prime \prime}(\omega)$ is an odd function of $\omega$.

Absolutely similar arguments show that the linear magnetic properties may be characterized with complex, frequency-dependent permeability $\mu(\omega)$. Now rewriting Eqs. (1) for the complex amplitudes of the fields at a particular frequency, we may repeat all calculations of Sec. 1, and verify that all its results are valid for monochromatic waves even for a dispersive (but necessarily linear!) medium. In particular, Eqs. (7) and (13) now become

$$
\begin{equation*}
Z(\omega)=\left(\frac{\mu(\omega)}{\varepsilon(\omega)}\right)^{1 / 2}, \quad k(\omega)=\omega[\varepsilon(\omega) \mu(\omega)]^{1 / 2} \tag{7.28}
\end{equation*}
$$

so that the wave impedance and wave number may be both complex functions of frequency.
This fact has important consequences for the electromagnetic wave propagation. First, plugging the presentation of the complex wave number as the sum of its real and imaginary parts, $k(\omega) \equiv k^{\prime}(\omega)+$ $i k^{\prime \prime}(\omega)$, into Eq. (11):

$$
\begin{equation*}
f=\operatorname{Re}\left\{f_{\omega} e^{i[k(\omega) z-\omega t]}\right\}=e^{-k^{\prime \prime}(\omega) z} \operatorname{Re}\left\{f_{\omega} e^{i\left[k^{\prime}(\omega) z-\omega t\right]}\right\} \tag{7.29}
\end{equation*}
$$

we see that $k^{\prime \prime}(\omega)$ describes the rate of wave attenuation in the medium at frequency $\omega .{ }^{9}$ Second, if the waveform is not sinusoidal (and hence should be presented as a sum of several/many sinusoidal components), the frequency dependence of $k^{\prime}(\omega)$ provides for wave dispersion, i.e. the waveform deformation at the propagation, because the propagation velocity (4) of component waves is now different. ${ }^{10}$

[^312]Let us consider a simple but very important Lorentz oscillator model of a dispersive medium. ${ }^{11}$ In dilute atomic or molecular systems (including gases), electrons respond to the external electric field especially strongly when frequency $\omega$ is close to certain eigenfrequencies $\omega_{j}$ corresponding to the spectrum of quantum transitions of a single atom/molecule. An approximate, phenomenological description of this behavior may be obtained from a classical model of several externally-driven harmonic oscillators with finite damping. For an oscillator, driven by electric field's force $F(t)=q E(t)$, we can write the $2^{\text {nd }}$ Newton law as

$$
\begin{equation*}
m\left(\ddot{x}+2 \delta \ddot{x}+\omega_{0}^{2} x\right)=q E(t) \tag{7.30}
\end{equation*}
$$

where $\omega_{0}$ is the own frequency of the oscillator, and $\delta$ its damping coefficient. For a sinusoidal field, $E(t)=\operatorname{Re}\left[E_{\omega} \exp \{-i \omega t\}\right]$, we can look for a particular, forced-oscillation solution in a similar form $x(t)=$ $\operatorname{Re}\left[x_{\omega} \exp \{-i \omega t\}\right] .{ }^{12}$ Plugging this solution into Eq. (30), we can readily find the complex amplitude of these oscillations:

$$
\begin{equation*}
x_{\omega}=\frac{q}{m} \frac{E_{\omega}}{\left(\omega_{0}^{2}-\omega^{2}\right)-2 i \omega \delta} . \tag{7.31}
\end{equation*}
$$

Using this result to calculate the complex amplitude of the dipole moment as $p_{\omega}=q x_{\omega}$, and then the electric polarization $P_{\omega}=n p_{\omega}$ of a dilute medium with $n$ independent oscillators for unit volume, for its frequency-dependent permittivity (27) we get

$$
\begin{equation*}
\varepsilon(\omega)=\varepsilon_{0}+\frac{n q^{2}}{m} \frac{1}{\left(\omega_{0}^{2}-\omega^{2}\right)-2 i \omega \delta} . \tag{7.32}
\end{equation*}
$$

This result may be readily generalized to the case when the system has several types of oscillators with different eigenfrequencies:
$\varepsilon(\omega)$ in Lorentz oscillator model

$$
\begin{equation*}
\varepsilon(\omega)=\varepsilon_{0}+n \frac{q^{2}}{m} \sum_{j} \frac{f_{j}}{\left(\omega_{j}^{2}-\omega^{2}\right)-2 i \omega \delta_{j}} \tag{7.33}
\end{equation*}
$$

where $f_{j} \equiv n_{j} / n$ is the fraction of oscillators with eigenfrequency $\omega_{j}$, so that the sum of all $f_{j}$ equals 1. Figure 5 shows a typical behavior of the real and imaginary parts of the complex dielectric constant, described by Eq. (33), as functions of frequency. The effect of oscillator resonances is clearly visible, and dominates the media response at $\omega \approx \omega_{j}$, especially in the case of low damping, $\delta_{j} \ll \omega_{j}$. Note that in the low-damping limit, the imaginary part of the dielectric constant $\varepsilon$ ", and hence the wave attenuation $k$ ", are negligibly small at all frequencies besides small vicinities of frequencies $\omega_{j}$, where derivative $d \varepsilon^{\prime}(\omega) / d \omega$ is negative. ${ }^{13}$ Thus, for a system of for weakly-damped oscillators, Eq. (33) may be approximated, at most frequencies, as a sum of odd singularities ("poles"):
these effects are discussed in more detail in the quantum-mechanics part of my lecture notes (QM Sec. 2.1), because they are the crucial factor of Schrödinger's wave mechanics. (See also CM Sec. 5.3.)
${ }^{11}$ This example is focused on the frequency dependence of $\varepsilon$, because electromagnetic waves interact with "usual" media via their electric field much more than via the magnetic field. However, as will be discussed in Sec. 7, forgetting about the possible dispersion of $\mu(\omega)$ might result in missing some remarkable opportunities for manipulating the waves.
${ }^{12}$ If this point is not absolutely clear, please see CM Sec. 3.1.
${ }^{13}$ In optics, such behavior is called the anomalous dispersion.

$$
\begin{equation*}
\varepsilon(\omega) \approx \varepsilon_{0}+n \frac{q^{2}}{2 m} \sum_{j} \frac{f_{j}}{\omega_{j}-\omega}, \quad \text { for } \delta_{j} \ll\left|\omega-\omega_{j}\right| \ll\left|\omega_{j}-\omega_{j^{\prime}}\right| . \tag{7.34}
\end{equation*}
$$

This result is especially important because, according to quantum mechanics, ${ }^{14}$ Eq. (34) is also valid for a set of non-interacting, similar quantum systems (whose dynamics may be completely different from that of a harmonic oscillator!), provided that $\omega_{j}$ are replaced with frequencies of possible quantum interstate transitions, and coefficients $f_{j}$ are replaced with the so-called oscillator strengths of the transitions - which obey the same sum rule, $\Sigma_{j} f_{j}=1$.


Fig. 7.5. Typical frequency dependence of the real and imaginary parts of the electric permittivity of a media in the Lorentz oscillator model.

At $\omega \rightarrow 0$, the imaginary part of the permittivity also vanishes (for any $\delta_{j}$ ), while its real part approaches its electrostatic ("dc") value

$$
\begin{equation*}
\varepsilon(0)=\varepsilon_{0}+q^{2} \sum_{j} \frac{n_{j}}{m_{j} \omega_{j}^{2}} . \tag{7.35}
\end{equation*}
$$

Note that according to Eq. (30), the denominator in Eq. (35) is just the effective spring constant $\kappa_{j}=$ $m_{j} \omega_{j}^{2}$ of the $j^{\text {th }}$ oscillator, so that the oscillator masses $m_{j}$ as such are actually (and quite naturally) not involved in the static dielectric response.

In the opposite limit $\omega \gg \omega_{j}, \delta_{j}$, permittivity (33) also becomes real, and may be presented as

$$
\begin{equation*}
\varepsilon(\omega)=\varepsilon_{0}\left(1-\frac{\omega_{p}^{2}}{\omega^{2}}\right), \quad \text { where } \omega_{p}^{2} \equiv \frac{q^{2}}{\varepsilon_{0}} \sum_{j} \frac{n_{j}}{m_{j}} \tag{7.36}
\end{equation*}
$$

The last result is very important, because it is also valid at all frequencies if all $\omega_{j}$ and $\delta_{j}$ vanish, i.e. for a gas of free charged particles, in particular for plasmas - ionized atomic gases, with negligible collision effects. (This is why the parameter $\omega_{p}$ defined by Eq. (36) is called the plasma frequency.) Typically, the plasma as a whole is neutral, i.e. the density $n$ of positive atomic ions is equal to that of

[^313]$\varepsilon(\omega)$ in plasma
the free electrons. Since the ratio $n_{j} / m_{j}$ for electrons is much higher than that for ions, the general formula (36) for the plasma frequency is usually well approximated by the following simple expression:
\[

$$
\begin{equation*}
\omega_{p}^{2} \equiv \frac{n e^{2}}{\varepsilon_{0} m_{e}} . \tag{7.37}
\end{equation*}
$$

\]

This expression has a simple physical sense: the effective spring constant $\kappa_{\mathrm{ef}}=m_{e} \omega_{p}{ }^{2}=n e^{2} / \varepsilon_{0}$ describes the Coulomb force that appears when the electron subsystem of a plasma is shifted, as a whole, from its positive-ion subsystem, thus violating the electroneutrality. Indeed, consider such a small shift, $\Delta x$, perpendicular to the plane surface of a broad, plane slab filled with plasma. The uncompensated charges, with equal and opposite surface densities $\sigma=\mp e n \Delta x$, that appear at the slab surfaces, create inside the it, according to Eq. (2.3), a uniform electric field $E_{x}=e n \Delta x / \varepsilon_{0}$. This field exerts force $e E=\left(n e^{2} / \varepsilon_{0}\right) \Delta x$ on each positively charged ion. According to the $3^{\text {rd }}$ Newton law, the ions pull each electron back to its equilibrium position with the equal and opposite force $F=-e E=-\left(n e^{2} / \varepsilon_{0}\right)$ $\Delta x$, justifying the above expression for $\kappa_{\text {eff }}$. Hence it is not surprising that $\varepsilon(\omega)$ described by the first of Eqs. (36) turns into zero at $\omega=\omega_{p}$ : at this resonance frequency, finite free oscillations of charge (and hence of $D=\varepsilon E$ ) do not require a finite force (and hence $E$ ).

The behavior of electromagnetic waves in a medium that obeys Eq. (36), is very remarkable. If the wave frequency $\omega$ is above $\omega_{p}$, the dielectric constant and hence the wave number (28) are positive and real, and waves propagate without attenuation, following the dispersion relation,

Plasma dispersion relation

$$
\begin{equation*}
k(\omega)=\omega\left[\varepsilon(\omega) \mu_{0}\right]^{1 / 2}=\frac{1}{c}\left(\omega^{2}-\omega_{p}^{2}\right)^{1 / 2} \tag{7.38}
\end{equation*}
$$

which is shown in Fig. 6. (As we will see later in this chapter, many wave transmission systems obey such dispersion law as well.)


At $\omega \rightarrow \omega_{p}$ the wave number $k$ tends to zero. Beyond that point (at $\omega<\omega_{p}$ ), we still can use Eq. (38), but it is more instrumental to rewrite it in the mathematically equivalent form

$$
\begin{equation*}
k(\omega)=\frac{i}{c}\left(\omega_{p}^{2}-\omega^{2}\right)^{1 / 2}=\frac{i}{\delta}, \quad \text { where } \delta \equiv \frac{c}{\left(\omega_{p}^{2}-\omega^{2}\right)^{1 / 2}} \tag{7.39}
\end{equation*}
$$

According to Eq. (29), this means that the electromagnetic field exponentially decreases with distance:

$$
\begin{equation*}
f=\operatorname{Re} f_{\omega} e^{i(k z-\omega t)}=\exp \left\{-\frac{z}{\delta}\right\} \operatorname{Re} f_{\omega} e^{-i \omega t} \tag{7.40}
\end{equation*}
$$

Does this mean that the wave is being absorbed in the plasma? Answering this question is a good pretext to calculate the time average of the Poynting vector $\mathbf{S}=\mathbf{E} \times \mathbf{H}$ of a monochromatic electromagnetic wave in an arbitrary dispersive (but still linear!) medium. First, let us spell out fields' time dependence:

$$
\begin{equation*}
E(t)=\operatorname{Re}\left[E_{\omega}(z) e^{-i \omega t}\right]=\frac{1}{2}\left[E_{\omega} e^{-i \omega t}+\text { c.c. }\right], \quad H(t)=\operatorname{Re}\left[H_{\omega}(z) e^{-i \omega t}\right]=\frac{1}{2}\left[\frac{E_{\omega}}{Z(\omega)} e^{-i \omega t}+\text { c.c. }\right] . \tag{7.41}
\end{equation*}
$$

Now, a straightforward calculation yields ${ }^{15}$

$$
\begin{equation*}
\bar{S}=\overline{E(t) H(t)}=\frac{E_{\omega} E_{\omega}^{*}}{4}\left[\frac{1}{Z(\omega)}+\frac{1}{Z^{*}(\omega)}\right]=\frac{E_{\omega} E_{\omega}^{*}}{2} \operatorname{Re} \frac{1}{Z(\omega)} \equiv \frac{\left|E_{\omega}\right|^{2}}{2} \operatorname{Re}\left(\frac{\varepsilon(\omega)}{\mu(\omega)}\right)^{1 / 2} \tag{7.42}
\end{equation*}
$$

Let us apply this important general formula to our simple model of plasma at $\omega<\omega_{p}$. In this case $\mu(\omega)=\mu_{0}$, i.e. is positive and real, while $\delta(\omega)$ is real and negative, so that $1 / Z(\omega)=[\varepsilon(\omega) / \mu(\omega)]^{1 / 2}$ is purely imaginary, and the average Poynting vector (42) vanishes. This means that energy, on the average, does not flow along axis $z$ - as it would if it was absorbed in plasma. As we will see in the next section, waves with $\omega<\omega_{p}$ are rather reflected from plasma's boundary, without energy loss. Note that in the limit $\omega \ll \omega_{p}$, Eq. (39) yields

$$
\begin{equation*}
\delta \rightarrow \frac{c}{\omega_{p}}=\left(\frac{c^{2} \varepsilon_{0} m_{e}}{n e^{2}}\right)^{1 / 2}=\left(\frac{m_{e}}{\mu_{0} n e^{2}}\right)^{1 / 2} . \tag{7.43}
\end{equation*}
$$

But this is just a particular case (for $q=e$ and $\mu=\mu_{0}$ ) of the expression (6.38) that we have derived for the depth of magnetic field penetration into a lossless (collision-free) conductor in the quasistatic approximation. We see again that, as was already discussed in Sec. 6.7, that approximation (in which we neglect the displacement currents) gives an adequate description of the time-dependent phenomena at $\omega$ $\ll \omega_{p}$, i.e. at $\delta \ll c / \omega=1 / k=\lambda / 2 \pi$.

There are two most important examples of plasmas. For the Earth's ionosphere, i.e. the upper part of the atmosphere that is almost completely ionized by the UV and X-ray components of Sun's radiation, the maximum value of $n$, reached at about 300 km over the Earth surface, is between $10^{10}$ and $10^{12} \mathrm{~m}^{-3}$ (depending on the time of the day and Sun's activity), so that that the maximum plasma frequency (37) is between 1 and 10 MHz . This is much higher than the particle's reciprocal collision time $\tau^{-1}$, so that Eq. (36) gives a very good description of plasma's electric polarization. The effect of reflection of waves with $\omega<\omega_{p}$ from the ionosphere enables long-range (over-the-globe) radio communications and broadcasting at the so-called short waves, with frequencies of the order of 10 MHz .

[^314]Such waves may propagate in the flat channel formed by the Earth surface and the ionosphere, reflected repeatedly by these "walls". Unfortunately, due to the random variations of Sun's activity, and hence $\omega_{p}$, such natural communication channel is not too reliable, and in our age of fiber optics cables its practical importance is diminishing.

Another important example of plasmas is free electrons in metals and other conductors. For a typical metal, $n$ is of the order of $10^{23} \mathrm{~cm}^{-3}=10^{29} \mathrm{~m}^{-3}$, so that Eq. (37) yields $\omega_{p} \sim 10^{16} \mathrm{~s}^{-1}$. Note that this value of $\omega_{p}$ is somewhat higher than mid-optical frequencies $\left(\omega \sim 3 \times 10^{15} \mathrm{~s}^{-1}\right)$. This explains why planar, even, clean metallic surfaces, such as aluminum and silver films used in mirrors, are so shiny: at these frequencies the permittivity is almost exactly real and negative, leading to light reflection, with very little absorption. However, the considered model, which neglects electron scattering, becomes inadequate at lower frequencies, $\omega \tau \sim 1$.

A phenomenological way of extending the model by account of scattering is to take, in Eq. (33), the lowest eigenfrequency $\omega_{j}$ to be equal zero (to describe free electrons), while keeping the damping coefficient $\delta_{0}$ of this mode finite, to account for their energy loss due to scattering. Then Eq. (33) is reduced to

$$
\begin{equation*}
\varepsilon_{\mathrm{ef}}(\omega)=\varepsilon_{\mathrm{opt}}(\omega)+\frac{n_{0} q^{2}}{m} \frac{1}{-\omega^{2}-2 i \omega \delta_{0}}=\varepsilon_{\mathrm{opt}}(\omega)+\frac{i}{\omega} \frac{n_{0} q^{2}}{2 \delta_{0} m} \frac{1}{1-i \omega / 2 \delta_{0}}, \tag{7.44}
\end{equation*}
$$

where response $\varepsilon_{\text {opt }}(\omega)$ at high (in practice, optical) frequencies is still given by Eq. (33), but now with $j$ $\neq 0$.

Result (44) allows for a simple interpretation. To show that, let us incorporate into our calculations the Ohmic conduction, generalizing Eq. (4.7) as $\mathbf{j}_{\omega}=\sigma(\omega) \mathbf{E}_{\omega}$ to account for the possible frequency dependence of the Ohmic conductivity. Plugging this relation into the Fourier image of the relevant Maxwell equation, $\nabla \times \mathbf{H}_{\omega}=\mathbf{j}_{\omega}-i \omega \mathbf{D}_{\omega}=\mathbf{j}_{\omega}-i \omega \delta(\omega) \mathbf{E}_{\omega}$, we get

$$
\begin{equation*}
\nabla \times \mathbf{H}_{\omega}=[\sigma(\omega)-i \omega \varepsilon(\omega)] \mathbf{E}_{\omega} . \tag{7.45}
\end{equation*}
$$

This relation shows that for a sinusoidal process, the addition of the Ohmic current density $\mathbf{j}_{\omega}$ to the displacement current density is equivalent to addition of $\sigma(\omega)$ to $-i \omega \varepsilon(\omega)$, i.e. to the following change of the ac electric permittivity: ${ }^{16}$

$$
\begin{equation*}
\varepsilon(\omega) \rightarrow \varepsilon_{\mathrm{ef}}(\omega) \equiv \varepsilon_{\mathrm{opt}}(\omega)+i \frac{\sigma(\omega)}{\omega} . \tag{7.46}
\end{equation*}
$$

Now the comparison of Eqs. (44) and (46) shows that they coincide if we take

Generalized
Drude formula

$$
\begin{equation*}
\sigma(\omega)=\frac{n_{0} q^{2} \tau}{m_{0}} \frac{1}{1-i \omega \tau}=\sigma(0) \frac{1}{1-i \omega \tau} \tag{7.47}
\end{equation*}
$$

where the dc conductivity $\sigma(0)$ is described by the Drude formula (4.13), and the phenomenologically introduced coefficient $\delta_{0}$ is associated with $1 / 2 \tau$. Relation (47), which is frequently called the

[^315]generalized (or "ac", or "rf") Drude formula, ${ }^{17}$ gives a very reasonable (semi-quantitative) description of the ac conductivity of many metals almost all the way up to optical frequencies.

### 7.3. Kramers-Kronig relations

The results for the simple model of dispersion, discussed in the last section, imply that the frequency dependences of the real $\left(\varepsilon^{\prime}\right)$ and imaginary $\left(\varepsilon^{\prime \prime}\right)$ parts of the permittivity are not quite independent. For example, let us have one more look at the resonance peaks in Fig. 5. Each time the real part drops with frequency, $d \varepsilon^{\prime} / d \omega<0$, its imaginary part $\varepsilon^{\prime \prime}$ has a positive peak. R. de L. Kronig in 1926 and H. A. Kramers in 1927 independently showed that this is not an occasional coincidence pertinent only to the Lorentz oscillator model. Moreover, the full knowledge of function $\varepsilon^{\prime}(\omega)$ allows one to calculate function $\varepsilon^{\prime \prime}(\omega)$, and vice versa. The reason is that both these functions are always related to a single real function $G(\theta)$ by Eqs. (28).

To derive the Kramers-Kronig relations, let us consider Eq. (27) on the complex frequency plane, $\omega \rightarrow \omega^{\prime}+i \omega^{\prime \prime}$ :

$$
\begin{equation*}
f(\omega) \equiv \varepsilon(\omega)-\varepsilon_{0}=\int_{0}^{\infty} G(\theta) e^{i \omega \theta} d \theta=\int_{0}^{\infty} G(\theta) e^{i \omega^{\prime} \theta} e^{-\omega^{\prime \prime} \theta} d \theta \tag{7.48}
\end{equation*}
$$

For all stable physical systems, $G(\theta)$ has to be finite for all important values of the integration variable $(\theta>0)$, and tend to zero at $\theta \rightarrow 0$ and $\theta \rightarrow \infty$. Because of that, and thanks to factor $e^{-\omega \prime \theta}$, the expression under the integral tends to zero at $|\omega| \rightarrow \infty$ in all upper half-plane ( $\omega^{\prime \prime} \geq 0$ ). As a result, we may claim that the complex-variable function $f(\omega)$ is analytical in that half-plane, and allows us to apply to it the Cauchy integral formula ${ }^{18}$

$$
\begin{equation*}
f(\omega)=\frac{1}{2 \pi i} \oint_{C} f(\Omega) \frac{d \Omega}{\Omega-\omega}, \tag{7.49}
\end{equation*}
$$

with the integration contour of the form shown in Fig. 7, with radius $R$ of the larger semicircle tending to infinity, and radius $r$ that of the smaller semicircle (about the singular point $\Omega=\omega$ ) tending to zero.


Fig. 7.7. Integration path $C$ used in the Cauchy integral formula to derive the Kramers-Kronig dispersion relations.

[^316]Due to the exponential decay of $|f(\Omega)|$ at $|\Omega| \rightarrow \infty$, the contribution to the integral from the larger semicircle vanishes, ${ }^{19}$ while the contribution from the small semicircle, where $\Omega=\omega+r \exp \{i \varphi\}$, with $-\pi \leq \varphi \leq 0$, is

$$
\begin{equation*}
\lim _{r \rightarrow 0} \frac{1}{2 \pi i} \int_{\Omega=\omega+r \exp \{i \varphi)} f(\Omega) \frac{d \Omega}{\Omega-\omega}=\frac{f(\omega)}{2 \pi i} \int_{-\pi}^{0} \frac{i r \exp \{i \varphi\} d \varphi}{r \exp \{i \varphi\}}=\frac{f(\omega)}{2 \pi} \int_{-\pi}^{0} d \varphi=\frac{1}{2} f(\omega) . \tag{7.50}
\end{equation*}
$$

As a result, for our contour $C$, Eq. (49) yields

$$
\begin{equation*}
f(\omega)=\lim _{r \rightarrow 0} \frac{1}{2 \pi i}\left(\int_{-\infty}^{\omega-r}+\int_{\omega+r}^{+\infty}\right) f(\Omega) \frac{d \Omega}{\Omega-\omega}+\frac{1}{2} f(\omega) . \tag{7.51}
\end{equation*}
$$

Such an integral, excluding a symmetric infinitesimal vicinity of the pole singularity, is called the principal value of the (formally, diverging) integral from $-\infty$ to $+\infty$, and is denoted by letter P before it. ${ }^{20}$ Using this notation, subtracting $f(\omega) / 2$ from both parts of Eq. (51), and multiplying them by 2 , we get

$$
\begin{equation*}
f(\omega)=\frac{1}{\pi i} \mathrm{P} \int_{-\infty}^{+\infty} f(\Omega) \frac{d \Omega}{\Omega-\omega} . \tag{7.52}
\end{equation*}
$$

Now plugging into this complex equality the polarization-related difference $f(\omega) \equiv \varepsilon(\omega)-\varepsilon_{0}$ in the form $\left[\varepsilon^{\prime}(\omega)-\varepsilon_{0}\right]+i\left[\varepsilon^{\prime \prime}(\omega)\right]$, and requiring both real and imaginary components of both parts of Eq. (52) to be equal separately, we get the famous Kramers-Kronig dispersion relations

$$
\begin{equation*}
\varepsilon^{\prime}(\omega)=\varepsilon_{0}+\frac{1}{\pi} \mathrm{P} \int_{-\infty}^{+\infty} \varepsilon^{\prime \prime}(\Omega) \frac{d \Omega}{\Omega-\omega}, \quad \varepsilon^{\prime \prime}(\omega)=-\frac{1}{\pi} \mathrm{P} \int_{-\infty}^{+\infty}\left[\varepsilon^{\prime}(\Omega)-\varepsilon_{0}\right] \frac{d \Omega}{\Omega-\omega} . \tag{7.53}
\end{equation*}
$$

Kramersdispersion relations

Now we may use the already mentioned fact that $\varepsilon^{\prime}(\omega)$ is always an even, while $\varepsilon^{\prime \prime}(\omega)$ an odd function of frequency, to rewrite these relations in the following form

$$
\begin{equation*}
\varepsilon^{\prime}(\omega)=\varepsilon_{0}+\frac{2}{\pi} \mathrm{P} \int_{0}^{+\infty} \varepsilon^{\prime \prime}(\Omega) \frac{\Omega d \Omega}{\Omega^{2}-\omega^{2}}, \quad \varepsilon^{\prime \prime}(\omega)=-\frac{2 \omega}{\pi} \mathrm{P} \int_{0}^{+\infty}\left[\varepsilon^{\prime}(\Omega)-\varepsilon_{0}\right] \frac{d \Omega}{\Omega^{2}-\omega^{2}}, \tag{7.54}
\end{equation*}
$$

which is more convenient for most applications, because it involves only physical (positive) frequencies.
Though the Kramers-Kronig relations are "global" in frequency, in certain cases they allow an approximate calculation of dispersion from experimental data for absorption, collected even in a limited frequency range. For example, if a medium has a sharp absorption peak at some frequency $\omega_{j}$, we may approximate it as

$$
\begin{equation*}
\varepsilon^{\prime \prime}(\omega) \approx c \delta\left(\omega-\omega_{j}\right)+\text { a more smooth function of } \omega \tag{7.55}
\end{equation*}
$$

and the first of Eqs. (54) immediately gives

[^317]$$
\varepsilon^{\prime}(\omega) \approx \varepsilon_{0}+\frac{2 c}{\pi} \frac{\omega_{j}}{\omega_{j}^{2}-\omega^{2}}+\text { another smooth function of } \omega
$$
thus predicting the anomalous dispersion near such a point. This calculation shows that such behavior observed in the Lorentz oscillator model (Fig. 5) is by no means occasional or model-specific.

Let me emphasize again that the general, and hence very powerful Kramers-Kronig relations hinge on the causal, linear relation (21) between polarization $P(t)$ with the electric field $E\left(t^{\prime}\right)$. Hence, these relations are also valid for the complex functions relating Fourier images of any cause/effectrelated pair of variables. In particular, at a measurement of any linear response $r(t)$ of any experimental sample to any external applied field $f(t)$, whatever the nature of this response and physics behind it, we may be confident that there is a causal relation between the variables $r$ and $f$, so that the complex function $\chi(\omega) \equiv r_{\omega} / f_{\omega}$ does obey the Kramers-Kronig relations. However, it is still important to remember that a linear relation between the Fourier amplitudes of two variables does not necessarily imply the causal relationship between them. ${ }^{21}$

### 7.4. Reflection

The most important new effect arising in nonuniform media is wave reflection. Let us start its discussion from the simplest case of a plane electromagnetic wave that is normally incident on an interface between two uniform, linear, isotropic media.

If the interface is an ideal mirror, the description of reflection is very simple. Indeed, let us assume that one of the two media (say, located at $z>0$, see Fig. 8) cannot sustain any electric field at all:

$$
\begin{equation*}
\left.E\right|_{z \geq 0}=0 . \tag{7.57}
\end{equation*}
$$

This condition is evidently incompatible with the single traveling wave (5). However, this solution may be readily corrected using the fact that the dispersion-free 1D wave equation,

$$
\begin{equation*}
\left(\frac{\partial^{2}}{\partial z^{2}}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) E=0 \tag{7.58}
\end{equation*}
$$

supports waves, propagating, with the same speed, in opposite directions. As a result, the following linear superposition of two such waves,

$$
\begin{equation*}
\left.E\right|_{z \leq 0}=f(z-v t)-f(-z-v t), \tag{7.59}
\end{equation*}
$$

satisfies both the equation and the boundary condition (57), for an arbitrary function $f$. The second term in Eq. (59) may be interpreted as the total reflection of the incident wave described by its first term, in this case with the change of electric field's sign. By the way, since vector $\mathbf{n}$ of the reflected wave is

[^318]opposite to that incident one (see arrows in Fig. 1), Eq. (6) shows that the magnetic field of the wave does not change its sign at the reflection:
\[

$$
\begin{equation*}
\left.H\right|_{z \leq 0}=\frac{1}{Z}[f(z-v t)+f(-z-v t)] . \tag{7.60}
\end{equation*}
$$

\]



Fig. 7.8. Spatial dependence of electric field at the reflection of a sinusoidal wave from a perfect conductor: the real pattern (red lines) and the crude, ideal-mirror approximation (blue lines). Dashed lines show the patterns after a half-period time delay $(\omega \Delta t=\pi)$.

Wave's total reflection
al red

Blue lines in Fig. 8 show the resulting pattern (59) for the simplest, sinusoidal waveform

$$
\begin{equation*}
\left.E\right|_{z \leq 0}=\operatorname{Re}\left[E_{\omega} e^{i(k z-\omega t)}-E_{\omega} e^{i(-k z-\omega t)}\right] \tag{7.61a}
\end{equation*}
$$

Depending on convenience in a particular context, this pattern may be legitimately interpreted either as a superposition (61a) of two traveling waves or a single standing wave,

$$
\begin{equation*}
\left.E\right|_{z \leq 0}=-2 \operatorname{Im}\left(E_{\omega} e^{-i \omega t}\right) \sin k z=2 \operatorname{Re}\left(i E_{\omega} e^{-i \omega t}\right) \sin k z \tag{7.61b}
\end{equation*}
$$

in which the electric and magnetic field oscillate with the phase shifts by $\pi / 2$ both in time and space:

$$
\begin{equation*}
\left.H\right|_{z \leq 0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z} e^{i(k z-\omega t)}+\frac{E_{\omega}}{Z} e^{i(-k z-\omega t)}\right]=2 \operatorname{Re}\left(\frac{E_{\omega}}{Z} e^{-i \omega t}\right) \cos k z . \tag{7.62}
\end{equation*}
$$

As the result of this shift, the time average of the Poynting vector's magnitude,

$$
\begin{equation*}
S(z, t)=E H=\frac{1}{Z} \operatorname{Re}\left[E_{\omega}^{2} e^{-2 i \omega t}\right] \sin 2 k z, \tag{7.63}
\end{equation*}
$$

equals zero, showing that at the total reflection there is no average power flow. (This is natural, because the perfect mirror can neither transmit the wave nor absorb it.) However, Eq. (63) shows that the standing wave provides local oscillations of energy, transferring it periodically between the concentrations of the electric and magnetic fields, separated by distance $\Delta z=\pi / 2 k=\lambda / 4$.

For the case of the sinusoidal waves, the reflection effects may be readily explored even for the more general case of dispersive and/or lossy media in which $\varepsilon(\omega)$ and $\mu(\omega)$, and hence the wave vector $k(\omega)$ and wave impedance $Z(\omega)$, defined by Eqs. (28), are certain complex functions of frequency. The "only" new factors we have to account for is that in this case the reflection may not be full, and that
inside the second media we have to use the traveling-wave solution as well. Both these factors may be taken care of by looking for the solution of our boundary problem in the form

$$
\begin{equation*}
\left.E\right|_{z \leq 0}=\operatorname{Re}\left[E_{\omega}\left(e^{i k_{-} z}+R e^{-i k_{-} z}\right) e^{-i \omega t}\right],\left.\quad E\right|_{z \geq 0}=\operatorname{Re}\left[E_{\omega} T e^{i k_{+} z} e^{-i \omega t}\right] \tag{7.64}
\end{equation*}
$$

and hence, according to Eq. (6),

$$
\begin{equation*}
\left.H\right|_{z \leq 0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{-}(\omega)}\left(e^{i k_{-} z}-R e^{-i k_{-} z}\right) e^{-i \omega t}\right],\left.\quad H\right|_{z \geq 0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{+}(\omega)} T e^{i k_{+} z} e^{-i \omega t}\right] \tag{7.65}
\end{equation*}
$$

(Indices + and - correspond to, respectively, the media at $z>0$ and $z<0$.) Please note the following important features of these relations:
(i) Due to the problem linearity, we could (and did :-) take the complex amplitudes of the reflected and transmitted wave proportional to that $\left(E_{\omega}\right)$ of the incident wave, describing them by the dimensionless coefficients $R$ and $T$. The total reflection from an ideal mirror, that was discussed above, corresponds to the particular case $R=-1$ and $T=0$.
(ii) Since the incident wave, that we are considering, arrives from one side only (from $z=-\infty$ ), there is no need to include a term proportional to $\exp \left\{-i k_{+} z\right\}$ into Eqs. (64)-(65) - in our current problem. However, we would need such a term if the medium at $z>0$ was non-uniform (e.g., had at least one more interface or any other inhomogeneity), because the wave reflected from that additional inhomogeneity would be incident on our interface (located at $z=0$ ) from the right.
(iii) Solution (64)-(65) is sufficient even for the description of the cases when waves cannot propagate at $z \geq 0$, for example a conductor or a plasma with $\omega_{p}>\omega$. Indeed, the exponential drop of the field amplitude at $z>0$ in such cases is automatically described by the imaginary part of wave number $k_{+}$- see Eq. (29).

In order to find coefficients $R$ and $T$, we need to use boundary conditions at $z=0$. Since the reflection does not change the transverse character of the partial waves, at the normal incidence both vectors $\mathbf{E}$ and $\mathbf{H}$ remain tangential to the interface plane (in our notation, $z=0$ ). Reviewing the arguments that has led us, in statics, to boundary conditions (3.47) and (5.118) for these components, we see that they remain valid for the time-dependent situation as well, ${ }^{22}$ so that for our current case of purely transverse waves we can write:

$$
\begin{equation*}
\left.E\right|_{z=-0}=\left.E\right|_{z=+0},\left.\quad H\right|_{z=-0}=\left.H\right|_{z=+0} . \tag{7.66}
\end{equation*}
$$

Plugging Eqs. (64)-(65) into these conditions, we get

$$
\begin{equation*}
1+R=T, \quad \frac{1}{Z_{-}}(1-R)=\frac{1}{Z_{+}} T . \tag{7.67}
\end{equation*}
$$

[^319]Solving this simple system of equations, we get ${ }^{23}$

$$
\begin{equation*}
R=\frac{Z_{+}-Z_{-}}{Z_{+}+Z_{-}}, \quad T=\frac{2 Z_{+}}{Z_{+}+Z_{-}} . \tag{7.68}
\end{equation*}
$$

These formulas are very important, and much more general than one may think, because they are applicable for virtually any 1D waves - electromagnetic or not, if only the impedance $Z$ is defined in a proper way. ${ }^{24}$ Since in the general case the wave impedances $Z_{ \pm}$, defined by Eq. (28) with the corresponding indices, are complex functions of frequency, Eqs. (68) show that coefficients $R$ and $T$ may have imaginary parts as well. This fact has most important consequences at $z<0$ where the reflected wave, proportional to $R$, interferes with the incident wave. Indeed, plugging $R=|R| e^{i \varphi}$ (where $\varphi \equiv \arg R$ is a real phase shift) into the expression in parentheses in the first of Eqs. (64), we may rewrite it as

$$
\begin{align*}
\left(e^{i k-z}+R e^{-i k_{-} z}\right) & =(1-|R|+|R|) e^{i k_{-} z}+|R| e^{i \varphi} e^{-i k_{-} z} \\
& =(1-|R|) e^{i k_{-} z}+2|R| e^{i \varphi / 2} \sin \left[k_{-}\left(z-\delta_{-}\right)\right], \quad \text { where } \delta_{-} \equiv \frac{\varphi-\pi}{2 k_{-}} \tag{7.69}
\end{align*}
$$

This means that the field may be presented as a sum of a traveling wave and a standing wave, with amplitude proportional to $|R|$, shifted by distance $\delta$. toward the interface, relatively to the ideal-mirror pattern (61b). This effect is frequently used for the experimental measurements of an unknown impedance $Z_{+}$of some medium, provided than $Z_{-}$is known (e.g., for the free space, $Z_{-}=Z_{0}$ ). For that, a small antenna (the probe), not disturbing the field distribution too much, is placed into the wave field, and the amplitude of the ac voltage induced in it by the wave in the probe is measured by some detector (e.g., a semiconductor diode with a quadratic $I-V$ curve), as a function of $z$ (Fig. 9). From this measurement, it is straightforward to find both $|R|$ and $\delta$, and hence restore complex $R$, and then use Eq. (68) to calculate both modulus and argument of $Z_{+} .{ }^{25}$


Fig. 7.9. Measurement of the complex impedance of a medium (schematically).

Now let us discuss what do these results give for waves incident from the free space ( $Z_{-}(\omega)=Z_{0}$ $=$ const, $k_{-}=k_{0}=\omega / c$ ) onto the surface of two particular media.

[^320](i) For a collision-free plasma (with negligible magnetization) we may use Eq. (36) with $\mu(\omega)=$ $\mu_{0}$, to present the impedance in either of two equivalent forms:
\[

$$
\begin{equation*}
Z_{+}=Z_{0} \frac{\omega}{\left(\omega^{2}-\omega_{p}^{2}\right)^{1 / 2}}=-i Z_{0} \frac{\omega}{\left(\omega_{p}^{2}-\omega^{2}\right)^{1 / 2}} \tag{7.70}
\end{equation*}
$$

\]

The former expression is more convenient in the case $\omega>\omega_{p}$, when the wave vector $k_{+}$and the wave impedance $Z_{+}$of plasma are real, so that a part of the incident wave propagates into the plasma. Plugging this expression into the latter of Eqs. (68), we see that the transmission coefficient is real:

$$
\begin{equation*}
T=\frac{2 \omega}{\omega+\left(\omega^{2}-\omega_{p}^{2}\right)^{1 / 2}} \tag{7.71}
\end{equation*}
$$

Note that according to this formula, somewhat counter-intuitively, $T>1$ for any frequency (above $\omega_{p}$ ). How can the transmitted wave be more intensive than the incident one that has induced it? For a better understanding of this result, let us compare the powers (rather than amplitudes) of these two waves, i.e. their average Poynting vectors (42):

$$
\begin{equation*}
\overline{S_{\text {incident }}}=\frac{\left|E_{\omega}\right|^{2}}{2 Z_{0}}, \quad \overline{S_{+}}=\frac{\left|T E_{\omega}\right|^{2}}{2 Z_{+}}=\frac{\left|E_{\omega}\right|^{2}}{2 Z_{0}} \frac{4 \omega\left(\omega^{2}-\omega_{p}^{2}\right)^{1 / 2}}{\left[\omega+\left(\omega^{2}-\omega_{p}^{2}\right)^{1 / 2}\right]^{2}} . \tag{7.72}
\end{equation*}
$$

It is easy to see that the ratio of these two values ${ }^{26}$ is always below 1 (and tends to zero at $\omega \rightarrow \omega_{p}$ ), so that only a fraction of the incident wave power may be transferred. Hence the result $T>1$ may be interpreted as follows: the interface between two media also works as an impedance transformer: though it can never transfer more power than the incident wave provides, i.e. can only decrease the product $S=$ $E H$, but since the ratio $Z=E / H$ changes at the interface, the amplitude of one of the fields may increase at the transfer.

Now let us proceed to case $\omega<\omega_{p}$, when the waves cannot propagate in the plasma. In this case, the latter of expressions (70) is more convenient, because it immediately shows that $Z_{+}$is purely imaginary, while $Z_{-}=Z_{0}$ is purely real. This means that $\left(Z_{+}-Z_{-}\right)=\left(Z_{+}+Z_{-}\right)^{*}$, i.e. according to the first of Eqs. (68), $|R|=1$, so that the reflection is total, i.e. no incident power (on the average) is transferred into the plasma - as was already discussed in Sec. 2. However, the complex $R$ has a finite argument,

$$
\begin{equation*}
\varphi=\arg R=2 \arg \left(Z_{+}-Z_{0}\right)=-2 \tan ^{-1} \frac{\omega}{\left(\omega_{p}^{2}-\omega^{2}\right)^{1 / 2}}, \tag{7.73}
\end{equation*}
$$

and hence provides a finite spatial shift (69) of the standing wave toward the plasma surface:

$$
\begin{equation*}
\delta_{-}=\frac{\varphi-\pi}{2 k_{0}}=\frac{c}{\omega} \tan ^{-1} \frac{\omega}{\left(\omega_{p}^{2}-\omega^{2}\right)^{1 / 2}} . \tag{7.74}
\end{equation*}
$$

On the other hand, we already know from Eq. (40) that the solution at $z>0$ is exponential, with the decay length $\delta$ that is described by Eq. (39). Calculating, from coefficient $T$, the exact coefficient before this exponent, it is straightforward to verify that the electric and magnetic fields are indeed

[^321]continuous at the interface, forming the pattern shown by red lines in Fig. 8. This penetration may be experimentally observed, for example, by bringing close to the interface the surface of another material transparent as frequency $\omega$. Even without solving this problem exactly, it is evident that if the distance between these two interfaces becomes comparable to $\delta$, a part of the exponential "tail" of the field is picked up by the second material, and induces a propagating wave. This is an electromagnetic analog of the quantum-mechanical tunneling through a potential barrier. ${ }^{27}$

Note that at $\omega \ll \omega_{p}$, both $\delta$ - and $\delta$ are reduced to the same frequency-independent value,

$$
\begin{equation*}
\delta, \delta_{-} \rightarrow \frac{c}{\omega_{p}}=\left(\frac{c^{2} \varepsilon_{0} m_{e}}{n e^{2}}\right)^{1 / 2}=\left(\frac{m_{e}}{\mu_{0} n e^{2}}\right)^{1 / 2} \tag{7.75}
\end{equation*}
$$

which is just the field penetration depth $\delta(6.38)$ calculated for a perfect conductor model (assuming $m=$ $m_{e}$ and $\mu=\mu_{0}$ ) in the quasistatic limit. This is natural, because the condition $\omega \ll \omega_{p}$ may be recast as $\lambda_{0}$ $=2 \pi c / \omega \gg 2 \pi c / \omega_{p}=2 \pi \delta$.
(ii) Now let us consider electromagnetic wave reflection from a nonmagnetic conductor. In the simplest low-frequency limit, when $\omega \tau$ is much less than 1 , the conductor may be described by a frequency-independent conductivity $\sigma .{ }^{28}$ According to Eq. (46), in this case we can take

$$
\begin{equation*}
Z_{+}=\left(\frac{\mu_{0}}{\varepsilon_{\mathrm{opt}}(\omega)+i \sigma / \omega}\right)^{1 / 2} . \tag{7.76}
\end{equation*}
$$

With this substitution, Eqs. (68) immediately give us all the results of interest. In particular, they show that now $R$ is complex, and hence some fraction $F$ of the incident wave is absorbed by the conductor. Using Eq. (42), we may calculate the fraction to be

$$
\begin{equation*}
F \equiv \frac{\overline{\left.S_{+}\right|_{z=+0}}}{\overline{S_{\text {incident }}}}=|T|^{2} \operatorname{Re} \frac{Z_{0}}{Z_{+}} . \tag{7.77}
\end{equation*}
$$

(Since power flow $S_{+}$into the conductor depends on $z$, tending to zero at distances $z \sim \delta$, it is important to calculate it directly at the interface to account for the absorption in the whole volume of the conductor.) Restricting ourselves, for the sake of simplicity, to the most important quasistatic limit, i.e. to $Z_{+}=\left(\mu_{0} \omega / i \sigma\right)^{1 / 2}$, and using Eq. (6.27) to express the impedance via the skin depth, $Z_{+}=$ $\pi(2 / i)^{1 / 2}\left(\delta_{s} / \lambda_{0}\right) Z_{0}$, we see that $\left|Z_{+}\right| \ll Z_{0}$, so that, according to Eq. (68), $T \approx 2 Z_{+} / Z_{0}$ and

Wave's
absorption conductor's surface

$$
\begin{equation*}
F \approx \frac{4\left|Z_{+}\right|^{2}}{Z_{0}^{2}} \operatorname{Re} \frac{Z_{0}}{Z_{+}}=2 \frac{\delta_{s}}{\lambda_{0}} \ll 1 \tag{7.78}
\end{equation*}
$$

Thus the absorbed power scales as the ratio of the skin depth to the free-space wavelength. This important result is widely used for the semi-qualitative evaluation of power losses in metallic waveguides and resonators, and immediately shows that in order to keep the losses low, the characteristic size of such systems (that gives a scale of the free-space wavelengths $\lambda_{0}$, at which they are

[^322]used) should be much larger than $\delta_{s}$. A more detailed theory of these structures will be discussed later in this chapter.

### 7.5. Refraction

Now let us consider the effects arising at the plane interface if the wave incidence angle $\theta$ (Fig. 10) is arbitrary, rather than equal to zero as in our previous analysis, for the simplest case of fully transparent media, with real $\varepsilon_{ \pm}$and $\mu_{ \pm}$.


Fig. 7.10. Plane wave reflection, transmission, and refraction at a plane interface. The plane of drawing is selected to contain all three wave vectors $\mathbf{k}_{+}, \mathbf{k}_{\text {-, }}$, and $\mathbf{k}^{\prime}$..

In contrast with the case of normal incidence, here the wave vectors $\mathbf{k}$., $\mathbf{k}_{-}^{\prime}$, and $\mathbf{k}_{+}$of the three component (incident, reflected, and transmitted) waves may have different directions. Hence now we have to start our analysis with writing a general expression for a single plane, monochromatic wave for the case when its wave vector $\mathbf{k}$ has all 3 Cartesian components, rather than one. An evident generalization of Eq. (11) to this case is

$$
\begin{equation*}
f(\mathbf{r}, t)=\operatorname{Re}\left[f_{\omega} e^{\left.i\left(k_{x} x+k_{y} y+k_{z} z\right)-\omega t\right)}\right]=\operatorname{Re}\left[f_{\omega} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)}\right] . \tag{7.79}
\end{equation*}
$$

This relation enables a ready analysis of "kinematic" relations that are independent of the media impedances. Indeed, it is sufficient to notice that in order to satisfy any linear, homogeneous boundary conditions at the interface $(z=0)$, all waves have the same temporal and spatial dependence on this plane. Hence if we select plane $x z$ so that vector $\mathbf{k}$. lies in it, then $\left(k_{-}\right)_{y}=0$, and $\mathbf{k}_{+}$and $\mathbf{k}_{\text {- ' cannot have }}$ any $y$-component either, i.e. all three vectors lie in the same plane - that is selected as the plane of drawing of Fig. 10. Moreover, due to the same reason their $x$-components should be equal:

$$
\begin{equation*}
k_{-} \sin \theta=k_{-}^{\prime} \sin \theta^{\prime}=k_{+} \sin r \text {. } \tag{7.80}
\end{equation*}
$$

From here we immediately have the well-known laws of reflection

$$
\begin{equation*}
\theta^{\prime}=\theta \tag{7.81}
\end{equation*}
$$

and refraction: ${ }^{29}$

[^323]Snell law

$$
\begin{equation*}
\frac{\sin r}{\sin \theta}=\frac{k_{-}}{k_{+}} \tag{7.82}
\end{equation*}
$$

In this form, the laws are valid for plane waves of any nature. In optics, the Snell law (82) is frequently presented in the form

$$
\begin{equation*}
\frac{\sin r}{\sin \theta}=\frac{n_{-}}{n_{+}} \tag{7.83}
\end{equation*}
$$

where $n_{ \pm}$is the index of refraction (also called the "refractive index") of the corresponding medium, defined as its wave number normalized so that of the free space (at wave's frequency):

$$
\begin{equation*}
n_{ \pm} \equiv \frac{k_{ \pm}}{k_{0}}=\left(\frac{\varepsilon_{ \pm} \mu_{ \pm}}{\varepsilon_{0} \mu_{0}}\right)^{1 / 2} \tag{7.84}
\end{equation*}
$$

Perhaps the most famous corollary of the Snell law is that if a wave propagates from a medium with a higher index of refraction to that with a lower one (i.e. if $n_{-}>n_{+}$in Fig. 10), for example from water into air, there is always a certain critical value $\theta_{c}$ of the incidence angle,
at which angle $r$ reaches $\pi / 2$. At a larger $\theta$, i.e. within the range $\theta_{c}<\theta<\pi / 2$, the boundary conditions cannot be satisfied with a refracted wave with a real wave vector, so that the wave experiences the socalled total internal reflection. This effect is very important for practice, because it shows that dielectric surfaces may be used as mirrors, in particular in optical fibers - to be discussed in more detail in Sec. 8 below. This is very fortunate for all the telecommunication technology, because the light reflection from metals is rather imperfect. Indeed, according to Eq. (78), in the optical range ( $\lambda_{0} \sim 0.5 \mu \mathrm{~m}$, i.e. $\omega \sim 10^{15}$ $\mathrm{s}^{-1}$ ), even the best conductors (with $\sigma \sim 6 \times 10^{8} \mathrm{~S} / \mathrm{m}$ and hence the normal skin depth $\delta_{\mathrm{s}} \sim 1.5 \mathrm{~nm}$ ) provide relatively high losses $F \sim 1 \%$ at each reflection.

Note, however, that even within the range $\theta_{\mathrm{c}}<\theta<\pi / 2$ the field at $z>0$ is not identically equal to zero: just as it does at the normal incidence $(\theta=0)$, it penetrates into the less dense media by a distance of the order of $\lambda_{0}$, exponentially decaying inside it. At $\theta \neq 0$ the penetrating field still changes sinusoidally, with wave number (80), along the interface. Such a field, exponentially dropping in one direction but still propagating as a wave in another direction, is frequently called the evanescent wave.

One more remark: just as at the normal incidence, the field penetration into another medium causes a phase shift of the reflected wave - see, e.g., Eq. (69) and its discussion. A new feature of this phase shift, arising at $\theta \neq 0$, is that it also has a component parallel to the interface - the so-called called the Goos-Hänchen effect. In geometric optics, this effect leads to an image shift (relative to that its position in a perfect mirror) with components both normal and parallel to the interface.

Now let us carry out an analysis of the "dynamic" relations that determine amplitudes of the refracted and reflected waves. For this we need to write explicitly the boundary conditions at the interface (i.e. plane $z=0$ ). Since now the electric and/or magnetic fields may have components normal to the plane, in addition to the continuity of their tangential components, which we have repeatedly discussed,

$$
\begin{equation*}
\left.E_{x, y}\right|_{z=-0}=\left.E_{x, y}\right|_{z=+0},\left.\quad H_{x, y}\right|_{z=-0}=\left.H_{x, y}\right|_{z=+0}, \tag{7.86}
\end{equation*}
$$

we also need relations for the normal components. As it follows from the homogeneous macroscopic Maxwell equations (6.94b), they are also the same as in statics ( $D_{n}=$ const, $B_{n}=$ const), for our reference frame choice (Fig. 10) giving

$$
\begin{equation*}
\left.\varepsilon_{-} E_{z}\right|_{z=-0}=\left.\varepsilon_{+} E_{z}\right|_{z=+0},\left.\quad \mu_{-} H_{z}\right|_{z=-0}=\left.\mu_{+} H_{z}\right|_{z=+0} . \tag{7.87}
\end{equation*}
$$

The expressions of these components via amplitudes $E_{\omega}, R E_{\omega}$, and $T E_{\omega}$ of the incident, reflected and transmitted waves depend on the incident wave's polarization. For example, for a linearly-polarized wave with the electric field vector perpendicular to the plane of incidence (Fig. 11a), i.e. parallel to the interface plane, the reflected and refracted waves are similarly polarized.

(b)

Fig. 7.11. Reflection and refraction at two different linear polarizations of the incident wave.

As a result, all $E_{z}$ are equal to zero (so that the first of Eqs. (87) is inconsequential), while the tangential components of the electric field are just equal to their full amplitudes, just as at the normal incidence, so we still can use Eqs. (64) to express these components via coefficients $R$ and $T$. However, at $\theta \neq 0$ the magnetic fields have not only tangential components

$$
\begin{equation*}
\left.H_{x}\right|_{z=-0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{-}}(1-R) \cos \theta e^{-i \omega t}\right],\left.\quad H_{x}\right|_{z=+0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{+}} T \cos r e^{-i \omega t}\right], \tag{7.88}
\end{equation*}
$$

but also normal components (Fig. 11a):

$$
\begin{equation*}
\left.H_{z}\right|_{z=-0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{-}}(1+R) \sin \theta e^{-i \omega t}\right],\left.\quad H_{z}\right|_{z=+0}=\operatorname{Re}\left[\frac{E_{\omega}}{Z_{+}} T \sin r e^{-i \omega t}\right] . \tag{7.89}
\end{equation*}
$$

Plugging these expressions into the boundary conditions expressed by Eqs. (86) (in this case, for $y$ components only) and the second of Eqs. (87), we get three equations for two unknown coefficients $R$ and $T$. However, two of these equations duplicate each other because of the Snell law, and we get just two independent equations,

$$
\begin{equation*}
1+R=T, \quad \frac{1}{Z_{-}}(1-R) \cos \theta=\frac{1}{Z_{+}} T \cos r, \tag{7.90}
\end{equation*}
$$

which are a very natural generalization of Eqs. (67), with replacements $Z_{-} \rightarrow Z_{-} \cos r, Z_{+} \rightarrow Z_{+} \cos \theta$. As a result, we can immediately use Eq. (68) to write the solution of system (90):30

$$
\begin{equation*}
R=\frac{Z_{+} \cos \theta-Z_{-} \cos r}{Z_{+} \cos \theta+Z_{-} \cos r}, \quad T=\frac{2 Z_{+} \cos \theta}{Z_{+} \cos \theta+Z_{-} \cos r} . \tag{7.91a}
\end{equation*}
$$

If we want to express the coefficients via the angle of incidence alone, we should use the Snell law (82) to eliminate angle $r$, getting

$$
\begin{equation*}
R=\frac{Z_{+} \cos \theta-Z_{-}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}}{Z_{+} \cos \theta+Z_{-}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}}, \quad T=\frac{2 Z_{+} \cos \theta}{Z_{+} \cos \theta+Z_{-}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}} . \tag{7.91b}
\end{equation*}
$$

However, my strong preference is to use the kinematic relation (82) and dynamic relations (91a) separately, because Eq. (91b) obscures the very important physical fact that and the ratio of $k_{ \pm}$, i.e. of the wave velocities of the two media, is only involved in the Snell law (79), while the dynamic relations essentially include only the ratio of wave impedances - just as in the case of normal incidence.

In the opposite case of the linear polarization of the electric field within the plane of incidence (Fig. 11b), it is the magnetic field that does not have a normal component, so it is now the second of Eqs. (87) that does not participate in the solution. However, now the electric fields in two media have not only tangential components,

$$
\begin{equation*}
\left.E_{x}\right|_{z=-0}=\left.\operatorname{Re}\left[E_{\omega}(1+R) \cos \theta e^{-i \omega t}\right] \quad E_{x}\right|_{z=+0}=\operatorname{Re}\left[E_{\omega} T \cos r e^{-i \omega t}\right], \tag{7.92}
\end{equation*}
$$

but also normal components (Fig. 11b):

$$
\begin{equation*}
\left.E_{z}\right|_{z=-0}=E_{\omega}(-1+R) \sin \theta,\left.\quad E_{z}\right|_{z=+0}=-E_{\omega} T \sin r . \tag{7.93}
\end{equation*}
$$

As a result, instead of Eqs. (90), the reflection and transmission coefficients are related as

$$
\begin{equation*}
(1+R) \cos \theta=T \cos r, \quad \frac{1}{Z_{-}}(1-R)=\frac{1}{Z_{+}} T . \tag{7.94}
\end{equation*}
$$

Again, the solution of this system may be immediately written using the analogy with Eq. (67):

$$
\begin{equation*}
R=\frac{Z_{+} \cos r-Z_{-} \cos \theta}{Z_{+} \cos r+Z_{-} \cos \theta}, \quad T=\frac{2 Z_{+} \cos \theta}{Z_{+} \cos r+Z_{-} \cos \theta}, \tag{7.95a}
\end{equation*}
$$

or, alternatively, using the Snell law:

$$
\begin{equation*}
R=\frac{Z_{+}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}-Z_{-} \cos \theta}{Z_{+}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}+Z_{-} \cos \theta}, \quad T=\frac{2 Z_{+} \cos \theta}{Z_{+}\left[1-\left(k_{-} / k_{+}\right)^{2} \sin ^{2} \theta\right]^{1 / 2}+Z_{-} \cos \theta} . \tag{7.95b}
\end{equation*}
$$

[^324]For the particular case $\mu_{+}=\mu_{-}=\mu_{0}$, when $Z_{+} / Z-=\left(\varepsilon_{-} / \varepsilon_{+}\right)^{1 / 2}=k_{l} / k_{+}=n_{-} / n_{+}($which is approximately correct for traditional optical media), Eqs. (91b) and (95b) are called the Fresnel formulas. ${ }^{31}$ Most textbooks are quick to point out that there is a major difference between these cases: while for the electric field polarization within the plane of incidence (Fig. 11b), the reflected wave amplitude (proportional to coefficient $R$ ) turns to zero at a special value of $\theta$ (the so-called Brewster angle):32

$$
\begin{equation*}
\theta_{\mathrm{B}}=\tan ^{-1} \frac{n_{+}}{n_{-}}, \tag{7.96}
\end{equation*}
$$

while there is no such angle in the opposite case (Fig. 11a). ${ }^{33}$ However, that this statement, as well as Eq. (96), is true only for the case $\mu_{+}=\mu$. In the general case of different $\varepsilon$ and $\mu$, Eqs. (91) and (95) show that the reflected wave vanishes at $\theta=\theta_{\mathrm{B}}$ with

$$
\tan ^{2} \theta_{B}=\frac{\varepsilon_{-} \mu_{+}-\varepsilon_{+} \mu_{-}}{\varepsilon_{+} \mu_{+}-\varepsilon_{-} \mu_{-}} \times \begin{cases}\left(\mu_{+} / \mu_{-}\right), & \text {for } \mathbf{E} \perp \mathbf{n}_{z} \text { (Fig.11a), }  \tag{7.97}\\ \left(-\varepsilon_{+} / \varepsilon_{-}\right), & \text {for } \mathbf{H} \perp \mathbf{n}_{z} \text { (Fig.11b) }\end{cases}
$$

## Brewster <br> angle

Note the natural $\varepsilon \leftrightarrow \mu$ symmetry of these relations, resulting from the $\mathbf{E} \leftrightarrow \mathbf{H}$ symmetry for these two polarization cases (Fig. 11). They also show that for any set of parameters of the two media (with $\varepsilon_{ \pm}, \mu_{ \pm}>0$ ), $\tan ^{2} \theta_{\mathrm{B}}$ is positive (and hence a real Brewster angle $\theta_{\mathrm{B}}$ exists) only for one of these two polarizations. In particular, if the interface is due to the change of $\mu$ alone (i.e. $\varepsilon_{+}=\varepsilon_{-}$), the first of Eqs. (97) is reduced to the simple form (96) again, while for the polarization shown in Fig. 11b there is no Brewster angle, i.e. the reflected wave has a nonvanishing amplitude for any $\theta$.

Such account of both media parameters on an equal footing is especially necessary to describe the so-called negative refraction effects. ${ }^{34}$ As was shown in Sec. 2, in a medium with electric-fielddriven resonances, function $\delta(\omega)$ may be almost real and negative, at least within limited frequency intervals - see, in particular, Eq. (34) and Fig. 5. As have already been discussed, if, at these frequencies, function $\mu(\omega)$ is real and positive, then $k^{2}(\omega)=\omega^{2} \varepsilon(\omega) \mu(\omega)<0$, and $k$ may be presented as $i / \delta$ with real $\delta$, meaning the exponential field decay into the medium. However, let consider the case when both $\varepsilon(\omega)<0$ and $\mu(\omega)<0$ at a certain frequency. (This is evidently possible in a medium with both E-driven and $\mathbf{H}$-driven resonances, at proper relations between their eigenfrequencies.) Since in this case $k^{2}(\omega)=\omega^{2} \varepsilon(\omega) \mu(\omega)>0$, the wave vector is real, so that Eq. (79) describes a traveling wave, and one could think that there is nothing new in this case. Not quite so!

[^325]First of all, for a sinusoidal, plane wave (79), operator $\nabla$ is equivalent to the multiplication by $i \mathbf{k}$. As the Maxwell equations (2a) show, this means that at a fixed direction of vectors $\mathbf{E}$ and $\mathbf{k}$, the simultaneous reversal of signs of $\varepsilon$ and $\mu$ means the reversal of the direction of vector $\mathbf{H}$. Namely, if both $\varepsilon$ and $\mu$ are positive, these equations are satisfied with mutually orthogonal vectors $\mathbf{E}, \mathbf{H}$, and $\mathbf{k}$ forming the usual, right-hand system (see Fig. 1 and Fig. 12a), the name stemming from the popular "right-hand rule" used to determine the vector product direction. However, if both $\varepsilon$ and $\mu$ are negative, the vectors form a left-hand system - see Fig. 12b. (Due to this fact, the media with $\varepsilon<0$ and $\mu<0$ are frequently called the left-handed materials, LHM for short.) According to Eq. (6.97), that does not involve media parameters, this means that for a plane wave in a left-hand material, the Poynting vector $\mathbf{S}$ $=\mathbf{E} \times \mathbf{H}$, i.e. of the energy flow, is directed opposite to the wave vector $\mathbf{k}$.


Fig. 7.12. Directions of main vectors of a plane wave inside a medium with (a) positive and (b) negative $\varepsilon$ and $\mu$.

This fact may seems strange, but is in no contradiction with any fundamental principle. Let me remind you that, according to the definition of vector $\mathbf{k}$, its direction shows the direction of the phase velocity $v_{\mathrm{ph}}=\omega / k$ of a sinusoidal (and hence infinitely long) wave that cannot be used, for example, for signaling. Such signaling (by sending wave packets - see Fig. 13) is possible with the group velocity $v_{\mathrm{gr}}$ $=d \omega / d k$. This velocity in left-hand materials is always positive (directed along vector $\mathbf{S}$ ).


Fig. 7.13. Example of a wave packet moving along axis $z$ with a negative phase velocity, but positive group velocity. Blue lines show a packet snapshot a short time interval after the first snapshot (red lines).

Maybe the most fascinating effect possible with left-hand materials is the wave refraction at their interfaces with the usual, right-handed materials - first predicted by V. Veselago. Consider the example shown in Fig. 14a. In the incident wave, coming from the usual material, the directions of vectors $\mathbf{k}$. and S. coincide, and so they are in the reflected wave characterized by vectors $\mathbf{k}^{\prime}$. and $\mathrm{S}^{\prime}$.. This means that the electric and magnetic fields in the interface plane $(z=0)$ are, at our choice of coordinates, proportional to $\exp \left\{i k_{x} x\right\}$, with positive component $k_{x}=k_{-} \cos \theta$. In order to satisfy any linear boundary conditions, the refracted wave, going into the left-handed material, should match that dependence, i.e.
have a positive $x$-component of its wave vector $\mathbf{k}_{+}$. But in this medium, this vector has to be antiparallel to vector $\mathbf{S}$ that, in turn, should be directed out of the interface, because it presents the power flow from the interface into the material bulk. These conditions cannot be reconciled by the refracted wave propagating along the usual Snell-law direction (shown by the dashed line in Fig. 13a), but are all satisfied at refraction in the direction given by Snell's angle with negative sign. (Hence the term "negative refraction"). ${ }^{35}$


Fig. 7.14. Negative refraction: (a) waves at the interface between media with positive and negative values of $\varepsilon \mu$, and (b) the hypothetical perfect lens: a parallel plate made of a material with $\varepsilon=-\varepsilon_{0}$ and $\mu=-\mu_{0}$.

In order to understand how unusual the results of the negative refraction may be, let us consider a parallel slab of thickness $d$, made of a hypothetical left-handed material with $\varepsilon=-\varepsilon_{0}, \mu=-\mu_{0}$ (Fig. 14b), placed in free space. For such a material, the refraction angle $r=-\theta$, so that the rays from a point source, located at a distance $a<d$ from the slab, propagate as shown in that figure, i.e. all meet again at distance $a$ inside the plate, and then continue to propagate to the second surface of the slab. Repeating our discussion for this surface, we see that a point's image is also formed beyond the plate at distance $2 a$ $+2 b=2 a+2(d-a)=2 d$ from the object. Superficially, this looks like the usual lens, but the wellknown lens formula, which relates $a$ and $b$ with the focal length $f$, is not satisfied. (In particular, a parallel beam is not focused into a point at any finite distance.)

As an additional difference from the usual lens, the system shown in Fig. 14b does not reflect any part of the incident light. Indeed, it is straightforward to check that in order for all above formulas for $R$ and $T$ to be valid, the sign of the wave impedance $Z$ in left-handed materials has to be kept positive. Thus, for our particular choice of parameters ( $\varepsilon=-\varepsilon_{0}, \mu=-\mu_{0}$ ), Eqs. (91a) and (95a) are valid with $Z_{+}=Z_{-}=Z_{0}$ and $\cos r=\cos \theta=1$, giving $R=0$ for any linear polarization, and hence for any other wave polarization - circular, elliptic, natural, etc.

The perfect lens suggestion has triggered a wave of efforts to implement left-hand materials experimentally. (Attempts to found such materials in nature have failed so far.) Most progress in this direction has been achieved using the so-called metamaterials, which are essentially quasi-periodic arrays of specially designed electromagnetic resonators, ideally with high density $n \gg \lambda^{-3}$. For example,

[^326]Fig. 15a shows the metamaterial that was used for the first demonstration of negative refractivity in the microwave region, i.e. a few-GHz frequencies - see Fig. 15b. It combines straight strips of a metallic film, working as lumped resonators with a large electric dipole moment (hence strongly coupled to wave's electric field $\mathbf{E}$ ), and several almost-closed film loops (so-called split rings), working as lumped resonators with large magnetic dipole moments, coupled to field $\mathbf{H}$. By designing the resonance frequencies close to each other, the negative refractivity may be achieved - see the black line in Fig. 15b, which shows experimental data. Recently, the negative refractivity was demonstrated in the optical range, albeit at relatively large absorption that spoils all potentially useful features of the left-handed materials.


Fig. 7.15. The first artificial left-hand material with experimentally demonstrated negative refraction in a microwave region. Adapted from R. Shelby et al., Science 292, 77 (2001). © AAAS.

This progress has stimulated the development of other potential uses of metamaterials (not necessarily the left-handed ones), in particular designs of nonuniform systems with engineered distributions $\varepsilon(\mathbf{r}, \omega)$ and $\mu(\mathbf{r}, \omega)$, which may provide electromagnetic wave propagation along the desired paths, e.g. around a certain region of space (Fig. 16), making it virtually invisible for an external observer - so far, within a limited frequency range, and a certain wave polarization only. Due to these restrictions, the practical value of this work on such invisibility cloaks in not yet clear (at least to this author); but so much attention is focused on this issue ${ }^{36}$ that the situation should become much more clear in just a few years.



Fig. 7.16. Experimental demonstration of a prototype 2D "invisibility cloak" in the microwave region. Adapted from D. Schurig et al., Science 314, 977 (2006). © AAAS.

[^327]
### 7.6. Transmission lines: TEM waves

So far, we have analyzed plane the electromagnetic waves with infinite cross-section. The crosssection may be limited, still sustaining wave propagation, using wave transmission lines (also called waveguides): cylindrically-shaped structures made of either good conductors or dielectrics. Let us first discuss the first option. In order to keep our analysis (relatively :-) simple, let us assume that:
(i) the structure is a cylinder (not necessarily with a round cross-section, see Fig. 17) filled with a usual (right-handed), uniform dielectric material with negligible losses: $\varepsilon=\varepsilon^{\prime}>0, \mu=\mu^{\prime}>0$, and
(ii) the wave attenuation due to the skin effect is also negligibly low. (As Eq. (78) indicates, for that the characteristic size $a$ of waveguide's cross-section has to be much larger than the skin-depth $\delta_{\mathrm{s}}$ of its wall material. The effect of skin-effect losses will be analyzed in Sec. 10 below.)

After such exclusion of attenuation, we may look for a particular solution of the Maxwell equations in the form of a monochromatic wave traveling along the waveguide:

$$
\begin{equation*}
\mathbf{E}(\mathbf{r}, t)=\operatorname{Re}\left[\mathbf{E}_{\omega}(x, y) e^{i\left(k_{z} z-\omega t\right)}\right] \quad \mathbf{H}(\mathbf{r}, t)=\operatorname{Re}\left[\mathbf{H}_{\omega}(x, y) e^{i\left(k_{z} z-\omega t\right)}\right], \tag{7.98}
\end{equation*}
$$

with real $k_{z}$. Note that this form allows an account for a substantial coordinate dependence of the electric and magnetic field in the plane $\{x, y\}$ of the waveguide's cross-section, as well as for longitudinal components of the fields, so that solution (98) is substantially more complex than the plane waves we have discussed above. We will see in a minute that as a result of this dependence, constant $k_{z}$ may be very much different from the plane-wave value (13), $k \equiv \omega(\varepsilon \mu)^{1 / 2}$, in the same material.


Fig. 7.17. Decomposition of the electric field in a waveguide.

In order to describe these effects explicitly, let us decompose the complex amplitudes of the fields into the longitudinal and transverse components (Fig. 17) ${ }^{37}$

$$
\begin{equation*}
\mathbf{E}_{\omega}=E_{z} \mathbf{n}_{z}+\mathbf{E}_{t}, \quad \mathbf{H}_{\omega}=H_{z} \mathbf{n}_{z}+\mathbf{H}_{t} . \tag{7.99}
\end{equation*}
$$

Plugging Eqs. (98)-(99) into the homogeneous Maxwell equations (2), and requiring the longitudinal and transverse components to be balanced separately, we get

[^328]\[

$$
\begin{array}{ll}
i k_{z} \mathbf{n}_{z} \times \mathbf{E}_{t}-i \omega \mu \mathbf{H}_{t}=-\nabla_{t} \times\left(E_{z} \mathbf{n}_{z}\right), & i k_{z} \mathbf{n}_{z} \times \mathbf{H}_{t}+i \omega \varepsilon \mathbf{E}_{t}=-\nabla_{t} \times\left(H_{z} \mathbf{n}_{z}\right), \\
\nabla_{t} \times \mathbf{E}_{t}=i \omega \mu H_{z} \mathbf{n}_{z}, & \nabla_{t} \times \mathbf{H}_{t}=-i \varepsilon \omega E_{z} \mathbf{n}_{z},  \tag{7.100}\\
\nabla_{t} \cdot \mathbf{E}_{t}=-i k_{z} E_{z}, & \nabla_{t} \cdot \mathbf{H}_{t}=-i k_{z} H_{z} .
\end{array}
$$
\]

where $\nabla_{t}$ is the 2D del operator acting in the transverse plane $[x, y]$ only (so that $\nabla=\nabla_{t}+\mathbf{n}_{z} \partial / \partial z$ ). These equations may look even more bulky than the original Maxwell equations, but actually are much simpler for analysis. Indeed, eliminating the transverse components from these equations (or, even simpler, just plugging Eq. (99) into Eqs. (3) and keeping just their $z$-components), we may get a pair of selfconsistent equations for the longitudinal components of the fields, ${ }^{38}$
where $k$ is still defined by Eq. (13), $k=(\varepsilon \mu)^{1 / 2} \omega$, and

After distributions $E_{z}(x, y)$ and $H_{z}(x, y)$ have been found from these equations, they provide right-hand parts for rather simple, closed system of equations (100) for the transverse components of field vectors. Moreover, as we will see below, each of the following three types of solutions:
(i) with $E_{z}=0$ and $H_{z}=0$ (called the transverse, or TEM waves),
(ii) with $E_{z}=0$, but $H_{z} \neq 0$ (called either $T E$ waves or, more frequently, $H$ modes), and
(iii) with $E_{z} \neq 0$, but $H_{z}=0$ (TM waves or $E$ modes),
has its own dispersion law and hence wave propagation velocity; as a result, these modes (the term meaning the field distribution pattern) may be considered separately.

Let us start with the simplest, TEM waves with no longitudinal components of either field. For them, the top two equations of system (100) immediately give Eqs. (6) and (13), and $k_{z}=k$. In plain English, this means that $\mathbf{E}=\mathbf{E}_{t}$ and $\mathbf{H}=\mathbf{H}_{t}$ are proportional to each other and mutually perpendicular (just as in the plane wave) at each point of the cross-section, and that the TEM wave impedance $Z \equiv E / \mathrm{H}$ and dispersion law $\omega(k)$, and hence the propagation speed, are the same as in a plane wave in the material filling the waveguide. In particular, if $\varepsilon$ and $\mu$ are frequency-independent within a certain frequency range, the dispersion law is linear, $\omega=k /(\varepsilon \mu)^{1 / 2}$, and wave's speed does not depend on its frequency. For practical applications to telecommunications, this is a very important advantage of TEM waves over their TM and TE counterparts - to be discussed below.

Unfortunately, such waves cannot propagate in every waveguide. In order to show this, let us have a look at the two last lines of Eqs. (100). For the TEM waves ( $E_{z}=0, H_{z}=0, k_{z}=k$ ), they yield

$$
\begin{array}{ll}
\nabla_{t} \times \mathbf{E}_{t}=0, & \nabla_{t} \times \mathbf{H}_{t}=0 \\
\nabla_{t} \cdot \mathbf{E}_{t}=0, & \nabla_{t} \cdot \mathbf{H}_{t}=0 \tag{7.103}
\end{array}
$$

In the macroscopic approximation of the boundary conditions (i. e., neglecting the screening and skin depths), we have to require that the wave does not penetrate the walls, so that inside them, $\mathbf{E}=\mathbf{H}=0$. Close to the wall but inside the waveguide, the normal component $E_{n}$ of the electric field may be

[^329]different from zero, because surface charges may sustain its jump (see Sec. 2.1). Similarly, the tangential component $H_{\tau}$ of the magnetic field may have a finite jump at the surface due to skin currents. However, the tangential component of the electric field and the normal component of magnetic field cannot experience such jump, and in order to have them vanishing inside the walls they have to equal zero near the walls inside the waveguide as well:
\[

$$
\begin{equation*}
\mathbf{E}_{\tau}=0, \quad H_{n}=0 . \tag{7.104}
\end{equation*}
$$

\]

But the left columns of Eqs. (103) and (104) coincide with the formulation of the 2D boundary problem of electrostatics for the electric field induced by electric charges of the conducting walls, with the only difference that in our current case the value of $\varepsilon$ should be replaced with $\varepsilon(\omega)$. Similarly, the right columns of those relations coincide with the formulation of the 2D boundary problem of magnetostatics for the magnetic field induced by currents in the walls, with $\mu=\mu(\omega)$. The only difference is that in our current case the magnetic fields should not penetrate inside the conductors.

Now we immediately see that in waveguides with a singly-connected wall topology (see, e.g., the particular example shown in Fig. 17), TEM waves are impossible, because there is no way to create a finite electrostatic field inside a conductor with such cross-section. Fortunately, such fields (and hence TEM waves) are possible in structures with cross-sections consisting of two or more disconnected (dcinsulated) parts - see, e.g., Fig. 18. (Such structures are more frequently called the transmission lines rather than waveguides, the last term being mostly reserved for the lines with singly-connected crosssections of the walls.)


Fig. 7.18. Example of the cross-section of a transmission line that may support the TEM wave propagation.

Now we can readily derive some "global" relations for each conductor, independent on the exact shape of its cross-section. Indeed, consider contour $C$ drawn very close to the conductor's surface (see, e.g., the red dashed line in Fig. 18). First, we can consider it as a cross-section of a cylindrical Gaussian volume of certain length $d z \ll \lambda \equiv 2 \pi / k$. Using the generalized Gauss law (3.29), get

$$
\begin{equation*}
\oint_{C}\left(\mathbf{E}_{t}\right)_{n} d r=\frac{\lambda_{\omega}}{\varepsilon}, \tag{7.105}
\end{equation*}
$$

where $\lambda_{\omega}$ (not to be confused with wavelength $\lambda!$ ) is the linear density of electric charge of the conductor. Second, the same contour $C$ may be used in the generalized Ampère law (5.131) to write

$$
\begin{equation*}
\oint_{C}\left(\mathbf{H}_{t}\right)_{\tau} d r=I_{\omega}, \tag{7.106}
\end{equation*}
$$

where $I_{\omega}$ is the total current flowing along the conductor (or rather its complex amplitude). But, as was mentioned above, in the TEM wave the ratio $E_{t} / H_{t}$ of the field components participating in these two integrals is constant and equal to $Z=(\mu / \varepsilon)^{1 / 2}$, so that Eqs. (105)-(106) give the following simple relation between the "global" characteristics of the conductor:

$$
\begin{equation*}
I_{\omega}=\frac{\lambda_{\omega} / \varepsilon}{Z}=\frac{\lambda_{\omega}}{(\varepsilon \mu)^{1 / 2}}=\frac{\omega}{k} \lambda_{\omega} \tag{7.107}
\end{equation*}
$$

This relation may be also obtained by a different means; let me describe it, because it has an independent value. Let us consider a small segment $d z \ll \lambda=2 \pi / k$ of the conductor (limited by the red dashed line in Fig. 18) and apply the electric charge conservation law (4.1) to the instant values of the linear charge density and current. The cancellation of $d z$ in both parts yields

$$
\begin{equation*}
\frac{\partial \lambda(z, t)}{\partial t}=-\frac{\partial I(z, t)}{\partial z} \tag{7.108}
\end{equation*}
$$

(If we accept the sinusoidal waveform, $\exp \{i(k z-\omega t)\}$, for both these variables, we immediately recover Eq. (107) for their complex amplitudes, so that the result just expresses the charge continuity law. However, Eq. (108) is valid for any waveform.)

The global equation (108) may be made more specific in the case when the frequency dependence of $\varepsilon$ and $\mu$ is negligible, and the transmission line consists of just two isolated conductors (see, e.g., Fig. 18). In this case, in order to have the wave well localized in the space near the two conductors, we need a sufficiently fast convergence of its electric field at large distances. ${ }^{39}$ For that, their linear charge densities for each value of $z$ should be equal and opposite, and we can simply relate them to the potential difference $V$ between the conductors:

$$
\begin{equation*}
\frac{\lambda(z, t)}{V(z, t)}=C_{0} \tag{7.109}
\end{equation*}
$$

where $C_{0}$ is the mutual capacitance of the conductors per unit length - that was repeatedly discussed in Chapter 2. Then Eq. (108) takes the form

$$
\begin{equation*}
C_{0} \frac{\partial V(z, t)}{\partial t}=-\frac{\partial I(z, t)}{\partial z} \tag{7.110}
\end{equation*}
$$

Next, let us consider the contour shown with the red dashed line in Fig. 19 (which shows a crosssection of the transmission line by a plane containing the wave propagation axis $z$ ), and apply to it the Faraday induction law (6.3). Since the electric field is zero inside the conductors (in Fig. 19, on the horizontal parts of the contour), the total e.m.f. equals the difference of voltages $V$ at the end of the segment $d z$, while the only source of the magnetic flux through the area limited by the contour are the (equal and opposite) currents $\pm I$ in the conductors, we can use Eq. (5.70) to express it. As a result, canceling $d z$ in both parts of the equation, we get

$$
\begin{equation*}
L_{0} \frac{\partial I(z, t)}{\partial t}=-\frac{\partial V(z, t)}{\partial z} \tag{7.111}
\end{equation*}
$$

[^330]where $L_{0}$ is the mutual inductance of the conductors per unit length. The only difference between $L_{0}$ and the dc mutual inductances discussed in Chapter 5 is that at the high frequencies we are analyzing now, $L_{0}$ should be calculated neglecting its penetration into the conductors. (In the dc case, we had the same situation for superconductor electrodes, within their crude, ideal-diamagnetic description.)


Fig. 7.19. Electric current, magnetic flux, and voltage in a two-conductor transmission line.

The system of Eqs. (110) and (111) is frequently called the telegrapher's equations. Combined, they give for any "global" variable $f$ (either $V$, or $I$, or $\lambda$ ) a 1 D wave equation,

$$
\begin{equation*}
\frac{\partial^{2} f}{\partial z^{2}}-L_{0} C_{0} \frac{\partial^{2} f}{\partial t^{2}}=0 \tag{7.112}
\end{equation*}
$$

which describes the dispersion-free TEM wave propagation. Again, this equation is only valid within the frequency range where the frequency dependence of both $\varepsilon$ and $\mu$ is negligible. If it is not so, the global approach may still be used for sinusoidal waves $f=\operatorname{Re}\left[f_{\omega} \exp \{i(k z-\omega t)\}\right]$. Repeating the above arguments, instead of Eqs. (110)-(111) we get algebraic equations

$$
\begin{equation*}
\omega C_{0} V_{\omega}=k I_{\omega}, \quad \omega L_{0} I_{\omega}=k V_{\omega}, \tag{7.113}
\end{equation*}
$$

in which $L_{0} \propto \mu$ and $C_{0} \propto \varepsilon$ may now depend on frequency.
Two linear equations (113) are consistent only if

$$
\begin{equation*}
L_{0} C_{0}=\frac{k^{2}}{\omega^{2}} \equiv \frac{1}{v^{2}} \equiv \varepsilon \mu \tag{7.114}
\end{equation*}
$$

```
LoCo
product
invariance
```

Besides the fact we have already known (that the TEM wave speed is the same as that of the plane wave), Eq. (114) gives us a result that I confess I have not emphasized enough in Chapter 5: the product $L_{0} C_{0}$ does not depend on the shape or size of line's cross-section (provided that the magnetic field penetration into the conductors is negligible). Hence, if we have calculated the mutual capacitance $C_{0}$ of a system of two cylindrical conductors, the result immediately gives us their mutual inductance: $L_{0}=$ $\varepsilon \mu / C_{0}$. This relation stems from the fact that both the electric and magnetic fields may be expressed via the solution of a 2D Laplace equation for system's cross-section.

With Eq. (114) satisfied, any of Eqs. (113) gives the same result for ratio

$$
\begin{equation*}
Z_{W} \equiv \frac{V_{\omega}}{I_{\omega}}=\left(\frac{L_{0}}{C_{0}}\right)^{1 / 2} \tag{7.115}
\end{equation*}
$$

Transmission line's TEM Impedance
that is called the transmission line's impedance. This parameter has the same dimensionality (in SI units, ohms) as the wave impedance (7),

$$
\begin{equation*}
Z \equiv \frac{E_{\omega}}{H_{\omega}}=\left(\frac{\mu}{\varepsilon}\right)^{1 / 2} \tag{7.116}
\end{equation*}
$$

but these parameters should not be confused, because $Z_{W}$ depends on cross-section's geometry, while $Z$ does not. In particular, $Z_{W}$ is the only important parameter of a transmission line for matching with a lumped load circuit (Fig. 20) in the important case when both the cable cross-section's size and the load's linear dimensions are much smaller than the wavelength. (The ability of TEM lines to have such a small cross-section is their another important advantage.) Indeed, in this case we may consider the load in the quasistatic limit and write

$$
\begin{equation*}
V_{\omega}\left(z_{0}\right)=Z_{L}(\omega) I_{\omega}\left(z_{0}\right), \tag{7.117}
\end{equation*}
$$

where $Z_{L}(\omega)$ is the (generally complex) impedance of the load. Taking $V(z, t)$ and $I(z, t)$ in the form similar to Eqs. (61) and (62), and writing two Kirchhoff's laws for point $z=z_{0}$, we get for the reflection coefficient a result similar to Eq. (68):

$$
\begin{equation*}
R=\frac{Z_{L}(\omega)-Z_{W}}{Z_{L}(\omega)+Z_{W}} . \tag{7.118}
\end{equation*}
$$

This formula shows that for the perfect matching (i.e. the total wave absorption in the load), load's impedance $Z_{L}(\omega)$ should be real and equal to $Z_{W}$ - but not necessarily to $Z$.


Fig. 7.20. Transmission line impedance matching.

As an example, let us consider one of the simplest (and the most important) transmission lines: the coaxial cable (Fig. 21). ${ }^{40}$


Fig. 7. 21. Cross-section of a coaxial cable with arbitrary (possibly, dispersive) dielectric filling.

For this geometry, we already know expressions for both $L_{0}$ and $C_{0}$, though they have to be modified for the dielectric constant and the magnetic field non-penetration into the conductors. After that modification,

[^331]$$
C_{0}=\frac{2 \pi \varepsilon}{\ln (b / a)}, \quad L_{0}=\frac{\mu}{2 \pi} \ln (b / a) .
$$

Coaxial
cable's $C_{0}$ and $L_{0}$

So, the universal relation (114) is indeed valid! For cable's impedance (115), Eqs. (119) yield

$$
\begin{equation*}
Z_{W}=\left(\frac{\mu}{\varepsilon}\right)^{1 / 2} \frac{\ln (b / a)}{2 \pi}=Z \frac{\ln (b / a)}{2 \pi} \neq Z . \tag{7.120}
\end{equation*}
$$

For standard TV antenna cables (such as RG-6/U, with $b / a \sim 3, \varepsilon / \varepsilon_{0} \approx 2.2$ ), $Z_{W}=75$ ohms, while for most computer component connections, cables with $Z_{W}=50$ ohms (such as RG-58/U) are prescribed by electronic engineering standards. Such cables are broadly used for transfer of electromagnetic waves with frequencies (limited mostly by cable attenuation; see Sec. 10 below) up to 1 GHz over distances of a few km , and up to $\sim 20 \mathrm{GHz}$ on the tabletop scale (a few meters).

Another important example of TEM transmission lines is the set of two parallel wires. In the form of twisted pairs, ${ }^{41}$ they allow communications, in particular long-range telephone and DSL Internet connections, at frequencies up to a few hundred kHz , as well as relatively short Ethernet and TV cables at frequencies up to $\sim 1 \mathrm{GHz}$, limited mostly by the mutual interference and parasitic radiation effects.

## 7.7. $H$ and $E$ waves in metallic waveguides

Let us now return to Eqs. (100) and explore the TE and TM waves - with, respectively, either $H_{z}$ or $E_{z}$ different from zero. At the first sight, they may seem more complex. However, equations (101), which determine the distribution of these longitudinal components over the cross-section, are just 2D Helmholtz equations for scalar functions. For simple cross-section geometries may be solved using the methods discussed for the Laplace equation in Chapter 2, in particular the variable separation. After the solution of such an equation has been found, the transverse components of the fields may be calculated by differentiation, using the simple formulas,

$$
\begin{equation*}
\mathbf{E}_{t}=\frac{i}{k_{t}^{2}}\left[k_{z} \nabla_{t} E_{z}-k Z\left(\mathbf{n}_{z} \times \nabla_{t} H_{z}\right)\right], \quad \mathbf{H}_{t}=\frac{i}{k_{t}^{2}}\left[k_{z} \nabla_{t} H_{z}+\frac{k}{Z}\left(\mathbf{n}_{z} \times \nabla_{t} E_{z}\right)\right], \tag{7.121}
\end{equation*}
$$

which follow from the two equations in the first line of Eqs. (100). ${ }^{42}$
In comparison with the electro- and magnetostatics problems, the only conceptually new feature of Eqs. (101), with appropriate boundary conditions, is that they form the so-called eigenproblems, with typically many solutions (eigenfunctions), each describing a specific wave mode, and corresponding to a specific eigenvalue of parameter $k_{t}$. The good news here is that these values of $k_{t}$ are determined by this 2D boundary problem and hence do not depend on $k_{z}$. As a result, the dispersion law $\omega\left(k_{z}\right)$ of each mode, that follows from the last form of Eq. (102),

$$
\begin{equation*}
\omega=\left(\frac{k_{z}^{2}+k_{t}^{2}}{\varepsilon \mu}\right)^{1 / 2}=\left(v^{2} k_{z}^{2}+\omega_{c}^{2}\right)^{1 / 2} \tag{7.122}
\end{equation*}
$$

[^332]is functionally the same as that of plane waves in a plasma (see Eq. (38), Fig. 6, and their discussion), with the only differences that $c$ is now replaced with $v=1 /(\varepsilon \mu)^{1 / 2}$, the speed of plane (or any TEM) waves in the medium filling the waveguide, and $\omega_{p}$ is replaced with the so-called cutoff frequency
\[

$$
\begin{equation*}
\omega_{c} \equiv v k_{t}, \tag{7.123}
\end{equation*}
$$

\]

specific for each mode. (As Eq. (101) implies, and as we will see from several examples below, $k_{t}$ has the order of $1 / a$, where $a$ is the characteristic dimension of waveguide's cross-section, so that the critical value of the free-space wavelength is of the order of $a$.) Below the cutoff frequency of each particular mode, it cannot propagate in the waveguide. ${ }^{43}$ As a result, modes with the lowest values of $\omega_{c}$ present special practical interest, because the choice of the signal frequency $\omega$ between two lowest values of cutoff frequency guarantees that the waves propagate in the form of only one mode, with the lowest $k_{t}$. Such a choice allows to simplify the excitation of the desired mode by wave generators, and to avoid the parasitic transfer of electromagnetic wave energy to undesirable modes by (unavoidable) small inhomogeneities of the system.

The boundary conditions for the Helmholtz equations (101) depend on the propagating wave type. For TM waves (i.e. $E$ modes, with $H_{z}=0$ but $E_{z} \neq 0$ ), in the macroscopic approximation the boundary condition $E_{\tau}=0$ immediately gives

$$
\begin{equation*}
\left.E_{z}\right|_{C}=0 \tag{7.124}
\end{equation*}
$$

where $C$ is the contour limiting the conducting wall's cross-section. For TE waves (the $H$ modes, with $E_{z}$ $=0$ but $H_{z} \neq 0$ ), the boundary condition is slightly less obvious and may be obtained using, for example, the second equation of system (100), vector-multiplied by $\mathbf{n}_{z}$. Indeed, for the component perpendicular to the conductor surface the equation gives

$$
\begin{equation*}
i k_{z}\left(\mathbf{H}_{t}\right)_{n}-i \frac{k}{Z}\left(\mathbf{n}_{z} \times \mathbf{E}_{t}\right)_{n}=\frac{\partial H_{z}}{\partial n} . \tag{7.125}
\end{equation*}
$$

But the first term in the left-hand part of this equation must be zero on the wall surface, because of the second of Eqs. (104), while according to the first of Eqs. (104), vector $\mathbf{E}_{t}$ in the second term cannot have a component tangential to the wall. As a result, the vector product in that term cannot have a normal component, so that the term should equal zero as well, and Eq. (125) is reduced to

$$
\begin{equation*}
\left.\frac{\partial H_{z}}{\partial n}\right|_{C}=0 . \tag{7.126}
\end{equation*}
$$

Let us see what does this approach give for a simple but practically important example of a metallic-wall waveguide with a rectangular cross-section. In this case it is natural to use the Cartesian coordinates shown in Fig. 22, so that both Eqs. (101) take the simple form

[^333]\[

\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+k_{t}^{2}\right) f=0, \quad f=\left\{$$
\begin{array}{lc}
E_{z}, & \text { for TM waves, }  \tag{7.127}\\
H_{z}, & \text { for TE waves }
\end{array}
$$\right.
\]

From Chapter 2 we know that the most effective way of solution of such equations in a rectangular region is the variable separation, in which the general solution is represented as a sum of partial solutions of the type

$$
\begin{equation*}
f=X(x) Y(y) \tag{7.128}
\end{equation*}
$$

Plugging this expression into Eq. (127), and dividing each term by $X Y$, we get the equation,

$$
\begin{equation*}
\frac{1}{X} \frac{d^{2} X}{d x^{2}}+\frac{1}{Y} \frac{d^{2} Y}{d y^{2}}+k_{t}^{2}=0 \tag{7.129}
\end{equation*}
$$

that should be satisfied for all values of $x$ and $y$ within the waveguide's interior. This is only possible if each term of the sum equals a constant. Taking the $X$-term and $Y$-term constants in the form $\left(-k_{x}^{2}\right)$ and ( $k_{y}{ }^{2}$ ), respectfully, and solving the corresponding ordinary differential equations, ${ }^{44}$ for eigenfunction (128) we get

$$
\begin{equation*}
f=\left(c_{x} \cos k_{x} x+s_{x} \sin k_{x} x\right)\left(c_{y} \cos k_{y} y+s_{y} \sin k_{y} y\right), \quad \text { with } k_{x}^{2}+k_{y}^{2}=k_{t}^{2}, \tag{7.130}
\end{equation*}
$$

where constants $c$ and $s$ should be found from the boundary conditions. Here the difference between the $H$ modes and $E$ modes pitches in.


Fig. 7.22. Rectangular waveguide, and the transverse field distribution in the basic mode $H_{10}$ (schematically).

For the former modes (TE waves), Eq. (130) is valid for $H_{z}$, and we should use condition (126) on all metallic walls of the waveguide ( $x=0$ and $a ; y=0$ and $b-$ see Fig. 22). As a result, we get very simple expressions for eigenfunctions and eigenvalues:

$$
\begin{gather*}
\left(H_{z}\right)_{n m}=H_{l} \cos \frac{\pi n x}{a} \cos \frac{\pi m y}{b}  \tag{7.131}\\
k_{x}=\frac{\pi n}{a}, \quad k_{y}=\frac{\pi m}{b}, \quad\left(k_{t}\right)_{n m}=\left(k_{x}^{2}+k_{y}^{2}\right)^{1 / 2}=\pi\left[\left(\frac{n}{a}\right)^{2}+\left(\frac{m}{b}\right)^{2}\right]^{1 / 2}, \tag{7.132}
\end{gather*}
$$

[^334]where $H_{l}$ is the longitudinal field amplitude, and $n$ and $m$ are two arbitrary integer numbers, besides that they cannot equal to zero simultaneously. (Otherwise, function $H_{z}(x, y)$ would be constant, so that, according to Eq. (121), the transverse components of the electric and magnetic field would equal zero. As a result, as the last two lines of Eqs. (100) show, the whole field would be zero for any $k_{z} \neq 0$.) Assuming, for certainty, that $a \geq b$ (as shown in Fig. 22), we see that the lowest eigenvalue of $k_{t}$, and hence the lowest cutoff frequency (123), is achieved for the so-called $H_{10}$ mode with $n=1$ and $m=0$, and hence
(thus confirming our prior estimate of $k_{t}$ ).
Depending on the $a / b$ ratio, the second lowest $k_{t}$ and cutoff frequency belong to either the $H_{11}$ mode with $n=1$ and $m=1$ :
\[

$$
\begin{equation*}
\left(k_{t}\right)_{11}=\pi\left(\frac{1}{a^{2}}+\frac{1}{b^{2}}\right)^{1 / 2}=\left[1+\left(\frac{a}{b}\right)^{2}\right]^{1 / 2}\left(k_{t}\right)_{10} \tag{7.134}
\end{equation*}
$$

\]

or to the $H_{20}$ mode with $n=2$ and $m=0$ :

$$
\begin{equation*}
\left(k_{t}\right)_{20}=\frac{2 \pi}{a}=2\left(k_{t}\right)_{10} . \tag{7.135}
\end{equation*}
$$

These values become equal at $a / b=\sqrt{ } 3 \approx 1.7$; in practical waveguides, the $a / b$ ratio is not too far from this value. For example, in the standard X-band waveguide WR90 with $a \approx 2.3 \mathrm{~cm}\left(f_{c} \equiv \omega_{c} / 2 \pi \approx 6.5\right.$ $\mathrm{GHz}), b \approx 1.0 \mathrm{~cm}$.

Now let us have a fast look at alternative TM waves ( $E$ modes). For them, we may still should use the general solution (130) with $f=E_{z}$, but now with boundary condition (124). This gives us eigenfunctions

$$
\begin{equation*}
\left(E_{z}\right)_{n m}=E_{l} \sin \frac{\pi n x}{a} \sin \frac{\pi m y}{b} \tag{7.136}
\end{equation*}
$$

and the same eigenvalue spectrum (132) as for the $H$ modes. However, now neither $n$ nor $m$ can be equal to zero; otherwise Eq. (136) would give the trivial solution $E_{z}(x, y)=0$. Hence the lowest cutoff frequency of TM waves is provided by the so-called $E_{11}$ mode with $n=1, m=1$, and the eigenvalue is again given by Eq. (134).

Thus the basic (or "fundamental") $H_{10}$ mode is certainly the most important wave in rectangular waveguides; let us have a better look at its field distribution. Plugging the corresponding solution (131) with $n=1$ and $m=0$ into the general Eqs. (121), we easily get

$$
\begin{align*}
& \left(H_{x}\right)_{10}=-i \frac{k_{z} a}{\pi} H_{l} \sin \frac{\pi x}{a}, \quad\left(H_{y}\right)_{10}=0,  \tag{7.137}\\
& \left(E_{x}\right)_{10}=0, \quad\left(E_{y}\right)_{10}=i \frac{k a}{\pi} Z H_{l} \sin \frac{\pi x}{a} . \tag{7.138}
\end{align*}
$$

This field distribution is (schematically) shown in Fig. 22. Neither of the fields depends on the vertical coordinate - which is very convenient, in particular, for microwave experiments with small samples.

The electric field has only one（vertical）component that vanishes at the side walls and reaches maximum at waveguide＇s center；its field lines are straight，starting and ending on wall surface charges （whose distribution propagates along the waveguide together with the wave）．In contrast，the magnetic field has two nonvanishing components $\left(H_{x}\right.$ and $H_{z}$ ），and its field lines are shaped as horizontal loops wrapped around the electric field maxima．

An important question is whether the $H_{10}$ wave may be usefully characterized by a unique impedance introduced similar to $Z_{W}$ of the TEM modes－see Eq．（115）．The answer is not，because the main value of $Z_{W}$ is a convenient description of the impedance matching of the transmission line with a lumped load－see Fig． 20 and Eq．（118）．As was discussed above，such simple description is possible （i．e．，does not depend on the exact geometry of the connection）only if both dimensions of line＇s cross－ section are much less than $\lambda$ ．But for the $H_{10}$ wave（and more generally，any non－TEM mode）this is impossible - see，e．g．，Eq．（129）：its lowest frequency corresponds to the TEM wavelength $\lambda_{\max }=$ $2 \pi /\left(k_{t}\right)_{\text {min }}=2 \pi /\left(k_{t}\right)_{10}=2 a .{ }^{45}$

Now let us consider metallic waveguides with round cross－section（Fig．23a）．In this single－ connected geometry，again，the TEM waves are impossible，while for the analysis of $H$ modes and $E$ modes the polar coordinates $\{\rho, \varphi\}$ are most natural．In these coordinates，the 2D Helmholtz equation （101）takes the form

$$
\left[\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2}}{\partial \varphi^{2}}+k_{t}^{2}\right] f=0, \quad f=\left\{\begin{array}{lc}
E_{z}, & \text { for TM waves, }  \tag{7.139}\\
H_{z}, & \text { for TE waves. }
\end{array}\right.
$$

Separating the variables as $f=尺(\rho) \notin(\varphi)$ ，we get

$$
\begin{equation*}
\frac{1}{\rho 尺} \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right)+\frac{1}{\rho^{2} \neq \frac{d^{2} \neq}{d \varphi^{2}}+k_{t}^{2}=0 . . . . . . ~} \tag{7.140}
\end{equation*}
$$



Fig．7．23．（a）Metallic and（b）dielectric waveguides with circular cross－sections．

But this is exactly the Eq．（2．127）that was studied in the context of electrostatics，just with a replacement of notation：$\gamma \rightarrow k_{t}$ ．So we already know that in order to have $2 \pi$－periodic functions $\pi \varphi$ ）， and finite values $\mathcal{R}(0)$（which are necessary for our current case－see Fig．23a），the general solution is

[^335]given by Eq. (2.136), i.e. the eigenfunctions may be expressed via integer-order Bessel functions of the first kind: ${ }^{46}$
\[

$$
\begin{equation*}
f_{n m}=\operatorname{const} \times J_{n}\left(k_{n m} \rho\right) e^{i n \varphi}, \tag{7.141}
\end{equation*}
$$

\]

with eigenvalues $k_{n m}$ of the transverse wave number $k_{t}$ to be determined from appropriate boundary conditions.

As for the rectangular waveguide, let us start from $H$ modes $\left(f=H_{z}\right)$. Then the boundary condition on the wall surface $(\rho=R)$ is given by Eq. (126), which, for solution (141), takes the form

$$
\begin{equation*}
\frac{d}{d \xi} J_{n}(\xi)=0, \quad \xi \equiv k R \tag{7.142}
\end{equation*}
$$

This means that eigenvalues of Eq. (139) are

$$
\begin{equation*}
k_{t}=k_{n m}=\frac{\xi_{n m}^{\prime}}{R} \tag{7.143}
\end{equation*}
$$

where $\xi^{\prime}{ }_{n m}$ is the $m^{\text {th }}$ root of function $d J_{n}(\xi) / d \xi$. The approximate values of these roots for several lowest $n$ and $m$ may be read out from the plots in Fig. 2.16; their more accurate values are presented in Table 1 below.

Table 7.1. Roots $\xi_{n m}$ of function $d J_{n}(\xi) / \mathrm{d} \xi$ for a few values of Bessel function's index $n$ and root's number $m$.

|  | $m=1$ | 2 | 3 |
| :---: | :---: | :---: | :---: |
| $n=0$ | 3.83171 | 7.015587 | 10.1735 |
| 1 | 1.84118 | 5.33144 | 8.53632 |
| 2 | 3.05424 | 6.70613 | 9.96947 |
| 3 | 4.20119 | 8.01524 | 11.34592 |

It shows, in particular, that the lowest of the roots is $\xi^{\prime}{ }_{11} \approx 1.84$. Thus, a bit counter-intuitively, the basic mode, providing the lowest cutoff frequency $\omega_{c}=v k_{n m}$, is $H_{11}$ corresponding to $n=1$ rather than $n=0: 47$

$$
\begin{equation*}
H_{z}=H_{l} J_{1}\left(\xi_{11}^{\prime} \frac{\rho}{R}\right) e^{i \varphi} \tag{7.144}
\end{equation*}
$$

with the transverse wave vector $k_{t}=k_{11}=\xi^{\prime}{ }_{11} / R \approx 1.84 / R$, and hence the cutoff frequency corresponding to the TEM wavelength $\lambda_{\max }=2 \pi / k_{11} \approx 3.41 R$. Thus the ratio of $\lambda_{\max }$ to the waveguide diameter $2 R$ is

[^336]about 1.7, i.e. is close to the ratio $\lambda_{\text {max }} / a=2$ for the rectangular waveguide. The origin of this proximity is clear from Fig. 24, which shows the transverse field distribution in the $H_{11}$ mode. (It may be readily calculated from Eqs. (121) with $E_{z}=0$ and $H_{z}$ given by the real part of Eq. (144).)


Fig. 7.24. Transverse field components in the basic $H_{11}$ mode of a metallic, circular waveguide (schematically).

One can see that the field structure is actually very similar to that of the basic mode in the rectangular waveguide, shown in Fig. 22, despite the different nomenclature (due to the different type of used coordinates). However, note the arbitrary argument of complex constant $H_{l}$ in Eq. (144), indicating that in circular waveguides the transverse field polarization is arbitrary. For some practical applications, the degeneracy of these "quasi-linearly-polarized" waves creates problems; they may be avoided by using waves with circular polarization. ${ }^{48}$

As Table 1 shows, the next lowest $H$ mode is $H_{21}$, for which $k_{t}=k_{21}=\xi^{\prime}{ }_{21} / R \approx 3.05 / R$, almost twice larger than that of the basic mode, and only then comes the first mode with no angular dependence of the any field, $H_{01}$, with $k_{t}=k_{01}=\xi^{\prime}{ }_{01} / R \approx 3.83 / R .{ }^{49}$

For the $E$ modes, we may still use Eq. (141) (with $f=E_{z}$ ), but with boundary condition (124) at $\rho$ $=R$. This gives the following equation for the problem eigenvalues:

$$
\begin{equation*}
J_{n}\left(k_{n m} R\right)=0, \text { i.e. } k_{n m}=\frac{\xi_{n m}}{R} \tag{7.145}
\end{equation*}
$$

where $\xi_{n m}$ is the $m$-th root of function $J_{n}(\xi)$ - see Table 2.1. The table shows that the lowest $k_{t}$ equals to $\xi_{01} / R \approx 2.405 / R$. Hence the corresponding mode $\left(E_{01}\right)$, with

$$
\begin{equation*}
E_{z}=E_{l} J_{0}\left(\xi_{01} \frac{\rho}{R}\right), \tag{7.146}
\end{equation*}
$$

has the second lowest cutoff frequency, approximately $30 \%$ higher than that of the basic mode $H_{11}$.
Finally, let us discuss one more topic of general importance - the number $N$ of electromagnetic modes that may propagate in a waveguide within a certain range of relatively large frequencies $\omega \gg \omega_{c}$. This is easy to calculate for a rectangular waveguide, with its simple expressions (132) for the eigenvalues of $\left\{k_{x}, k_{y}\right\}$. Indeed, these expressions describe a rectangular mesh on the [ $k_{x}, k_{y}$ ] plane, so

[^337]that each point corresponds to the plane area $\Delta A_{k}=(\pi / a)(\pi / b)$, and the number of modes in a large $k$ plane area $A_{k} \gg \Delta A_{k}$ is $N=A_{k} / \Delta A_{k}=a b A_{k} / \pi^{2}=A A_{k} / \pi^{2}$, where $A$ is the waveguide's cross-section area. ${ }^{50}$ However, it is frequently more convenient to discuss transverse wave vectors $\mathbf{k}_{t}$ of arbitrary direction, i.e. with arbitrary sign their components $k_{x}$ and $k_{y}$. Taking into account that the opposite values of each component actually give the same wave, the actual number of different modes of each type $(E$ or $H$ ) is a factor of 4 lower than was calculated above. This means that the number of modes of both types is
\[

$$
\begin{equation*}
N=2 \frac{A_{k} A}{(2 \pi)^{2}} . \tag{7.147}
\end{equation*}
$$

\]

It may be convincingly argued that this mode counting rule is valid for waveguides with crosssection of any shape, and any boundary conditions on the walls, provided that $N \gg 1$.

### 7.8. Dielectric waveguides and optical fibers

Now let us discuss electromagnetic wave propagation in dielectric waveguides. The simplest, step-index waveguide (Figs. 23, 25) consists of an inner core and an outer shell (in the optical fiber technology, called cladding) with a higher wave propagation speed, i.e. lower index of refraction:

$$
\begin{equation*}
v_{+}>v_{-}, \quad \text { i.e. } k_{+}<k_{-}, \quad \varepsilon_{+} \mu_{+}<\varepsilon_{-} \mu_{-} . \tag{7.148}
\end{equation*}
$$

(In most cases the difference is achieved due to that in the dielectric constant, $\varepsilon_{-}<\varepsilon_{+}$, while magnetically both materials are almost passive: $\mu_{-} \approx \mu_{+} \approx \mu_{0}$, and I will assume that in my narrative.) The idea of the waveguide operation may be readily understood in the case when wavelength $\lambda$ is much smaller than the characteristic size $R$ of core's cross-section. If this "geometric optics" limit, at the distances of the order of $\lambda$ from the core-to-cladding interface, which determines the wave reflection, we can consider the interface as a plane. As we know from Sec. 5, if angle $\theta$ of plane wave incidence on such an interface is larger than the critical value $\theta_{c}$ specified by Eq. (82), the wave is totally reflected. As a result, the waves launched into the fiber core at such "grazing" angles, propagate inside the core, repeatedly reflected from the cladding - see Fig. 25.


Fig. 7.25. Wave propagation in a thick optical fiber.

The most important type of dielectric waveguides are optical fibers. ${ }^{51}$ Due to a heroic technological effort, in about three decades starting from the mid-1960s, the attenuation of glass fibers

[^338]has been decreased from the values of the order of $20 \mathrm{db} / \mathrm{km}$ (typical for the window glass) to the fantastically low values about $0.2 \mathrm{db} / \mathrm{km}$ (meaning a virtually perfect transparency of $10-\mathrm{km}$-long fiber segments!) - see Fig. 26a. It is remarkable that this ultralow power loss may be combined with an extremely low frequency dispersion, especially for near-infrared waves (Fig. 26b). In conjunction with the development of inexpensive erbium-based quantum amplifiers, this breakthrough has enabled intercontinental (undersea), broadband ${ }^{52}$ optical cables, which are the backbone of all the modern telecommunication infrastructure. The only bad news is that these breakthroughs were achieved for just one kind of materials (silica-based glasses) ${ }^{53}$ within a very narrow range of their chemical composition. As a result, the dielectric constants $\varepsilon_{ \pm} / \varepsilon_{0}$ of the cladding and core of practical optical fibers are both close to $2.2\left(n_{ \pm} \approx 1.5\right)$ and are very close to each other, so that the relative difference of the refraction indices,
\[

$$
\begin{equation*}
\Delta \equiv \frac{n_{-}-n_{+}}{n_{-}} \approx \frac{\varepsilon_{-}-\varepsilon_{+}}{2 \varepsilon_{ \pm}} \tag{7.149}
\end{equation*}
$$

\]

is typically below $0.5 \%$, thus limiting the fiber bandwidth - see below.


Fig. 7.26. (a) Attenuation and (b) dispersion of representative single-mode optical fibers. (Adapted, respectively, from http://olson-technology.com and http://www.timbercon.com.)

Practical optical fibers come in two flavors: multi-mode and single-mode ones. Multi-mode fibers, used for transfer of high optical power (up to as much as $\sim 10$ watts), have relatively thick cores, with a diameter $2 R$ of the order of $50 \mu \mathrm{~m}$, much larger than $\lambda \sim 1 \mu \mathrm{~m}$. In this case, the "geometricoptics" picture of the wave propagation discussed above is quantitatively correct, and we may use it to calculate the number of quasi-plane-wave modes that may propagate in the fiber. Indeed, for the complementary angle (Fig. 25)

[^339]\[

$$
\begin{equation*}
\vartheta \equiv \frac{\pi}{2}-\theta \tag{7.150}
\end{equation*}
$$

\]

Eq. (82) gives the propagation condition

$$
\begin{equation*}
\cos \vartheta>\frac{n_{+}}{n_{-}}=1-\Delta . \tag{7.151}
\end{equation*}
$$

For the case $\Delta \ll 1$, when the incidence angles $\theta>\theta_{c}$ of all propagating waves are close to $\pi / 2$, and hence the complimentary angles are small, we can keep only two first terms in the Taylor expansion of the left-hand part of Eq. (151) and get

$$
\begin{equation*}
\vartheta_{\max }^{2} \approx 2 \Delta \tag{7.152}
\end{equation*}
$$

Even for the higher-end value $\Delta=0.005$, this critical angle is only $\sim 0.1$ radian, i.e. close to $5^{\circ}$. Due to this smallness, we can approximate the maximum transverse component of the wave vector as

$$
\begin{equation*}
\left(k_{t}\right)_{\max }=k(\sin \vartheta)_{\max } \approx k \vartheta_{\max } \approx \sqrt{2} k \Delta, \tag{7.153}
\end{equation*}
$$

and use Eq. (147) to calculate number $N$ of propagating modes:

$$
\begin{equation*}
N \approx 2 \frac{\left(\pi R^{2}\right)\left(\pi k^{2} \vartheta_{\max }^{2}\right)}{(2 \pi)^{2}}=(k R)^{2} \Delta . \tag{7.154}
\end{equation*}
$$

For typical values $k=0.73 \times 10^{7} \mathrm{~m}^{-1}$ (corresponding to the free-space wavelength $\lambda_{0}=n \lambda=2 \pi n / k \approx 1.3$ $\mu \mathrm{m}$ ), $R=25 \mu \mathrm{~m}$, and $\Delta=0.005$, this formula gives $N \approx 150$.

The largest problem with using multi-mode fibers for communications is their high geometric dispersion, i.e. the difference of the mode propagation speed, which is usually characterized in terms of the signal delay time difference (traditionally measured in picoseconds per kilometer) between the fastest and the slowest mode. Within the geometric optics approximation, the difference of time delays of the fastest mode (with $k_{z}=k$ ) and the slowest mode (with $k_{z}=k \sin \theta_{c}$ ) at distance $l$ is

$$
\begin{equation*}
\Delta t=\Delta\left(\frac{l}{v_{z}}\right)=\Delta\left(\frac{k_{z} l}{\omega}\right)=\frac{l}{\omega} \Delta k_{z}=\frac{l}{v}\left(1-\sin \theta_{c}\right)=\frac{l}{v}\left(1-\frac{n_{+}}{n_{-}}\right)=\frac{l}{v} \Delta . \tag{7.155}
\end{equation*}
$$

For the example considered above, the TEM wave speed $v=c / n \approx 2 \times 10^{8} \mathrm{~m} / \mathrm{s}$, and the geometric dispersion $\Delta t / l$ is close to $25 \mathrm{ps} / \mathrm{m}$, i.e. $25,000 \mathrm{ps} / \mathrm{km}$. (This means, for example, that a $1-\mathrm{ns}$ pulse, being distributed between the modes, would spread to a $\sim 25-\mathrm{ns}$ pulse after passing a just $1-\mathrm{km}$ fiber segment.) Such disastrous dispersion should be compared with chromatic dispersion that is due to the frequency dependence of $\varepsilon_{ \pm}$, and has the steepness $(d t / d \lambda) / l$ of the order of $10 \mathrm{ps} / \mathrm{km} \cdot \mathrm{nm}$ (see the solid pink line in Fig. 26b). One can see that through the whole frequency band ( $d \lambda \sim 100 \mathrm{~nm}$ ) the total chromatic dispersion $d t / l$ is of the order of only $1,000 \mathrm{ps} / \mathrm{km}$.

Due to the large geometric dispersion, the multimode fibers are used for signal transfer over only short distances ( $\sim 100 \mathrm{~m}$ ), while long-range communications are based on single-mode fibers, with thin cores (typically with diameters $2 R \sim 5 \mu \mathrm{~m}$, i. e. of the order of $\lambda / \Delta^{1 / 2}$ ). For such structures, Eq. (154) yields $N \sim 1$, but in this case the geometric optics approximation is not quantitatively valid, and we should get back to the Maxwell equations. In particular, this analysis should take into an explicit
account the evanescent wave propagating in the cladding, because its penetration depth may be comparable with $R .{ }^{54}$

Since the cross-section of an optical fiber is not uniform and lacks metallic conductors, the Maxwell equations cannot be exactly satisfied with either a TEM, or a TE, or a TM solutions. Instead, the fibers can carry so-called $H E$ and $E H$ modes, with both fields having longitudinal components simultaneously. In such modes, both $E_{z}$ and $H_{z}$ inside the core $(\rho \leq R)$ have the form similar to Eq. (141):

$$
\begin{equation*}
f_{-}=f_{l} J_{n}\left(k_{t} \rho\right) e^{i n \varphi}, \text { with } k_{t}^{2}=k_{-}^{2}-k_{z}^{2}>0, \quad k_{-}^{2} \equiv \omega^{2} \varepsilon_{-} \mu_{-}, \tag{7.156}
\end{equation*}
$$

where amplitudes $f_{l}$ (i.e., $E_{l}$ and $H_{1}$ ) may be complex to account for the possible angular shift between these components. On the other hand, for the evanescent wave in the cladding, we may rewrite Eq. (102) as

$$
\begin{equation*}
\left(\nabla^{2}-\kappa_{t}^{2}\right) f_{+}=0, \quad \text { with } \quad \kappa_{t}^{2} \equiv k_{z}^{2}-k_{+}^{2}>0, \quad k_{+}^{2} \equiv \omega^{2} \varepsilon_{+} \mu_{+} \tag{7.157}
\end{equation*}
$$

Figure 27 illustrates the relation between $k_{t}, \kappa_{t}, k_{z}$, and $k_{ \pm}$; note that the following sum,

$$
\begin{equation*}
k_{t}^{2}+\kappa_{t}^{2} \equiv \omega^{2}\left(\varepsilon_{-}-\varepsilon_{+}\right) \mu_{0} \tag{7.158}
\end{equation*}
$$

is fixed (at fixed frequency) and, for typical fibers, very small ( $\sim 2 \Delta k^{2} \ll k^{2}$ ). By the way, Fig. 27 shows that neither of $k_{t}$ and $\kappa_{t}$ can be larger than $\omega\left[\left(\varepsilon_{-}-\varepsilon_{+}\right) \mu_{0}\right]^{1 / 2}=k \Delta^{1 / 2}$. In particular, this means that the depth $\delta=1 / \kappa_{t}$ of wave penetration into the cladding is at least $1 / k \Delta^{1 / 2}=\lambda / 2 \pi \Delta^{1 / 2} \gg \lambda / 2 \pi$. This is why the cladding layers in practical optical fibers are made as thick as $\sim 50 \mu \mathrm{~m}$, so that only a negligibly small tail of this evanescent wave field reaches their outer surfaces.


Fig. 7.27. Relation between the transverse exponents $k_{t}$ and $\kappa_{t}$ for waves in optical fibers.

In the polar coordinates, Eq. (157) becomes

$$
\begin{equation*}
\left[\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2}}{\partial \varphi^{2}}-\kappa_{t}^{2}\right] f_{+}=0 \tag{7.159}
\end{equation*}
$$

instead of Eq. (139). From Sec. 2.5 we know that the eigenfunctions of Eq. (159) are the products of the angular factor $\exp \{\operatorname{in} \varphi\}$ by a linear combination of the modified Bessel functions $I_{n}$ and $K_{n}$, shown in

[^340]Fig. 2.20, now of argument $\kappa_{t} \rho$. In our case, the fields should vanish at $\rho \rightarrow \infty$, so that only the latter functions (of the second kind) can participate:

$$
\begin{equation*}
f_{+} \propto K_{n}\left(\kappa_{t} \rho\right) e^{i n \varphi} \tag{7.160}
\end{equation*}
$$

Now we have to reconcile Eqs. (156) and (160), using the boundary conditions at $\rho=R$ for both longitudinal and transverse components of both fields, with the latter fields first calculated from using Eqs. (121). Such a conceptually simple, but a bit bulky calculation (which I am leaving for reader's exercise :-), yields a system of two linear, homogeneous equations for complex amplitudes $E_{l}$ and $H_{l}$, that are compatible if

$$
\begin{equation*}
\left(\frac{k_{-}^{2}}{k_{t}} \frac{J_{n}{ }^{\prime}}{J_{n}}+\frac{k_{+}^{2}}{\kappa_{t}} \frac{K_{n}{ }^{\prime}}{K_{n}}\right)\left(\frac{1}{k_{t}} \frac{J_{n}{ }^{\prime}}{J_{n}}+\frac{1}{\kappa_{t}} \frac{K_{n}{ }^{\prime}}{K_{n}}\right)=\frac{n^{2}}{R^{2}}\left(\frac{k_{-}^{2}}{k_{t}^{2}}+\frac{k_{+}^{2}}{\kappa_{t}^{2}}\right)\left(\frac{1}{k_{t}^{2}}+\frac{1}{\kappa_{t}^{2}}\right), \tag{7.161}
\end{equation*}
$$

where prime means the derivative of each function over its full argument: $k_{t} \rho$ for $J_{n}$, and $\kappa_{t} \rho$ for $K_{n}$.
For any given frequency $\omega$, the system of Eqs. (158) and (161) determines the values of $k_{t}$ and $\kappa_{t}$, and hence $k_{z}$. Actually, for any $n>0$, this system provides two different solutions: one corresponding to the so-called $H E$ wave with larger ratio $E_{z} / H_{z}$, and the $E H$ wave, with a smaller value of that ratio. For angular-symmetric modes with $n=0$ (for whom we might naively expect the lowest cutoff frequency), the equations may be satisfied by fields having just one finite longitudinal component (either $E_{z}$ or $H_{z}$ ), and the $H E$ modes are the usual $E$ waves, while the $E H$ modes are the $H$ waves. For the $H$ modes, the characteristic equation is reduced to the requirement that the second parentheses in the left-hand part of Eq. (161) equals to zero. Using the identities $J^{\prime}{ }_{0}=-J_{1}$ and $K_{0}^{\prime}=-K_{1}$, this equation may be rewritten as

$$
\begin{equation*}
\frac{1}{k_{t}} \frac{J_{1}\left(k_{t} R\right)}{J_{0}\left(k_{t} R\right)}=-\frac{1}{\kappa_{t}} \frac{K_{1}\left(\kappa_{t} R\right)}{K_{0}\left(\kappa_{t} R\right)} . \tag{7.162}
\end{equation*}
$$

Using the simple relation between $k_{t}$ and $\kappa_{t}$ given by Eq. (158), we may plot both parts of Eq. (162) as a function of the same argument, say, $\xi \equiv k_{t} R$ - see Fig. 28.


Fig. 7.28. Two sides of the characteristic equation (162), plotted as a function of $k_{1} R$, for two values of its dimensionless parameter: $V=8$ (blue line) and $V=3$ (red line). Note that according to Eq. (158), the argument of functions $K_{0}$ and $K_{1}$ is just
$\kappa_{t} R=\left[V^{2}-\left(k_{t} R\right)^{2}\right]^{1 / 2}=\left(V^{2}-\xi^{2}\right)^{1 / 2}$.

The right-hand part of Eq. (162) depends not only on $\xi$ but also on the dimensionless parameter $V$ defined as the normalized right-hand part of Eq. (158):

$$
\begin{equation*}
V^{2} \equiv \omega^{2}\left(\varepsilon_{-}-\varepsilon_{+}\right) \mu_{0} R^{2} \approx 2 \Delta k_{ \pm}^{2} R^{2} . \tag{7.163}
\end{equation*}
$$

(According to Eq. (155), if $V \gg 1$, it gives the doubled number of the fiber modes - the conclusion confirmed by Fig. 28, taking into account that it describes only the $H$ modes.) Since the ratio $K_{1} / K_{0}$ is positive for all values of their argument (see, e.g., the right panel of Fig. 2.20), the right-hand part of Eq. (162) is always negative, so that the equation may have solutions only in the intervals where the ratio $J_{1} / J_{0}$ is negative, i.e. at

$$
\begin{equation*}
\xi_{01}<k_{t} R<\xi_{11}, \quad \xi_{02}<k_{t} R<\xi_{12}, \ldots \tag{7.164}
\end{equation*}
$$

where $\xi_{n m}$ is the $m$-th zero of function $J_{n}(\xi)$ - see Table 2.1. The right-hand part of the characteristic equation diverges at $\kappa_{t} R \rightarrow 0$, i.e. at $k_{t} R \rightarrow V$, so that no solutions are possible if $V$ is below the critical value $V_{c}=\xi_{01} \approx 2.405$. At this cutoff point, Eq. (163) yields $k_{ \pm} \approx \xi_{01} / R(2 \Delta)^{1 / 2}$. Hence, the cutoff frequency for the lowest $H$ mode corresponds to the TEM wavelength

$$
\begin{equation*}
\lambda_{\max }=\frac{2 \pi R}{\xi_{01}}(2 \Delta)^{1 / 2} \approx 3.7 R \Delta^{1 / 2} \tag{7.165}
\end{equation*}
$$

For typical parameters $\Delta=0.005$ and $R=2.5 \mu \mathrm{~m}$, this result yields $\lambda_{\max } \sim 0.65 \mu \mathrm{~m}$, corresponding to the free-space wavelength $\lambda_{0} \sim 1 \mu \mathrm{~m}$. A similar analysis of the first parentheses in the left-hand part of Eq. (161) shows that at $\Delta \rightarrow 0$, the cutoff frequency for the $E$ modes is similar.

This situation may look exactly like that in metallic waveguides, with no waves possible at frequencies below $\omega_{c}$, but this is not so. The basic reason for the difference is that in metallic waveguides, the approach to $\omega_{c}$ results in the divergence of the longitudinal wavelength $\lambda_{z} \equiv 2 \pi / k_{z}$. On the contrary, in dielectric waveguides this approach leaves $\lambda_{z}$ finite $\left(k_{z} \rightarrow k_{+}\right)$. Due to this difference, a certain linear superposition of $H E$ and $E H$ modes with $n=1$ can propagate at frequencies well below the cutoff frequency for $n=0$, which we have just calculated. ${ }^{55}$ This mode, in the limit $\varepsilon_{+} \approx \varepsilon_{-}$(i.e. $\Delta \ll 1$ ) allows a very interesting and simple description using the Cartesian (rather than polar) components of the fields, but still expressed as functions of polar coordinates $\rho$ and $\varphi$. The reason is that this mode is very close to a linearly polarized TEM wave. (Due to this reason, this mode is referred to as $L P_{01}$.)

Let us select axis $x$ parallel to the transverse component of the magnetic field vector, so that $\left.E_{x}\right|_{\rho=0}=0$, but $\left.E_{y}\right|_{\rho=0} \neq 0$, and $\left.H_{x}\right|_{\rho=0} \neq 0$, but $\left.H_{y}\right|_{\rho=0}=0$. The only suitable solutions of the 2D Helmholtz equation (that should be obeyed not only by $z$-components of the field, but also their $x$ - and $y$ components) are proportional to $J_{0}\left(k_{t} \rho\right)$, with zero coefficients for $E_{x}$ and $H_{y}$ :

$$
\begin{equation*}
E_{x}=0, \quad E_{y}=E_{0} J_{0}\left(k_{t} \rho\right), \quad H_{x}=H_{0} J_{0}\left(k_{t} \rho\right), \quad H_{y}=0, \quad \text { for } \rho \leq R . \tag{7.166}
\end{equation*}
$$

Now we can readily calculate the longitudinal components, using the last two equations of Eqs. (100):

$$
\begin{equation*}
E_{z}=\frac{1}{-i k_{z}} \frac{\partial E_{y}}{\partial y}=-i \frac{k_{t}}{k_{z}} E_{0} J_{1}\left(k_{t} \rho\right) \sin \varphi, \quad H_{z}=\frac{1}{-i k_{z}} \frac{\partial H_{x}}{\partial x}=-i \frac{k_{t}}{k_{z}} H_{0} J_{1}\left(k_{t} \rho\right) \cos \varphi \tag{7.167}
\end{equation*}
$$

where I have used mathematical identities $J_{0}^{\prime}=-J_{1}, \partial \rho / \partial x=x / \rho=\cos \varphi$, and $\partial \rho / \partial y=y / \rho=\sin \varphi$. As a sanity check, we see that the longitudinal component or each field is a (legitimate!) eigenfunction of the

[^341]type (141) with $n=1$. Note also that if $k_{t} \ll k_{z}$ (this relation is always true if $\Delta \ll 1-$ see Fig. 27), the longitudinal components of the fields are much smaller than their transverse counterparts, so that the wave is indeed very close to the TEM one. Because of that, the ratio of the electric and magnetic field amplitudes is also close to that in the TEM wave: $E_{0} / H_{0} \approx Z_{-} \approx Z_{+}$.

Now in order to ensure the continuity of the fields at the core-to-cladding interface $(\rho=R)$, we need to have a similar angular dependence of these components at $\rho \geq R$. The longitudinal components of the fields are tangential to the interface and thus should be continuous. Using the solutions similar to Eq. (160) with $n=1$, we get

$$
\begin{equation*}
E_{z}=-i \frac{k_{t}}{k_{z}} \frac{J_{1}\left(k_{t} R\right)}{K_{1}\left(\kappa_{t} R\right)} E_{0} K_{1}\left(\kappa_{t} \rho\right) \sin \varphi, \quad H_{z}=-i \frac{k_{t}}{k_{z}} \frac{J_{1}\left(k_{t} R\right)}{K_{1}\left(\kappa_{t} R\right)} H_{0} K_{1}\left(\kappa_{t} \rho\right) \cos \varphi, \quad \text { for } \rho \geq R \tag{7.168}
\end{equation*}
$$

For the transverse components, we should require the continuity of the normal magnetic field $\mu H_{n}$, for our simple field structure equal to just $\mu H_{x} \cos \varphi$, of the tangential electric field $E_{\tau}=E_{y} \sin \varphi$, and of the normal component of $D_{n}=\varepsilon E_{n}=\varepsilon E_{y} \cos \varphi$. Assuming that $\mu_{-}=\mu_{+}=\mu_{0}$, and $\varepsilon_{+} \approx \varepsilon_{-}{ }^{56}$ we can satisfy these conditions with the following solutions

$$
\begin{equation*}
E_{x}=0, \quad E_{y}=\frac{J_{0}\left(k_{t} R\right)}{K_{0}\left(\kappa_{t} R\right)} E_{0} K_{0}\left(\kappa_{t} \rho\right), \quad H_{x}=\frac{J_{0}\left(k_{t} R\right)}{K_{0}\left(k_{t} R\right)} H_{0} K_{0}\left(\kappa_{t} \rho\right), \quad H_{y}=0, \quad \text { for } \rho \geq R . \tag{7.169}
\end{equation*}
$$

From here, we can calculate components from $E_{z}$ and $H_{z}$, using the same approach as for $\rho \leq R$ :

$$
\begin{align*}
& E_{z}=\frac{1}{-i k_{z}} \frac{\partial E_{y}}{\partial y}=-i \frac{\kappa_{t}}{k_{z}} \frac{J_{0}\left(k_{t} R\right)}{K_{0}\left(\kappa_{t} R\right)} E_{0} K_{1}\left(\kappa_{t} \rho\right) \sin \varphi,  \tag{7.170}\\
& H_{z}=\frac{1}{-i k_{z}} \frac{\partial H_{x}}{\partial x}=-i \frac{\kappa_{t}}{k_{z}} \frac{J_{0}\left(k_{t} R\right)}{K_{0}\left(\kappa_{t} R\right)} H_{0} K_{1}\left(\kappa_{t} \rho\right) \cos \varphi, \quad \text { for } \rho \geq R .
\end{align*}
$$ equation

We see that this equation provides the same functional dependence of the fields as Eqs. (166), i.e. the internal and external fields are compatible, but their amplitudes coincide only if

$$
\begin{equation*}
k_{t} \frac{J_{1}\left(k_{t} R\right)}{J_{0}\left(k_{t} R\right)}=\kappa_{t} \frac{K_{1}\left(\kappa_{t} R\right)}{K_{0}\left(\kappa_{t} R\right)} . \tag{7.171}
\end{equation*}
$$

This characteristic equation (which may be also derived from Eq. (161) with $n=1$ in the limit $\Delta \rightarrow 0$ ) looks close to Eq. (162), but functionally is much different from it - see Fig. 29. Indeed, its righthand part is always positive, and the left-hand part tends to zero at $k_{t} R \rightarrow 0$. Due to this, Eq. (171) may have a solution for arbitrary small values of parameter $V$, defined by Eq. (163), i.e. for arbitrary low frequencies. This is why this mode is used in practical single-mode fibers: there are no other modes that can propagate at $\omega<\omega_{c}$, so that the geometric dispersion problem is avoided.

It is easy to use the Bessel function approximations given by the first term of the expansion (2.132) and also Eq. (2.157) to show that in the limit $V \rightarrow 0$ (i.e. $V \ll 1$ ), $\kappa_{t} R$ tends to zero much faster

[^342]than $k_{t} R \approx V: \kappa_{t} R \rightarrow 2 \exp \{-1 / V\} \ll V$. This means that the scale $\rho_{c} \equiv 1 / \kappa_{t}$ of the radial distribution of the $L P_{01}$ wave's fields in the cladding becomes very large. In this limit, this mode may be interpreted as a virtually TEM wave propagating in the cladding, just slightly deformed (and guided) by the fiber core. The drawback of this feature is that it requires very thick cladding, in order to avoid energy losses in outer ("buffer" and "jacket") layers that defend the silica components from the elements, but lack their low optical absorption. Due to this reason, the core radius is usually selected so that parameter $V$ is just slightly less than the critical value $V_{c}=\xi_{01} \approx 2.4$ for higher modes, thus ensuring the single-mode operation and eliminating the geometric dispersion problem.


Fig. 7.29. Two sides of the characteristic equation (167) for the $L P_{01}$ mode, plotted as a function of $k_{t} R$, for two values of the dimensionless parameter: $V=8$ (blue line) and $V=1$ (red line).

In order to reduce the field spread into the cladding, the step-index fibers considered above may be replaced with graded-index fibers whose the dielectric constant $\varepsilon_{r}$ is gradually and slowly decreased from the center to the periphery. Keeping only the main two terms in the Taylor expansion of the function $\varepsilon(\rho)$ at $\rho=0$, we may approximate such reduction as

$$
\begin{equation*}
\varepsilon(\rho) \approx \varepsilon(0)\left(1-\frac{\zeta}{2} \rho^{2}\right) \tag{7.172}
\end{equation*}
$$

where $\zeta \equiv-\left[\left(d^{2} \varepsilon / d \rho^{2}\right) / \varepsilon\right]_{\rho=0}$ is a positive constant characterizing the fiber composition gradient. ${ }^{57}$ Moreover, if this constant is sufficiently small $\left(\zeta \ll k^{2}\right)$, the field distribution across the fiber's crosssection may be described by the same 2D Helmholtz equation, but with the space-dependent transverse wave vector: ${ }^{58}$

$$
\begin{equation*}
\left[\nabla_{t}^{2}+k_{t}^{2}(\rho)\right] f=0, \quad \text { where } k_{t}^{2}(\rho) \equiv k^{2}(\rho)-k_{z}^{2}=\omega^{2} \varepsilon(\rho) \mu_{0}-k_{z}^{2}=k_{t}^{2}(0)\left(1-\frac{\zeta}{2} \rho^{2}\right) \tag{7.173}
\end{equation*}
$$

Surprisingly for such axially-symmetric problem, because of its special dependence on the radius, this equation may be most readily solved in Cartesian coordinates. Indeed, rewriting it as

[^343]\[

$$
\begin{equation*}
\left[\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+k_{t}^{2}(0)\left(1-\frac{\zeta}{2} x^{2}-\frac{\zeta}{2} y^{2}\right)\right] f=0 \tag{7.174}
\end{equation*}
$$

\]

and separating variables as $f=X(x) Y(y)$, we get

$$
\begin{equation*}
\frac{1}{X} \frac{d^{2} X}{d x^{2}}+\frac{1}{Y} \frac{d^{2} Y}{d y^{2}}+k_{t}^{2}(0)\left(1-\frac{\zeta}{2} x^{2}-\frac{\zeta}{2} y^{2}\right)=0 \tag{7.175}
\end{equation*}
$$

so that functions $X$ and $Y$ obey similar differential equations, for example

$$
\begin{equation*}
\frac{d^{2} X}{d x^{2}}+\left[k_{x}^{2}-k_{t}^{2}(0) \frac{\zeta}{2} x^{2}\right] X=0 \tag{7.176}
\end{equation*}
$$

with the separation constants satisfying the following relation:

$$
\begin{equation*}
k_{x}^{2}+k_{y}^{2}=k_{t}^{2}(0) \equiv \omega^{2} \varepsilon(0) \mu_{0}-k_{z}^{2} . \tag{7.177}
\end{equation*}
$$

Equation (176) is well known from the elementary quantum mechanics, because the Schrödinger equation for the perhaps most important quantum system, a 1D harmonic oscillator, may be rewritten in this form. Their eigenvalues are described by a simple formula

$$
\begin{equation*}
\left(k_{x}^{2}\right)_{n}=k_{t}(0)\left(\frac{\zeta}{2}\right)^{1 / 2}(2 n+1), \quad\left(k_{y}^{2}\right)_{m}=k_{t}(0)\left(\frac{\zeta}{2}\right)^{1 / 2}(2 m+1), \quad n, m=0,1,2, \ldots \tag{7.178}
\end{equation*}
$$

but eigenfunctions $X_{n}(x)$ and $Y_{m}(y)$ have to be expressed via not quite elementary functions - the Hermite polynomials. ${ }^{59}$ For our purposes, however, the lowest eigenfunctions $X_{0}(x)$ and $Y_{0}(y)$ are sufficient, because they correspond to the lowest $k_{x, y}$ and hence to the lowest cutoff frequency:

$$
\begin{equation*}
\omega_{c}^{2} \varepsilon(0) \mu_{0}=\left(k_{x}^{2}\right)_{0}+\left(k_{y}^{2}\right)_{0}=\zeta . \tag{7.179}
\end{equation*}
$$

(Note that at $\zeta \rightarrow 0$, the cutoff frequency tends to zero, as it should be for a wave in a uniform medium.) The eigenfunctions corresponding to the lowest eigenvalues are simple:

$$
\begin{equation*}
f_{0}(x)=\text { const } \times \exp \left\{-\frac{\zeta x^{2}}{2}\right\} \tag{7.180}
\end{equation*}
$$

so that the field distribution follows the Gaussian ("bell curve") function

$$
\begin{equation*}
f_{0}(\rho)=f_{0}(0) \exp \left\{-\frac{\zeta\left(x^{2}+y^{2}\right)}{2}\right\}=f_{0}(0) \exp \left\{-\frac{\zeta \rho^{2}}{2}\right\} . \tag{7.181}
\end{equation*}
$$

This is the so-called Gaussian beam, very convenient for some applications. Still, the graded-index fibers have higher attenuation than their step-index counterparts, and are not used as broadly.

Speaking of the Gaussian beams (or more generally, any beams with axially-symmetric profile $f_{0}(\rho)$ ), I cannot help noticing the very curious option of forming so-called helical waves with complex amplitude $f_{0}(\rho) \exp \{i l \varphi\}$, where $l$ is an integer constant, and $\varphi$ is the azimuthal angle (so that in our notation $x=\rho \cos \varphi, y=\rho \sin \varphi$ ). Let me leave it for reader's exercise to prove that the electromagnetic

[^344]field of such a wave has an angular momentum vector $\mathbf{L}=L_{z} \mathbf{n}_{z}$, with $L_{z}$ proportional to $l .{ }^{60}$ Quantization of the helical field gives $L_{z}=l \hbar$ per photon. The case $l= \pm 1$ is possible for infinite-width beams (i.e. plane waves) and means their circular polarization, quantum-mechanically corresponding to spin $\pm 1$ of their photons - see the discussion in the end of Sec. 1. In contrast, the implementation of higher values of $|l|$ requires space-limited beams (with $f_{0} \rightarrow 0$ at $\rho \rightarrow \infty$ ) and may be interpreted as giving the wave an additional "orbital" angular momentum. ${ }^{61}$

### 7.9. Resonators

Resonators are the distributed oscillators, i.e. structures that may sustain standing waves (in electrodynamics, oscillations of the electric and magnetic field at each point) even without a source, until the oscillation amplitude slowly decreases in time due to unavoidable energy losses. If the resonator quality (described by the so-called $Q$-factor, which will be defined and discussed in the next section) is high, this decay takes many oscillation periods. Alternatively, high- $Q$ resonators may sustain oscillating fields permanently, if fed with a relatively weak incident wave.

Conceptually the simplest resonator is the Fabry-Pérot interferometer ${ }^{62}$ that may be obtained by placing two well-conducting planes parallel to each other. ${ }^{63}$ Indeed, in Sec. 1 we have seen that if a plane wave is normally incident on such a "perfect mirror", located at $z=0$, its reflection, at negligible skin depth, results in a standing wave described by Eq. (61) - that may be rewritten as

$$
\begin{equation*}
E(z, t)=\operatorname{Re}\left(2 E_{\omega} e^{-i \omega t+i \pi / 2}\right) \sin k z \tag{7.182}
\end{equation*}
$$

Hence the wave would not change if we had suddenly put the second mirror (isolating the segment of length $l$ from the external wave source) at any position $z=l$ with $\sin k l=0$, i.e.

$$
\begin{equation*}
k l=p \pi, \quad \text { where } p=1,2, \ldots \tag{7.183}
\end{equation*}
$$

This condition, which also determines the eigen- (or resonance) frequency spectrum of the resonator of fixed length $l$,

$$
\begin{equation*}
\omega_{p}=v k_{p}=\frac{\pi v}{a} p, \quad v=\frac{1}{(\varepsilon \mu)^{1 / 2}} \tag{7.184}
\end{equation*}
$$

[^345]has a simple physical sense: the resonator length $l$ equals exactly $p$ half-waves of frequency $\omega_{p}$. Though this is all very simple, please note a considerable change of philosophy from what we have been doing in the previous sections: the main task in resonator analysis is finding its eigenfrequencies $\omega_{p}$ that are now determined by the system geometry rather than by an external wave source.

Before we move to more complex resonators, let us use Eq. (62) to present the magnetic field in the Fabry-Pérot interferometer:

$$
\begin{equation*}
H(z, t)=\operatorname{Re}\left(2 \frac{E_{\omega}}{Z} e^{-i \omega t}\right) \cos k z \tag{7.185}
\end{equation*}
$$

Expressions (182) and (185) show that in contrast to traveling waves, each field of the standing wave changes simultaneously (proportionately) at all points of the Fabry-Pérot resonator, turning to zero everywhere twice a period. At those instants the electric field energy of the resonator vanishes, but the total energy stays constant, because the magnetic field oscillates (also simultaneously at all points) with the phase shift $\pi / 2$. Such behavior is typical for all electromagnetic resonators.

Another, more technical remark is that we can readily get the same results (182)-(185) by solving the Maxwell equations from the scratch. For example, we already know that in the absence of dispersion, losses, and sources, they are reduced to wave equations (3) for any field components. For the Fabry-Pérot resonator's analysis, we can use their 1D form, say, for the transverse component of the electric field:

$$
\begin{equation*}
\left(\frac{\partial^{2}}{\partial z^{2}}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) E=0 \tag{7.186}
\end{equation*}
$$

and solve it as a part of an eigenvalue problem with the corresponding boundary conditions. Indeed, separating time and space variables as $E(z, t)=Z(z) \pi t)$, we get

$$
\begin{equation*}
\frac{1}{Z} \frac{d^{2} Z}{d z^{2}}-\frac{1}{v^{2}} \frac{1}{T} \frac{d^{2} T}{d t^{2}}=0 \tag{7.187}
\end{equation*}
$$

Calling the separation constant $k^{2}$, we get two similar ordinary differential equations,

$$
\begin{gather*}
\frac{d^{2} Z}{d z^{2}}+k^{2} Z=0  \tag{7.188}\\
\frac{d^{2} T}{d t^{2}}+k^{2} v^{2} T=0 \tag{7.189}
\end{gather*}
$$

both with sinusoidal solutions, so that their product is a standing wave with a wave vector $k$ and frequency $\omega=k v$, which may be presented by Eq. (182). ${ }^{64}$ Now using the boundary conditions $E(0, t)=$ $\mathrm{E}(l, t)=0,{ }^{65}$ we get the eigenvalue spectrum for $k_{p}$ and hence for $\omega_{p}=\nu k_{p}$, given by Eqs. (183) and (184).

[^346]Lessons from this simple case study may be readily generalized for an arbitrary resonator: there are (at least :-) two methods of finding the eigenfrequency spectrum:
(i) We may look at a traveling wave solution and find where reflecting mirrors may be inserted without affecting the wave's structure. Unfortunately, this method is limited to simple geometries.
(ii) We may solve the general 3D wave equation,

$$
\begin{equation*}
\left(\nabla^{2}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) f(\mathbf{r}, t)=0 \tag{7.190}
\end{equation*}
$$

for field components, as an eigenvalue problem with appropriate boundary conditions. If system parameters (and hence coefficient $v$ ) do not change in time, the spatial and temporal variables of Eq. (185) may be always separated by taking

$$
\begin{equation*}
f(\mathbf{r}, t)=R(\mathbf{r}) T(t), \tag{7.191}
\end{equation*}
$$

where function $\pi t$ ) always obeys the same equation (189), having the sinusoidal solution of frequency $\omega$ $=v k$. Plugging this solution back into Eq. (190), for the spatial distribution of the field we get the $3 D$ Helmholtz equation,

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) 尺(\mathbf{r})=0 \tag{7.192}
\end{equation*}
$$

whose solution (for non-symmetric geometries) may be much more complex.
Let us use these methods to find the eigenfrequency spectrum of a few simple, but practically important resonators. First of all, the first method is completely sufficient for the analysis of any resonator formed as a fragment of a uniform TEM transmission line (e.g., a coaxial cable) between two conducting lids perpendicular to the line direction. Indeed, since in such lines $k_{z}=k=\omega / v$, and the electric field is perpendicular to the propagation axis, e.g., parallel to the lid surface, the boundary conditions are exactly the same as in the Fabry-Pérot resonator, and we again arrive at the eigenfrequency spectrum (184).

Now let us analyze a slightly more complex system: a rectangular metallic-wall cavity of volume $a \times b \times l$ - see Fig. 30. In order to use the first method, let us consider the resonator as a finite-length ( $\Delta \mathrm{z}=$ $l$ ) of the rectangular waveguide stretched along axis $z$, which was analyzed in detail in Sec. 7. As a reminder, for $a<b$, in the basic $H_{10}$ traveling wave mode, both $\mathbf{E}$ and $\mathbf{H}$ do not depend on $y$, with vector E having only $y$-component. On the contrary, vector $\mathbf{H}$ has both components $H_{x}$ and $H_{z}$, with the phase shift $\pi / 2$ between them, with component $H_{x}$ having the same phase as $E_{y}$ - see Eqs. (131), (137), and (138). Hence, if a plane, perpendicular to axis $z$, is placed so that the electric field vanishes on it, $H_{x}$ also vanishes, so that all the boundary conditions (104) pertinent to a perfect metallic wall are fulfilled simultaneously.


Fig. 7.30. Rectangular metallic resonator as a finite section of a waveguide with the crosssection shown in Fig. 25.

As a result, the $H_{10}$ wave would not be perturbed by two metallic walls separated by an integer number of half-wavelength $\lambda_{z} / 2$ corresponding to the wave number given by Eqs. (102) and (133):

$$
\begin{equation*}
k_{z}=\left(k^{2}-k_{t}^{2}\right)^{1 / 2}=\left(\frac{\omega^{2}}{v^{2}}-\frac{\pi^{2}}{a^{2}}\right) . \tag{7.193}
\end{equation*}
$$

Using this expression, we see that the smallest of these distances, $l=\lambda_{z} / 2=\pi / k_{z}$, gives resonance frequency ${ }^{66}$

$$
\begin{equation*}
\omega_{101}=v\left[\left(\frac{\pi}{a}\right)^{2}+\left(\frac{\pi}{l}\right)^{2}\right]^{1 / 2} \tag{7.194}
\end{equation*}
$$

with the indices showing the number of half-waves along each dimension of the system. This is the lowest (fundamental) eigenfrequency of the resonator (if $b<a, l$ ).

The field distribution in this mode is close to that in the corresponding waveguide mode $H_{10}$ (Fig. 22), with the important difference that phases of the magnetic and electric fields are shifted by phase $\pi / 2$ both in space and time, just as in the Fabry-Pérot resonator - see Eqs. (182) and (185). Such time shift allows for a very simple interpretation of the $H_{101}$ mode that is especially adequate for very flat resonators, with $b \ll a, l$. At the instant when the electric field reaches maximum (Fig. 31a), i.e. the magnetic field vanishes in the whole volume, the surface electric charge of the walls (with density $\sigma=$ $E_{n} / \varepsilon$ ) is largest, being localized mostly in the middle of the broadest (in Fig. 31, horizontal) faces of the resonator. At later times, the walls start to recharge via surface currents whose density $J$ is largest in the side walls, and reaches its maximal value in a quarter period of the oscillation period of frequency $\omega_{101}-$ see Fig. 31b. The currents generate the vortex magnetic field, with looped field lines in the plane of the broadest face. The surface currents continue to flow in this direction until (in one more quarter period) the broader walls of the resonator are fully recharged in the polarity opposite to that shown in Fig. 31a. After that, the surface currents stat to flow in the direction opposite to that shown in Fig. 31b. This process, that repeats again and again, is conceptually similar to the well-known oscillations in a lumped $L C$ circuit, with the role of (now, distributed) capacitance played mostly by the broadest faces of the resonator, and that of distributed inductance, mostly by its narrower walls.
(a)


(b)

Fig. 7.31. Fields, charges, and currents in the basic $H_{101}$ mode of a rectangular metallic resonator, at two instants separated by $\Delta t=\pi / 2 \omega_{101}$ schematically.

In order to generalize result (194) to higher oscillation modes, the second method discussed above is more prudent. Separating variables as $\mathbb{Z}(\mathbf{r})=X(x) Y(y) Z(z)$ in the Helmholtz equation (192), we

[^347]see that $X, Y$, and $Z$ have to be sinusoidal functions of their arguments, with wave vector components satisfying the characteristic equation
\[

$$
\begin{equation*}
k_{x}^{2}+k_{y}^{2}+k_{z}^{2}=k^{2} \equiv \frac{\omega^{2}}{v^{2}} . \tag{7.195}
\end{equation*}
$$

\]

In contrast to the wave propagation problem, now we are dealing with standing waves along all three dimensions, and have to satisfy the boundary conditions on all sets of parallel walls. It is straightforward to check that the macroscopic boundary conditions $\left(E_{\tau}=0, H_{n}=0\right)$ are fulfilled at the following field component distribution:

$$
\begin{array}{lll}
E_{x}=E_{1} \cos k_{x} x \sin k_{y} y \sin k_{z} z, & H_{x}=H_{1} \sin k_{x} x \cos k_{y} y \cos k_{z} z, \\
E_{y}=E_{2} \sin k_{x} x \cos k_{y} y \sin k_{z} z, & H_{y}=H_{2} \cos k_{x} x \sin k_{y} y \cos k_{z} z,  \tag{7.196}\\
E_{z}=E_{3} \sin k_{x} x \sin k_{y} y \cos k_{z} z, & H_{z}=H_{3} \cos k_{x} x \cos k_{y} y \sin k_{z} z,
\end{array}
$$

with each of the wave vector components having the equidistant spectrum similar to the one given by Eq. (183):

$$
\begin{equation*}
k_{x}=\frac{\pi n}{a}, \quad k_{y}=\frac{\pi m}{b}, \quad k_{z}=\frac{\pi p}{l} \tag{7.197}
\end{equation*}
$$

so that the full spectrum of eigenfrequencies is given by the following formula,

$$
\begin{equation*}
\omega_{n m p}=v k=v\left[\left(\frac{\pi n}{a}\right)^{2}+\left(\frac{\pi m}{b}\right)^{2}+\left(\frac{\pi p}{l}\right)^{2}\right]^{1 / 2} \tag{7.198}
\end{equation*}
$$

which is a natural generalization of Eq. (194). Note, however, that of 3 integers $m, n$, and $p$ at least two have to be different from zero, in order to keep the fields (196) nonvanishing.

Let us use Eq. (199) to evaluate the number of different modes in a relatively small region $d^{3} k$ $\ll k^{3}$ (which is still much larger than the reciprocal volume, $1 / V=1 / a b l$, of the resonator) of the wave vector space. Taking into account that each eigenfrequency (198), with $n m l \neq 0$, corresponds to two field modes with different polarizations, ${ }^{67}$ the argumentation absolutely similar to the one used in the end of Sec. 7 for the 2D case yields

$$
\begin{equation*}
d N=2 V \frac{d^{3} k}{(2 \pi)^{3}} \tag{7.199}
\end{equation*}
$$

[^348]This property, valid for resonators of arbitrary shape, is broadly used in classical and quantum statistical physics, ${ }^{68}$ in the following form. If some electromagnetic mode property, $f(\mathbf{k})$, is a smooth function of the wave vector, and volume $V$ is large enough, then Eq. (199) may be used to approximate the sum over the modes by an integral:

[^349]\[

$$
\begin{equation*}
\sum_{\mathbf{k}} f(\mathbf{k}) \approx \int_{N} f(\mathbf{k}) d N=\int_{\mathbf{k}} f(\mathbf{k}) \frac{d N}{d^{3} k} d^{3} k=2 \frac{V}{(2 \pi)^{3}} \int_{\mathbf{k}} f(\mathbf{k}) d^{3} k . \tag{7.200}
\end{equation*}
$$

\]

Finally, note that low-loss resonators may be also formed by finite-length sections of not only metallic waveguides with different cross-sections, but also of the dielectric waveguides. Moreover, even the a simple slab of a dielectric material with a $\mu / \varepsilon$ ratio substantially different from that of its environment (say, the free space) may be used as a high- $Q$ Fabry-Pérot interferometer (Fig. 32), due to an effective wave reflection from its surfaces at normal and especially inclined incidence - see, respectively, Eqs. (68) and Eqs. (91) and (95).


Fig. 7.32. Dielectric Fabry-Pérot interferometer.

Actually, such dielectric Fabry-Pérot interferometer is frequently more convenient for practical purposes than a metallic resonator, due to its natural coupling to environment, that enables a ready way of wave insertion and extraction. The back side of the same medal is that this coupling to environment provides an additional mechanism of power losses, limiting the resonance quality - see the next section.

### 7.10. Energy loss effects

Inevitable energy losses ("power dissipation") in passive media lead, in two different situations, to two different effects. In a long transmission line fed by a constant wave source at one end, the losses lead to a gradual attenuation of the wave, i.e. to the decrease of its amplitude, and hence power $\mathcal{P}$, with the distance $z$ along the line. In linear materials, the losses are proportional to the wave amplitude squared, i.e. to the time- average of the power itself, so that the energy balance on a small segment $d z$ takes the form

$$
\begin{equation*}
d \mathcal{P}=-\frac{d \mathcal{P}_{\text {loss }}}{d z} d z=-\alpha \mathcal{P} d z \tag{7.201}
\end{equation*}
$$

Coefficient $\alpha$, participating in the last form of Eq. (201) and defined by relation

$$
\begin{equation*}
\alpha \equiv \frac{d \mathcal{P}_{\text {loss }} / d z}{\mathcal{P}} \tag{7.202}
\end{equation*}
$$

is called the attenuation constant. ${ }^{69}$ Comparing the evident solution of Eq. (201),
${ }^{69}$ In engineering, attenuation is frequently measured in decibels per meter (acronymed as $\mathrm{db} / \mathrm{m}$ or just dbm ):

$$
\left.\alpha\right|_{\mathrm{db} / \mathrm{m}} \equiv 10 \log _{10} \frac{\mathcal{P}(z=0)}{\mathcal{P}(z=1 \mathrm{~m})}=10 \log _{10} e^{\alpha[1 / \mathrm{m}]}=\frac{10}{\ln 10} \alpha\left[\mathrm{~m}^{-1}\right] \approx 4.34 \alpha\left[\mathrm{~m}^{-1}\right] .
$$

$$
\begin{equation*}
\mathcal{P}(z)=\mathbb{P}(0) e^{-\alpha z} \tag{7.203}
\end{equation*}
$$

with Eq. (29), where $k$ is replaced with $k_{z}$, we see that $\alpha$ may expressed as

$$
\begin{equation*}
\alpha=2 \operatorname{Im} k_{z}, \tag{7.204}
\end{equation*}
$$

where $k_{z}$ is the component of the wave vector along the transmission line. In the most important limit when the losses are low in the sense $\alpha \ll\left|k_{z}\right| \approx \operatorname{Re} k_{z}$, its effects on the field distributions along the line's cross-section are negligible, making the calculation of $\alpha$ rather straightforward. In particular, in this limit the contributions to attenuation from two major sources, energy losses in the filling dielectric, and the skin effect in conducting walls, are independent and additive.

The dielectric losses are especially simple to describe. Indeed, a review of our calculations in Secs. 6-8 shows that all of them remain valid if either $\varepsilon(\omega)$, or $\mu(\omega)$, or both, and hence $k(\omega)$, have small imaginary parts:

$$
\begin{equation*}
k^{\prime \prime}=\omega \operatorname{Im}\left[\varepsilon^{1 / 2}(\omega) \mu^{1 / 2}(\omega)\right] \ll k^{\prime} \tag{7.205}
\end{equation*}
$$

In TEM transmission lines, $k=k_{z}$, and hence Eq. (205) yields

$$
\begin{equation*}
\alpha_{\text {dielectric }}=2 k^{\prime \prime}=2 \omega \operatorname{Im}\left[\varepsilon^{1 / 2}(\omega) \mu^{1 / 2}(\omega)\right] \tag{7.206}
\end{equation*}
$$

[^350]For dielectric waveguides, in particular optical fibers, these losses are the main attenuation mechanism. As we already know from Sec. 8, in practical optical fibers $\kappa_{t} R \gg$ 1, i.e. most of the field propagates (as the evanescent wave) in the cladding, and the wave mode is very close to TEM. This is why it is sufficient to use Eq. (206) for the cladding material alone.

In waveguides with non-TEM waves, we can readily use the relations between $k_{z}$ and $k$ derived above to re-calculate $k$ " into $\operatorname{Im} k_{z}$. (Note that as such re-calculation, values of $k_{t}$ stay real, because they are just the eigenvalues of the Helmholtz equation (101), which does not include $k$.).

In waveguides and transmission lines with metallic conductors, much higher energy losses may come from the skin effect. Let us calculate them, assuming that we know the field distribution in the wave, in particular, the tangential component $H$ of the magnetic field at conductor surface. Then, if the wavelength $\lambda$ is much larger than $\delta_{s}$, as it usually is, ${ }^{70}$ we may use the results of the quasistatic approximation derived in Sec. 6.2, in particular Eqs. (6.27)-(6.28) for the relation between the complex amplitudes of the current density in the conductor and the tangential magnetic field

$$
\begin{equation*}
j_{\omega}(x)=k_{-} H_{\omega}(x), \quad k_{-}=-\frac{(1-i)}{\delta_{s}}, \quad \delta_{s}^{2}=\frac{2}{\mu \omega \sigma} . \tag{7.207}
\end{equation*}
$$

The power loss density (per unit volume) may be now calculated by time averaging of Eq. (4.39):

$$
\begin{equation*}
\mathcal{P}_{\text {loss }}(x)=\frac{\left|j_{\omega}(x)\right|^{2}}{2 \sigma}=\frac{\left|k_{-}\right|^{2}\left|H_{\omega}(x)\right|^{2}}{2 \sigma}=\frac{\left|H_{\omega}(x)\right|^{2}}{\delta_{s}^{2} \sigma} \tag{7.208}
\end{equation*}
$$

[^351]and its integration along the normal to the surface (through all the skin depth), using the exponential law (6.26). This (elementary) integration yields the following power loss per unit area: ${ }^{71}$
\[

$$
\begin{equation*}
\frac{d \mathcal{P}_{\text {loss }}}{d A} \equiv \int_{0}^{\infty} p_{\text {loss }}(x) d x=\left|H_{\omega}(0)\right|^{2} \frac{\mu \omega \delta_{s}}{4} . \tag{7.209}
\end{equation*}
$$

\]

The total power loss $d \mathcal{P}_{\text {loss }} / d z$ per unit length of a waveguide, i.e. the right-hand part of Eq. (201), now may be calculated by the integration of the ratio $\mathcal{P}_{\text {loss }} / A$ along the contour(s) limiting the cross-section of all conductors of the line. Since our calculation is only valid for low losses, we may ignore their effect on the field distribution, so that the unperturbed distribution may be used both in Eq. (209), i.e. the numerator of Eq. (202), and also for the calculation of the average propagating power, i.e. the denominator of Eq. (202), as the integral of the Poynting vector over the cross-section of the waveguide.

Let us see how this approach works for the TEM mode in one of the simplest TEM transmission lines, the coaxial cable (Fig. 19). As we already know from Sec. 6, in the absence of losses, the distribution of TEM mode fields is the same as in statics, namely:

$$
\begin{equation*}
H_{z}=0, \quad H_{\rho}=0, \quad H_{\varphi}(\rho)=H_{0} \frac{a}{\rho}, \tag{7.210}
\end{equation*}
$$

where $H_{0}$ is the field's amplitude on the surface of the inner conductor, and

$$
\begin{equation*}
E_{z}=0, \quad E_{\rho}(\rho)=Z H_{\varphi}(\rho)=Z H_{0} \frac{a}{\rho}, \quad E_{\varphi}=0, \quad Z \equiv\left(\frac{\mu}{\varepsilon}\right)^{1 / 2} . \tag{7.211}
\end{equation*}
$$

Now we can, neglecting losses for now, use Eq. (42) to calculate the time-averaged Poynting vector

$$
\begin{equation*}
\bar{S}=\frac{Z\left|H_{\varphi}(\rho)\right|^{2}}{2}=\frac{Z\left|H_{0}\right|^{2}}{2}\left(\frac{a}{\rho}\right)^{2} \tag{7.212}
\end{equation*}
$$

and from it, the total power propagating through the cross-section:

$$
\begin{equation*}
\mathcal{P}=\int_{A} \bar{S} d^{2} r=\frac{Z\left|H_{0}\right|^{2} a^{2}}{2} 2 \pi \int_{a}^{b} \frac{\rho d \rho}{\rho^{2}}=\pi Z\left|H_{0}\right|^{2} a^{2} \ln \frac{b}{a} . \tag{7.213}
\end{equation*}
$$

For the particular case of the coaxial cable (Fig. 19), the contours limiting the wall cross-sections are circles of radii $\rho=a$ (where the surface field amplitude $H_{\omega}(0)$ equals, in our notation, $H_{0}$ ), and $\rho=b$ (where, according to Eq. (204), the field is a factor of $b / a$ lower). As a result, for the power loss per unit length, Eq. (209) yields

$$
\begin{equation*}
\frac{d \mathcal{P}_{\text {loss }}}{d z}=\left(2 \pi a\left|H_{0}\right|^{2}+2 \pi b\left|H_{0} \frac{a}{b}\right|^{2}\right) \frac{\mu_{0} \omega \delta_{s}}{4}=\frac{\pi}{2} a\left(1+\frac{a}{b}\right) \mu \omega \delta_{s}\left|H_{0}\right|^{2} . \tag{7.214}
\end{equation*}
$$

Note that at $a \ll b$, the losses in the inner conductor dominate, despite its smaller surface, because of the higher surface field. Now we may plug Eqs. (213)-(214) into the definition (202) of $\alpha$, to calculate the part of the attenuation constant associated with the skin effect:

[^352]\[

$$
\begin{equation*}
\alpha_{\text {skin }} \equiv \frac{d \mathcal{P}_{\text {loss }} / d z}{\mathcal{P}}=\frac{1}{2 \ln (b / a)}\left(\frac{1}{a}+\frac{1}{b}\right) \frac{\mu \omega \delta_{s}}{Z}=\frac{k \delta_{s}}{2 \ln (b / a)}\left(\frac{1}{a}+\frac{1}{b}\right) . \tag{7.215}
\end{equation*}
$$

\]

We see that the relative (dimensionless) attenuation, $\alpha / k$, scales approximately as the ratio $\delta_{s} / \min [a, b]$. This result is should be compared with Eq. (78) for the normal incidence of plane waves on a conducting surface.

Let us evaluate $\alpha$ for the standard TV cable RG-6/U (with copper conductors of diameters $2 a=$ $1 \mathrm{~mm}, 2 b=4.7 \mathrm{~mm}$, and $\left.\varepsilon \approx 2.2 \varepsilon_{0}, \mu \approx \mu_{0}\right)$. According to Eq. ( 6.27 a ), for $f=100 \mathrm{MHz}\left(\omega \approx 6.3 \times 10^{8} \mathrm{~s}^{-1}\right)$ the skin depth of pure copper at room temperature (with $\sigma \approx 6.0 \times 10^{7} \mathrm{~S} / \mathrm{m}$ ) is close to $6.5 \times 10^{-6} \mathrm{~m}$, while $k=\omega(\varepsilon \mu)^{1 / 2}=\left(\varepsilon / \varepsilon_{0}\right)^{1 / 2}(\omega / c) \approx 3.1 \mathrm{~m}^{-1}$. As a result, the attenuation is rather low: $\alpha_{\text {skin }} \approx 0.016 \mathrm{~m}^{-1}$, so that the attenuation length scale $\mathcal{L} \equiv 1 / \alpha$ is about 60 m . Hence the attenuation in a cable connecting a roof TV antenna to a TV set in the same house is not a big problem, though using a worse conductor, e.g., steel, would make the losses rather noticeable. (Hence the current worldwide shortage of copper.) However, an attempt to use the same cable in the X-band ( $f \sim 10 \mathrm{GHz}$ ) is more problematic. Indeed, though the skin depth $\delta_{\mathrm{s}} \propto \omega^{-1 / 2}$ decreases with frequency, the wave length drops, i.e. $k$ increases, even faster $(k \propto \omega)$, so that the attenuation $\alpha_{\text {skin }} \propto \omega^{1 / 2}$ becomes close to 0.16 m , and $\mathcal{L}$ to $\sim 6 \mathrm{~m}$. This is why at such frequencies, it is more customary to use rectangular waveguides, with their larger internal dimensions $a, b \sim 1 / k$, and hence lower attenuation. Let me leave the calculation of this attenuation, using Eq. (209) and the results derived in Sec. 9, for reader's exercise.

The power loss effect on free oscillations in resonators is different: there it leads to a gradual decay of oscillation energy $\varepsilon$ in time. The useful measure of this decay, called the $Q$ factor, may be introduced by writing the temporal analog of Eq. (201):

$$
\begin{equation*}
d \varepsilon=-\mathcal{P}_{\text {loss }} d t=-\frac{\omega}{Q} \varepsilon d t \tag{7.216}
\end{equation*}
$$

where $\omega$ in the eigenfrequency in the loss-free limit, and the dimensional $Q$ factor is defined by a relation parallel to Eq. (202): ${ }^{72}$

$$
\begin{equation*}
\frac{\omega}{Q} \equiv \frac{\mathcal{P}_{\text {loss }}}{\varepsilon} . \tag{7.217}
\end{equation*}
$$

The solution to Eq. (216),

$$
\begin{equation*}
\varepsilon(t)=\varepsilon(0) e^{-t / \tau}, \quad \text { with } \tau \equiv \frac{Q}{\omega}=\frac{Q / 2 \pi}{\omega / 2 \pi}=\frac{Q T}{2 \pi}, \tag{7.218}
\end{equation*}
$$

which is an evident temporal analog of Eq. (203), shows the physical meaning of the $Q$ factor: the characteristic time $\tau$ of the oscillation energy decay is $(Q / 2 \pi)$ times longer than the oscillation period $T$ $=2 \pi / \omega$. (Another interpretation of $Q$ comes from the relation ${ }^{73}$

$$
\begin{equation*}
Q=\frac{\omega}{\Delta \omega}, \tag{7.219}
\end{equation*}
$$

[^353]$Q$-factor's definition

Oscillation energy decay

FWHM bandwidth
where $\Delta \omega$ is the so-called $F W H M^{74}$ bandwidth of the resonance, namely the difference between the two values of the external signal frequency, one above and one below $\omega$, at which the energy of forced oscillations induced in the resonator by an input signal is twice lower than its resonant value.)

In the important particular case of resonators formed by insertion of metallic walls into a TEM transmission line of small cross-section (with the linear size scale $a$ much less than the wavelength $\lambda$ ), there is no need to calculate the $Q$ factor directly if the line attenuation coefficient $\alpha$ is already known. In fact, as was discussed in Sec. 9 above, the standing waves in such a resonator, of the length given by Eq. (183): $l=p(\lambda / 2)$ with $p=1,2, \ldots$, may be understood as an overlap of two TEM waves running in opposite directions, or in other words, a traveling wave and its reflection from one of the ends, the whole roundtrip taking time $\Delta t=2 l / v=p \lambda / v=2 \pi p / \omega=p T$. According to Eq. (201), at this distance the wave's power should drop by $\exp \{-2 \alpha l\}=\exp \{-p \alpha \lambda\}$. On the other hand, the same decay may be viewed as happening in time, and according to Eq. (216), result in the drop by $\exp \{-\Delta t / \tau\}=\exp \{-$ $(p T) /(Q / \omega)\}=\exp \{-2 \pi p / Q\}$. Comparing these two exponents, we get

$$
\begin{equation*}
Q=\frac{2 \pi}{\alpha \lambda}=\frac{k}{\alpha} \tag{7.220}
\end{equation*}
$$

This simple relation neglects the losses at wave reflection from the walls limiting the resonator length. Such approximation is indeed legitimate at $a \ll \lambda$; if this relation is violated, or if we are dealing with more complex resonator modes (such as those based on the reflection of $E$ or $H$ waves), the $Q$ factor may be smaller than that given by Eq. (220), and needs to be calculated directly. A substantial relief for such a direct calculation is that, just at the calculation of small attenuation in waveguides, in the low-loss limit ( $Q \gg 1$ ), both the numerator and denominator of the right-hand part of Eq. (217) may be calculated neglecting the effects of the power loss on the field distribution in the resonator. I am leaving such a calculation, for the simplest (rectangular and circular) resonators, for reader's exercise.

To conclude this chapter, the last remark: in some resonators (including certain dielectric resonators and metallic resonators with holes in their walls), additional losses due to wave radiation into the environment are also possible. In some simple cases (say, the Fabry-Pérot interferometer shown in Fig. 32) the calculation of these radiative losses is straightforward, but sometimes it requires more elaborated approaches, which will be discussed in the next chapter.

### 7.11. Exercise problems

7.1.* Find the temporal Green's function of a medium whose complex dielectric constant obeys Eq. (32), using:
(i) the Fourier transform, and
(ii) the direct solution of Eq. (30), which describes the corresponding model of the medium.

Hint: For the Fourier transform, you may like to use the Cauchy integral. ${ }^{75}$
7.2. The electric polarization of a material responds in the following way to an electric field step: ${ }^{76}$

[^354]\[

P(t)=\varepsilon_{1} E_{0}\left(1-e^{-t / \tau}\right), \quad if E(t)=E_{0} \times $$
\begin{cases}0, & \text { for } t<0, \\ 1, & \text { for } 0<t\end{cases}
$$
\]

where $\tau$ is a positive constant. Calculate the complex permittivity $\varepsilon(\omega)$ of this material, and discuss a possible simple physical model giving such dielectric response.
7.3. Calculate the complex dielectric constant $\varepsilon(\omega)$ for a material whose dielectric-response Green's function, defined by Eq. (23), is

$$
G(\theta)=G_{0}\left(1-e^{-\theta / \tau}\right)
$$

with some positive constants $G_{0}$ and $\tau$. What is the difference between this dielectric response and the apparently similar one considered in the previous problem?
7.4. Use the Lorentz oscillator model of an atom, given by Eq. (30), to calculate the average potential energy of the atom in a uniform, sinusoidal ac electric field, and use the result to calculate the potential profile created for the atom by a standing electromagnetic wave with the electric field amplitude $E_{\sigma}(\mathbf{r})$. Discuss the conditions of validity of your result.
7.5. The solution of the previous problem shows that a standing plane wave exerts a timeaveraged force on a non-relativistic charged particle. Reveal the physics of this force by writing and solving the equations of motion of a free particle in:
(i) a linearly-polarized, monochromatic, plane traveling wave, and
(ii) a similar but standing wave.

Discuss the conditions of validity of your result.
7.6. Calculate, sketch and discuss the dispersion relation for electromagnetic waves propagating in a Lorentz oscillator medium described by Eq. (32), for the case of negligible damping.
7.7. As was briefly discussed in Sec. $2,{ }^{77}$ a wave pulse of a finite but relatively large spatial extension $\Delta r \gg \lambda \equiv 2 \pi / k$ may be represented with a wave packet - a sum of sinusoidal waves with wave vectors $\mathbf{k}$ within a relatively narrow interval. Consider an electromagnetic plane wave packet of this type, with the electric field distribution

$$
\mathbf{E}(\mathbf{r}, t)=\operatorname{Re} \int_{-\infty}^{+\infty} \mathbf{E}_{k} e^{i\left(k z-\omega_{k} t\right)} d k, \quad \text { with } \omega_{k}\left[\varepsilon\left(\omega_{k}\right) \mu\left(\omega_{k}\right)\right]^{1 / 2} \equiv|k|
$$

propagating along axis $z$ in an isotropic, linear, and loss-free (but not necessarily dispersion-free) medium. Express the full energy of the packet (per unit area of wave's front) via complex amplitudes $\mathbf{E}_{k}$, and discuss its dependence of time.

[^355]7.8. ${ }^{*}$ Analyze the effect of a constant, uniform magnetic field $\mathbf{B}_{0}$, parallel to the direction $\mathbf{n}$ of electromagnetic wave propagation, on the wave dispersion in plasma, within the same simple model that was used in the lecture notes for derivation of Eq. (7.38). (Limit your analysis to relatively weak waves, whose magnetic field is negligible in comparison with $\mathbf{B}_{0}$.)

Hint: You may like to represent the incident wave as a linear superposition of two circularly polarized waves, with the left- and right-hand polarization.
7.9. A monochromatic, plane electromagnetic wave is normally incident from free space on a uniform slab of a material with electric permittivity $\varepsilon$ and magnetic permeability $\mu$, with the slab thickness $d$ comparable with the wavelength.
(i) Calculate the power transmission coefficient $T$, i.e. the fraction of the incident power, that is transmitted through the slab.
(ii) Assuming that $\varepsilon$ and $\mu$ are frequency-independent and positive, analyze in detail the frequency dependence of $\tau$. In particular, how does function $\pi(\omega)$ depend on the film thickness $d$ and the wave impedance $Z=(\mu / \varepsilon)^{1 / 2}$ of its material?
7.10. A monochromatic, plane electromagnetic wave with free-space wave number $k_{0}$ is normally incident on a plane conducting film of thickness $d \sim \delta_{\mathrm{s}} \ll 1 / k_{0}$. Calculate the power transmission coefficient of the system, i.e. the fraction of incident wave's power propagating beyond the film. Analyze the result in the limits of small and large ratios $d / \delta_{\text {s }}$.
7.11. A plane wave of frequency $\omega$ is normally incident, from free space, on a plane surface of a material with real values of the electric permittivity $\varepsilon^{\prime}$ and magnetic permeability $\mu^{\prime}$. To minimize wave reflection from the surface, you may cover it with a layer, of thickness $d$, of another transparent material - see Fig. on the right. Calculate the optimal values of $\varepsilon, \mu$, and $d$.

7.12. A monochromatic, plane wave is incident from inside a medium with $\varepsilon \mu>\varepsilon_{0} \mu_{0}$ on its plane surface, at the angle of incidence $\theta$ larger than the critical angle $\theta_{\mathrm{c}}=$ $\sin ^{-1}\left(\varepsilon_{0} \mu_{0} / \varepsilon \mu\right)^{1 / 2}$. Calculate the depth $\delta$ of the evanescent wave penetration into the free space and analyze its dependence on $\theta$. Does the result depend on the wave polarization?
7.13. Analyze the possibility of propagation of surface electromagnetic waves along a plane boundary between plasma and free space. In particular, calculate and analyze the dispersion relation of the waves.

Hint: Assume that the magnetic field of the wave is parallel to the boundary and perpendicular to the wave propagation direction. (After solving the problem, justify this mode choice.)
7.14. Calculate the characteristic impedance $Z_{W}$ of the long, straight TEM transmission lines formed by metallic electrodes with cross-sections shown in Fig. below:

(iii)
(i) two round, parallel wires, separated by distance $d \gg R$,
(ii) microstrip line of width $w \gg d$,
(iii) stripline with $w \gg d_{1} \sim d_{2}$,
in all cases using the macroscopic boundary conditions on metallic surfaces. Assume that the conductors are embedded into a linear dielectric with constant $\varepsilon$ and $\mu$.
7.15. Modify results of Problem 10(ii) for a superconductor microstrip line, taking into account the magnetic field penetration into both the strip and the ground plane.
7.16. * What lumped ac circuit would be equivalent to the system shown in Fig. 20, with incident wave's power $\mathcal{P}_{i}$ ? Assume that the wave reflected from the load circuit does not return to it.
7.17. Find the lumped ac circuit equivalent to a loss-free TEM transmission line of length $l \sim \lambda$, with a small cross-section area $A \ll \lambda^{2}$, as "seen" (measured) from one end, if the line's conductors are galvanically connected ("shortened") at the other end
 - see Fig. on the right. Discuss result's dependence on the signal frequency.
7.18. Represent the fundamental $H_{10}$ wave in a rectangular waveguide (Fig. 22) with a sum of two plane waves, and discuss the physics behind such a representation .
7.19. ${ }^{*}$ For a metallic coaxial cable with the circular cross-section (Fig. 21), find the lowest nonTEM mode and calculate its cutoff frequency.
7.20. Two coaxial cable sections are connected coaxially - see Fig. on the right, which shows system's cut along its symmetry axis. Relations (118) and (120) seem to imply that if the ratios $b / a$ of these sections are equal, their impedance matching is perfect, i.e. a TEM wave incident from one side on the connection would pass it without any reflection at all: $R=0$. Is this statement correct?

7.21. * Use the recipe outlined in Sec. 8 to prove the characteristic equation (161) for the $H E$ and EH modes in a round, step-index optical fiber.
7.22. Find the lowest eigenfrequencies, and corresponding oscillation modes, of a round cylindrical resonator (see Fig. on the right) with perfectly conducting walls.

7.23. A plane, monochromatic wave propagates through a medium whose Ohmic conductance $\sigma$ dominates the power losses, while the electric and magnetic polarization effects are negligible. Calculate the wave attenuation coefficient and relate the result with some calculation carried out in Chapter 6.
7.24. Generalize the telegrapher's equations (110)-(111) by taking into account small energy losses in:
(i) transmission line's conductors, and
(ii) the media separating the conductors, using their simplest (Ohmic) models. Formulate the conditions of validity of the resulting equations.
7.25. Calculate the skin-effect contribution to the attenuation coefficient $\alpha$, defined by Eq. (202), for the basic $\left(H_{10}\right)$ mode propagating in a waveguide with the rectangular cross-section - see Fig. 22. Use the results to evaluate $\alpha$ and $L$ for a 10 GHz wave in the standard X-band waveguide WR-90 (with copper walls, $a=23 \mathrm{~mm}, b=10 \mathrm{~mm}$, and no dielectric filling), at room temperature. Compare the estimate with that, made in Sec. 10, for a standard coaxial cable, for the same frequency.
7.26. ${ }^{*}$ Calculate the skin-effect contribution to the attenuation coefficient $\alpha$ of
(i) the basic $\left(H_{11}\right)$ mode, and
(ii) the $H_{01}$ mode
in a metallic waveguide with the circular cross-section (Fig. 23a), and analyze the low-frequency ( $\omega$ $\left.\rightarrow \omega_{\mathrm{c}}\right)$ and high-frequency $\left(\omega \gg \omega_{\mathrm{c}}\right)$ behaviors of $\alpha$ for each of these modes.
7.27. For a rectangular metallic-wall resonator with dimensions $a \times b \times l(b \leq a, l)$, calculate the $Q$ factor in the fundamental (lowest) oscillation mode, due to the skin-effect losses in the walls. Evaluate the factor (and the lowest eigenfrequency) for a $23 \times 23 \times 10 \mathrm{~mm}^{3}$ resonator with copper walls, at room temperature.
7.28.* Calculate the lowest eigenfrequency and $Q$ factor (due to the skin-effect losses) of the toroidal (axially-symmetric) resonator with metallic walls and interior's cross-section shown in Fig. on the right, within the limit $d \ll r, R$.

7.29. Express the contribution to the damping coefficient (the reciprocal $Q$-factor) of a resonator, due to small energy losses in the dielectric that fills it, via dielectric's complex functions $\varepsilon(\omega)$ and $\mu(\omega)$ of the material.
7.30. For the dielectric Fabry-Pérot resonator (Fig. 32) with the normal wave incidence, find the $Q$-factor due to radiation losses in the limit of strong impedance mismatch ( $Z \gg Z_{0}$ ), using two methods:
(i) from the energy balance, using Eq. (217), and
(ii) from the frequency dependence of the power transmission coefficient, using Eq. (219). Compare the results.

## Chapter 8. Radiation, Scattering, Interference, and Diffraction

This chapter continues the discussion of the electromagnetic wave propagation, now focusing on the results of wave incidence on a passive object. Depending on the object's shape, the result of this interaction is called either scattering, or diffraction, or interference. However, as we will see below, the boundary between these effects is blurry, and their mathematical description may be conveniently based on a single key calculation - the electric dipole radiation of a spherical wave by a small source. Naturally, I will start the chapter from this calculation, deriving it from an even more general result the "retarded potentials" solution of the Maxwell equations.

### 8.1. Retarded potentials

Let us start from the general solution of the Maxwell equations in a dispersion-free, linear, uniform, isotropic medium, characterized by frequency-independent, real $\varepsilon$ and $\mu$ - for example, free space. ${ }^{1}$ The easiest way to perform this calculation is to use the scalar $(\phi)$ and vector (A) potentials of electromagnetic field, that are defined via the electric and magnetic fields by Eqs. (6.106):

$$
\begin{equation*}
\mathbf{E}=-\nabla \phi-\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B}=\nabla \times \mathbf{A} . \tag{8.1}
\end{equation*}
$$

As was discussed in Chapter 6, imposing upon the potentials the Lorenz gauge condition (6.108),

$$
\begin{equation*}
\nabla \cdot \mathbf{A}+\frac{1}{v^{2}} \frac{\partial \phi}{\partial t}=0, \quad v^{2} \equiv \frac{1}{\varepsilon \mu}, \tag{8.2}
\end{equation*}
$$

(which does not affect fields $\mathbf{E}$ and $\mathbf{B}$ ) the macroscopic Maxwell equations for the fields may be recast into a pair of very similar, simple equations (6.109) for the potentials:

$$
\begin{align*}
& \nabla^{2} \phi-\frac{1}{v^{2}} \frac{\partial^{2} \phi}{\partial t^{2}}=-\frac{\rho}{\varepsilon}  \tag{8.3a}\\
& \nabla^{2} \mathbf{A}-\frac{1}{v^{2}} \frac{\partial^{2} \mathbf{A}}{\partial t^{2}}=-\mu \mathbf{j} \tag{8.3b}
\end{align*}
$$

Let us calculate the fields induced by the stand-alone electric charge and current densities $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$, thinking of them as known functions. ${ }^{2}$ The idea how this may be done may be borrowed from electro- and magnetostatics. Indeed, for the stationary case $(\partial / \partial t=0)$, the solutions of Eqs. (8.3) are given, by the evident generalization of, respectively, Eq. (1.38) and by Eq. (5.28) to the uniform, linear medium:

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon} \int \rho\left(\mathbf{r}^{\prime}\right) \frac{d^{3} r^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}, \tag{8.4a}
\end{equation*}
$$

[^356]\[

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}) \equiv \frac{\mu}{4 \pi} \int \mathbf{j}\left(\mathbf{r}^{\prime}\right) \frac{d^{3} r^{\prime}}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \tag{8.4b}
\end{equation*}
$$

\]

As we know, these expressions may be derived by, first, calculating the potential of a point source, and then using the linear superposition principle for a system of such sources.

Let us do the same for the time-dependent case, starting from the field induced by a timedependent point charge at origin: ${ }^{3}$

$$
\begin{equation*}
\rho(\mathbf{r}, t)=q(t) \delta(\mathbf{r}) \tag{8.5}
\end{equation*}
$$

In this case Eq. (3a) is homogeneous everywhere but the origin:

$$
\begin{equation*}
\nabla^{2} \phi-\frac{1}{v^{2}} \frac{\partial^{2} \phi}{\partial t^{2}}=0, \quad \text { at } r \neq 0 \tag{8.6}
\end{equation*}
$$

Due to the spherical symmetry of the problem, it is natural to look for a spherically-symmetric solution to this equation. ${ }^{4}$ Thus, we may simplify the Laplace operator ${ }^{5}$ correspondingly, and reduce Eq. (6) to

$$
\begin{equation*}
\left[\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial}{\partial r}\right)-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right] \phi=0, \quad \text { at } r \neq 0 . \tag{8.7}
\end{equation*}
$$

If we now introduce a new variable $\chi \equiv r \phi$, Eq. (7) is reduced to the 1 D wave equation

$$
\begin{equation*}
\left(\frac{\partial^{2}}{\partial r^{2}}-\frac{1}{v^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) \chi=0, \quad \text { at } r \neq 0 . \tag{8.8}
\end{equation*}
$$

From the discussion in Chapter $7,{ }^{6}$ we know that its general solution may be presented as

$$
\begin{equation*}
\chi(r, t)=\chi_{\text {out }}\left(t-\frac{r}{v}\right)+\chi_{\text {in }}\left(t+\frac{r}{v}\right) \tag{8.9}
\end{equation*}
$$

where $\chi_{\text {in }}$ and $\chi_{\text {out }}$ are (so far) arbitrary functions of one variable. The physical sense of $\phi_{\text {out }}=\chi_{\text {out }} / r$ is a spherical wave propagating from our source (at $r=0$ ) to outer space, i.e. exactly the solution we are looking for. On the other hand, $\phi_{\text {in }}=\chi_{\text {in }} / r$ describes a spherical wave that could be created by some distant spherically-symmetric source, that converges on our charge located at the origin - evidently not the effect we want to consider here. Discarding this term, and returning to $\phi=\chi / r$, we can write the solution (7) as

$$
\begin{equation*}
\phi(r, t)=\frac{1}{r} \chi_{\text {out }}\left(t-\frac{r}{v}\right) \tag{8.10}
\end{equation*}
$$

[^357]In order to find function $\chi_{\text {out }}$, let us consider distances $r$ so small that the time derivative in Eq. (3a), with the right-hand part (5),

$$
\begin{equation*}
\nabla^{2} \phi-\frac{1}{v^{2}} \frac{\partial^{2} \phi}{\partial t^{2}}=-\frac{q(t)}{\varepsilon} \delta(\mathbf{r}) \tag{8.11}
\end{equation*}
$$

is much smaller that the spatial derivative (that diverges at $r \rightarrow 0$ ). Then Eq. (11) is reduced to the electrostatic equation whose solution (4a), for source (5), is

$$
\begin{equation*}
\phi(r \rightarrow 0, t)=\frac{q(t)}{4 \pi \varepsilon r} . \tag{8.12}
\end{equation*}
$$

Now requiring the two solutions, (10) and (12), to coincide at $r \ll \nu t$, we get $\chi_{\text {out }}(t)=q(t) / 4 \pi \varepsilon r$, so that Eq. (10) becomes

$$
\begin{equation*}
\phi(r, t)=\frac{1}{4 \pi \varepsilon r} q\left(t-\frac{r}{v}\right) \tag{8.13}
\end{equation*}
$$

Just as had been done in statics, this result may be readily generalized for the arbitrary position $r^{\prime}$ of the point charge:

$$
\begin{equation*}
\rho(\mathbf{r}, t)=q(t) \delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \equiv q(t) \delta(\mathbf{R}), \tag{8.14}
\end{equation*}
$$

where $R$ is the distance between the field observation point $\mathbf{r}$ and the source position point $\mathbf{r}$ ', i.e. the length of the vector,

$$
\begin{equation*}
\mathbf{R} \equiv \mathbf{r}-\mathbf{r}^{\prime} \tag{8.15}
\end{equation*}
$$

connecting these points - see Fig. 1.


Now we can use the linear superposition principle to write, for the arbitrary charge distribution $\rho(\mathbf{r}, t)$,

$$
\begin{equation*}
\phi(\mathbf{r}, t)=\frac{1}{4 \pi \varepsilon} \int \rho\left(\mathbf{r}^{\prime}, t-\frac{R}{v}\right) \frac{d^{3} r^{\prime}}{R} \tag{8.17a}
\end{equation*}
$$

where integration is extended over all charges of the system under analysis. Acting absolutely similarly, for the vector potential we get

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}, t)=\frac{\mu}{4 \pi} \int \mathbf{j}\left(\mathbf{r}^{\prime}, t-\frac{R}{v}\right) \frac{d^{3} r^{\prime}}{R} \tag{8.17b}
\end{equation*}
$$

(Now nothing prevents functions $\rho(\mathbf{r}, t)$ and $\boldsymbol{j}(\mathbf{r}, t)$ from satisfying the continuity relation.)
Solutions (17) are called the retarded potentials, the name signifying that the observed fields are "retarded" (delayed) in time by $\Delta t=R / v$ relative to the source variations, due to the finite speed $v$ of the electromagnetic wave propagation. These solutions are so important that they deserve at least a couple of general remarks.

First, remarkably, these simple expressions are exact solutions of the Maxwell equations (93) in a uniform medium for an arbitrary distribution of stand-alone charges and currents. They also may be considered as the general solutions of these equations, provided that the integration is extended over all field sources in the Universe - or at least in its part that affects our observations.

Second, if functions $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$ include the microscopic (bound) charges and currents as well, the macroscopic Maxwell equations (6.93) are valid with the replacement $\varepsilon \rightarrow \varepsilon_{0}$ and $\mu \rightarrow \mu_{0}$, so that the retarded potentials solutions (17) are also valid - with the same replacement.

Finally, Eqs. (17) may be plugged into Eqs. (1), giving (after an explicit differentiation) the socalled Jefimenko equations for fields $\mathbf{E}$ and $\mathbf{B}$ - similar in structure to Eqs. (17), but more cumbersome. Conceptually, the existence of such equations is a good news, because they are free from the gauge ambiguity pertinent to potentials $\phi$ and $\mathbf{A}$. However, the practical value of these explicit expressions for the fields is not too high: for all applications I am aware of, it is easier to use Eqs. (17) to calculate the particular expressions for the potentials first, and only then calculate the fields from Eqs. (1). Let me present the (apparently most important) example of this approach.

### 8.2. Electric dipole radiation

Consider again the problem that was discussed in electrostatics (Sec. 3.1), namely the field of a localized source with linear dimensions $a \ll r$ (Fig. 1), but now with time-dependent charge and/or current distribution. Using the arguments of that discussion, in particular the condition expressed by Eq. (3.1), $r^{\prime} \ll r$, we may apply the Taylor expansion (3.3),

$$
\begin{equation*}
f(\mathbf{R})=f(\mathbf{r})-\mathbf{r}^{\prime} \cdot \nabla f(\mathbf{r})+\ldots \tag{8.18}
\end{equation*}
$$

to function $f(\mathbf{R}) \equiv R$ (for which $\nabla f(\mathbf{r})=\nabla R=\mathbf{n}$, where $\mathbf{n} \equiv \mathbf{r} / r$ is the unit vector directed toward the observation point, see Fig. 1) to approximate distance $R$ as

$$
\begin{equation*}
R \approx r-\mathbf{r}^{\prime} \cdot \mathbf{n} . \tag{8.19}
\end{equation*}
$$

In each of the retarded potential formulas (17), $R$ participates in two places: in the denominator and in the source time argument. If $\rho$ and $\mathbf{j}$ change in time on scale $\sim 1 / \omega$, where $\omega$ is some characteristic frequency, then any change of argument $(t-R / v)$ on that time scale, for example due to a change of $R$ on the spatial scale $\sim v / \omega=1 / k$, may substantially change these functions. Thus, expansion (18) may be applied to $R$ in the argument $(t-R / v)$ only if $k a \ll 1$, i.e. if the system size $a$ is much smaller than the radiation wavelength $\lambda=2 \pi / k$. On the other hand, function $1 / R$ changes relatively slowly, and for it even the first term expansion (19) gives a good approximation as soon as $a \ll r, R$. In this approach, Eq. (17a) yields

$$
\begin{equation*}
\phi(\mathbf{r}, t) \approx \frac{1}{4 \pi \varepsilon r} \int \rho\left(\mathbf{r}^{\prime}, t-\frac{R}{v}\right) d^{3} r^{\prime}=\frac{1}{4 \pi \varepsilon r} Q\left(t-\frac{R}{v}\right) \tag{8.20}
\end{equation*}
$$

where $Q(t)$ is the net electric charge of the localized system Due to the charge conservation, this charge cannot change with time, so that the approximation (20) describes gives just a static Coulomb field of our localized source, rather than a radiated wave.

Let us, however, apply a similar approximation to the vector potential (17b):

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}, t) \approx \frac{\mu}{4 \pi r} \int \mathbf{j}\left(\mathbf{r}^{\prime}, t-\frac{R}{v}\right) d^{3} r^{\prime} \tag{8.21}
\end{equation*}
$$

According to Eq. (5.87), in statics the right-hand part of this expression would vanish, but in dynamics this is no longer true. For example, if the current is due to a non-relativistic motion ${ }^{7}$ of a system of charges $q_{k}$, we can write

$$
\begin{equation*}
\int \mathbf{j}\left(\mathbf{r}^{\prime}, t\right) d^{3} r^{\prime}=\sum_{k} q_{k} \dot{\mathbf{r}}_{k}(t)=\frac{d}{d t} \sum_{k} q_{k} \mathbf{r}_{k}(t) \equiv \dot{\mathbf{p}}(t), \tag{8.22}
\end{equation*}
$$

where $\mathbf{p}(t)$ is the dipole moment of the localized system, defined by Eq. (3.6). Now, after the integration, we may keep only the first term of approximation (19) in the argument $(t-R / v)$ as well, getting

$$
\begin{equation*}
\mathbf{A}(\mathbf{r}, t) \approx \frac{\mu}{4 \pi r} \dot{\mathbf{p}}\left(t-\frac{r}{v}\right) \tag{8.23}
\end{equation*}
$$

Let us analyze what exactly does this result, valid in the limit $k a \ll 1$, describe. The second of Eqs. (1) allows us to calculate the magnetic field by the spatial differentiation of A. At large distances $r$ $\gg \lambda$ (i.e. in the so-called far field zone), where Eq. (23) describes a virtually plane wave, the main contribution into this derivative is given by the dipole moment factor:

$$
\begin{equation*}
\mathbf{B}(\mathbf{r}, t)=\frac{\mu}{4 \pi r} \nabla \times \dot{\mathbf{p}}\left(t-\frac{r}{v}\right)=-\frac{\mu}{4 \pi r v} \mathbf{n} \times \ddot{\mathbf{p}}\left(t-\frac{r}{v}\right) \tag{8.24}
\end{equation*}
$$

This expression means that the magnetic field, at the observation point, is perpendicular to vectors $\mathbf{n}$ and (the retarded value of) $\ddot{\mathbf{p}}$, and its magnitude is

$$
\begin{equation*}
B=\frac{\mu}{4 \pi r v} \ddot{p}\left(t-\frac{r}{v}\right) \sin \theta, \quad \text { i.e. } H=\frac{1}{4 \pi r v} \ddot{p}\left(t-\frac{r}{v}\right) \sin \theta \tag{8.25}
\end{equation*}
$$

where $\theta$ is the angle between those two vectors - see Fig. 2. ${ }^{8}$

[^358]The most important feature of this result is that the time-dependent field decreases very slowly (only as $1 / r$ ) with the distance from the source, so that the radial component of the corresponding Poynting vector (7.7), $S_{r}=Z H^{2}$, drops as $1 / r^{2}$, i.e. the full power $\mathcal{P}$ of the emitted spherical wave, that scales as $r^{2} S_{r}$, does not depend on the distance from the source - as it should for radiation. Equation (25) allows us to be more quantitative; for the instantaneous radiation intensity we may plug it into Eq. (7.9) to get

$$
\begin{equation*}
S_{r}=Z H^{2}=\frac{Z}{(4 \pi v r)^{2}}\left[\ddot{p}\left(t-\frac{r}{v}\right)\right]^{2} \sin ^{2} \theta . \tag{8.26}
\end{equation*}
$$



Fig. 8.2. Far zone fields of a localized source, contributing into its electric dipole radiation.

This is the famous formula for the electric dipole radiation; this is the dominating component of radiation by a localized system of charges - unless $\ddot{\mathbf{p}}=0$. Please notice its angular dependence: the radiation vanishes at the axis of the retarded vector $\ddot{\mathbf{p}}$ (where $\theta=0$ ), and reaches its maximum in the plane perpendicular to that axis. Integration of $S_{r}$ over all directions, i.e. over the whole sphere of radius $r$, gives the total instant power of the dipole radiation: ${ }^{9}$

$$
\begin{equation*}
\mathcal{P} \equiv \oint_{r=\text { const }} S_{r} d^{2} r=\frac{Z}{(4 \pi v)^{2}} \ddot{p}^{2} 2 \pi \int_{0}^{\pi} \sin ^{3} \theta d \theta=\frac{Z}{6 \pi v^{2}} \ddot{p}^{2} \tag{8.27}
\end{equation*}
$$

In order to find the average power, this expression has to be averaged over a sufficiently long time. In particular, if the source is monochromatic, $\mathbf{p}(t)=\operatorname{Re}\left[\mathbf{p}_{\omega} \exp \{-i \omega t\}\right.$, with time-independent vector $\mathbf{p}_{\omega}$, such averaging may be carried out just over one period, giving an extra factor 2 in the denominator:

$$
\begin{equation*}
\overline{\mathcal{P}}=\frac{Z \omega^{4}}{12 \pi v^{2}}\left|p_{\omega}\right|^{2} \tag{8.28}
\end{equation*}
$$

[^359]The easiest example of application of the formula is to a point charge oscillating, with frequency $\omega$, along a straight line (that we may take for axis $z$ ), with amplitude $a$. In this case, $\mathbf{p}=q \mathbf{n}_{z} z(t)=q a \operatorname{Re}$ [ $\exp \{-i \omega t\}$ ], and if the charge velocity amplitude, $a \omega$, is much less than the wave speed $v$, we may use Eq. (28) with $p_{\omega}=q a$, giving

[^360]\[

$$
\begin{equation*}
\overline{\mathcal{P}}=\frac{Z q^{2} a^{2} \omega^{4}}{12 \pi v^{2}} . \tag{8.29}
\end{equation*}
$$

\]

Applied to an electron ( $q=-e \approx-1.6 \times 10^{-19} \mathrm{C}$ ), rotating about a nuclei at an atomic distance $a \sim 10^{-10} \mathrm{~m}$, the Larmor formula shows ${ }^{10}$ that the energy loss due to the dipole radiation is so large that it would cause electron's collapse on atom's nuclei in just $\sim 10^{-10} \mathrm{~s}$. In the beginning of the 1900 s , this classical result was one of the main arguments for the development of quantum mechanics that prevents such collapse of electrons in their lowest-energy (ground) state.

Another example of a very useful application of Eq. (28) is the radio wave radiation by a short, straight, symmetric antenna which is fed, for example, by a TEM transmission line such as a coaxial cable - see Fig. 3.


Fig. 8.3. Dipole antenna.

The exact solution of this problem is rather complex, because the law $I_{\omega}(z)$ of the current variation along antenna's length should be calculated self-consistently with the distribution of the electromagnetic field that is induced by the current in the surrounding space. (This fact is unfortunately ignored in some textbooks.) However, one may argue that at $l \ll \lambda$, the current should be largest in the feeding point (in Fig. 3, taken for $z=0$ ), vanish at antenna's ends ( $z= \pm l / 2$ ), and that the only possible scale of the current variation in the antenna is $l$ itself, so that the linear function,

$$
\begin{equation*}
I_{\omega}(z)=I_{\omega}(0)\left(1-\frac{2}{l}|z|\right), \tag{8.30}
\end{equation*}
$$

gives a good approximation - as it indeed does. Now we can use the continuity equation $\partial Q / \partial t=I$, i.e. $i \omega Q_{\omega}=I_{\omega}$, to calculate the complex amplitude $Q_{\omega}(z)=i I_{\omega}(z) \operatorname{sgn}(z) / \omega$ of the electric charge $Q(z, t)=$ $\operatorname{Re}\left[Q_{\omega} \exp \{-i \omega t\}\right]$ of the wire beyond point $z$, and from it, the amplitude of the linear density of charge

$$
\begin{equation*}
\lambda_{\omega}(z) \equiv \frac{d Q_{\omega}(z)}{d|z|}=-i \frac{2 I_{\omega}(0)}{\omega l} \operatorname{sgn} z . \tag{8.31}
\end{equation*}
$$

From here, the dipole moment's amplitude is

$$
\begin{equation*}
p_{\omega}=2 \int_{0}^{l / 2} \lambda_{\omega}(z) z d z=-i \frac{I_{\omega}(0)}{2 \omega} l \tag{8.32}
\end{equation*}
$$

[^361]so that Eq. (28) yields
\[

$$
\begin{equation*}
\bar{P}=Z \frac{\omega^{4}}{12 \pi v^{2}} \frac{\left|I_{\omega}(0)\right|^{2}}{4 \omega^{2}} l^{2}=\frac{Z(k l)^{2}}{24 \pi} \frac{\left|I_{\omega}(0)\right|^{2}}{2} \tag{8.33}
\end{equation*}
$$

\]

where $k=\omega / \mathrm{v}$. The analogy between this result and the dissipation power, $\mathcal{P}=\operatorname{Re} Z\left(I_{\omega}{ }^{2} / 2\right)$, in a lumped linear circuit element, allows the interpretation of the first fraction in the last form of Eq. (33) as the real part of antenna's impedance:

$$
\begin{equation*}
\operatorname{Re} Z_{A}=Z \frac{(k l)^{2}}{24 \pi} \tag{8.34}
\end{equation*}
$$

as felt by the transmission line. (Indeed, according to Eq. (7.118), the wave traveling along the line toward the antenna is fully radiated, i.e. not reflected back, only if $Z_{A}$ equals to $Z_{W}$ of the line.) As we know from Chapter 7, for typical TEM lines, $Z_{W} \sim Z_{0}$, while Eq. (34), that is only valid in the limit $k l \ll$ 1 , shows that for radiation into free space $\left(Z=Z_{0}\right), \operatorname{Re} Z_{A}$ is much less than $Z_{0}$.

Hence in order to reach the impedance matching condition $Z_{W}=Z_{A}$, antenna's length should be increased - as a more involved theory shows, to $l \sim \lambda / 2$. However, in many cases, practical considerations make short antennas necessary. The most frequently met example met nowadays are the cell phone antennas, which use frequencies close to 1 or 2 GHz , with free-space wavelengths $\lambda$ between 15 and 30 cm , i.e. much larger than the phone size. The quadratic dependence of antenna's efficiency on $l$, following from Eq. (34), explains why every millimeter counts in the design of such antennas, and why the designs are carefully optimized using software packages for (virtually exact) numerical solution of time-dependent Maxwell equations for the specific shape of the antenna and other phone parts. ${ }^{11}$

To conclude this section, let me note that if the wave source is not monochromatic, so that $\mathbf{p}(t)$ should presented as a Fourier series,

$$
\begin{equation*}
\mathbf{p}(t)=\operatorname{Re} \sum_{\omega} \mathbf{p}_{\omega} e^{-i \omega t} \tag{8.35}
\end{equation*}
$$

the terms corresponding to interference of spectral components with different frequencies $\omega$ are averaged out at the time averaging of the Poynting vector, so that the average radiated power is just a sum of contributions (28) from all substantial frequency components.

### 8.3. Wave scattering

The formalism described above may be immediately used in the theory of scattering - the phenomenon illustrated by Fig. 4. Generally, scattering is a complex problem. However, in many cases it allows the so-called Born approximation, ${ }^{12}$ in which scattered wave's field applied to the scattering object is assumed to be much weaker than that of the incident wave, and is neglected.

[^362]

Fig. 8.4. Scattering (schematically).

As the first example of this approach, let us consider scattering of a plane wave, propagating in free space $\left(Z=Z_{0}, v=c\right)$, by a free ${ }^{13}$ charged particle whose motion may be described by non-relativistic classical mechanics. (This requires, in particular, the incident wave to be of a modest intensity, so that the speed of the induced charge motion is much less than the speed of light.) In this case the magnetic component of the Lorentz force (5.8),

$$
\begin{equation*}
\mathbf{F}_{m}=q \dot{\mathbf{r}} \times \mathbf{B}, \tag{8.36}
\end{equation*}
$$

exerted on the charge by the magnetic field of a plane wave, is much smaller than force $\mathbf{F}_{e}=q \mathbf{E}$ exerted by its electric field. Indeed, according to Eq. (7.8), $H=E / Z=E /(\mu / \varepsilon)^{1 / 2}, B=\mu H=E / v$, so that the ratio $F_{m} / F_{e}$ equals to the ratio of particle'e speed, $|\dot{\mathbf{r}}|$, to wave's speed $v \sim c$.

Thus, assuming that the incident wave is linearly-polarized along axis $x$, the equation of particle's motion in the Born approximation is just $m \ddot{x}=q E(t)$, so that for the $x$-component $p_{x}=q x$ of its dipole moment we can write

$$
\begin{equation*}
\ddot{p}=q \ddot{x}=\frac{q^{2}}{m} E(t) . \tag{8.37}
\end{equation*}
$$

As we already know from Sec. 2, oscillations of the dipole moment lead to radiation of a wave with a wide angular distribution of intensity; in our case this is the scattered wave - see Fig. 4. Its full power may be found by plugging Eq. (37) into Eq. (27):

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0}}{6 \pi c^{2}} \ddot{p}^{2}=\frac{Z_{0} q^{4}}{6 \pi c^{2} m^{2}} E^{2}(t), \text { i.e. } \bar{P}=\frac{Z_{0} q^{4}}{12 \pi c^{2} m^{2}}\left|E_{\omega}\right|^{2} . \tag{8.38}
\end{equation*}
$$

Since the power is proportional to incident wave's intensity $S$, it is customary to characterize scattering ability of the object by the ratio,

Full crosssection: definition

$$
\begin{equation*}
\sigma \equiv \frac{\overline{\mathcal{P}}}{\overline{S_{\text {incident }}}}=\frac{\bar{P}}{\left|E_{\omega}\right|^{2} / 2 Z_{0}} \tag{8.39}
\end{equation*}
$$

which evidently has the dimension of area and is called the full cross-section of scattering. For this measure, Eq. (38) yields the famous result

[^363]\[

$$
\begin{equation*}
\sigma=\frac{Z_{0}^{2} q^{4}}{6 \pi c^{2} m^{2}}=\frac{\mu_{0}^{2} q^{4}}{6 \pi m^{2}} \tag{8.40}
\end{equation*}
$$

\]

which is called the Thomson scattering formula, ${ }^{14}$ especially when applied to an electron. This relation is most frequently presented in the form ${ }^{15}$

$$
\begin{equation*}
\sigma=\frac{8 \pi}{3} r_{c}^{2}, \quad \text { with } r_{c} \equiv \frac{q^{2}}{4 \pi \varepsilon_{0}} \cdot \frac{1}{m c^{2}}=10^{-7} \frac{q^{2}}{m} \text {. } \tag{8.41}
\end{equation*}
$$

Thomson scattering formula

Constant $r_{c}$ is called the classical radius of the particle (or sometimes the "Thomson scattering length"); for electron $\left(q=-e, m=m_{e}\right)$ it is close to $2.82 \times 10^{-15} \mathrm{~m}$. Its possible interpretation is evident from the first form of Eq. (41) for $r_{c}$ : at that distance between two similar particles, the potential energy $q^{2} / 4 \pi \varepsilon_{0} r$ of their electrostatic interaction is equal to particle's rest-mass energy $m c^{2}{ }^{2} .{ }^{16}$

Now we have to go back and establish the conditions at which the Born approximation, when the field of the scattered wave is negligible, is indeed valid for a point-object scattering. Since the scattered wave's intensity, described by Eq. (26), diverges as $1 / r^{2}$, according to the definition (39) of the crosssection, it may become comparable to $S_{\text {incident }}$ at $r^{2} \sim \sigma$. However, Eq. (38) itself is only valid if $r \gg \lambda$, so that the Born approximation does not lead to any contradiction if

$$
\begin{equation*}
\sigma \ll \lambda^{2} \tag{8.42}
\end{equation*}
$$

For the Thompson scattering by an electron, this condition means $\lambda \gg r_{c} \sim 3 \times 10^{-15} \mathrm{~m}$ and is fulfilled for all frequencies up to very hard $\gamma$ rays with energies $\sim 100 \mathrm{MeV}$.

Possibly the most notable feature of result (40) is its independence of the wave frequency. As it follows from its derivation, particularly from Eq. (37), this independence is intimately related with the unbound character of charge motion. For bound charges, say for electrons in a gas molecule, this result is only valid if the wave frequency $\omega$ is much higher all eigenfrequencies $\omega_{j}$ of molecular resonances. In the opposite limit, $\omega \ll \omega_{j}$, the result is dramatically different. Indeed, in this limit we can approximate the molecule's dipole moment by its static value (3.39)

$$
\begin{equation*}
\mathbf{p}=4 \pi \varepsilon_{0} \alpha_{\mathrm{mol}} \mathbf{E} \tag{8.43}
\end{equation*}
$$

In the Born approximation, and in the absence of the molecular field effects discussed in Sec. 3.5, E in this expression is just the incident wave's field, and we can use Eq. (28) to calculate the power of the wave scattered by a single molecule:

[^364]\[

$$
\begin{equation*}
\overline{\mathcal{P}}=\frac{4 \pi Z_{0} \omega^{4} \varepsilon_{0}^{2}}{c^{2}} \alpha_{\mathrm{mol}}^{2}\left|E_{\omega}\right|^{2} . \tag{8.44}
\end{equation*}
$$

\]

Now, using the last form of definition (39) of the cross-section, we get a very simple result,

$$
\begin{equation*}
\sigma=\frac{8 \pi Z_{0}^{2} \varepsilon_{0}^{2} \omega^{4}}{3 c^{2}} \alpha_{\mathrm{mol}}^{2}=\frac{8 \pi k^{4}}{3} \alpha_{\mathrm{mol}}^{2}, \tag{8.45}
\end{equation*}
$$

showing that in contrast to Eq. (40), at low frequencies $\sigma$ grows as fast as $\omega^{4}$.
Now let us explore the effect of such Rayleigh scattering ${ }^{17}$ on wave propagation in a gas, with relatively low density $n_{1}$. We can expect (and will prove in the next section) that due to the randomness of molecule positions, the waves scattered by each molecules may be treated as incoherent, so that the total scattering power may be calculated just as the sum of those scattered by each molecule. We can use this additivity to write the balance of the incident's wave intensity on a small volume $d V$ of length (along the incident wave direction) $d z$, and area $A$ in across it. Since such a segment includes $n d V=$ $n A d z$ molecules, and, according to definition (39), each of them scatters power $S \sigma=\mathcal{P} / A$, the total scattered power is $n$ Podz; hence the incident power's change is

$$
\begin{equation*}
d \mathcal{P} \equiv-n \sigma \mathcal{P} d z \tag{8.46}
\end{equation*}
$$

Comparing this equation with the general definition (7.202) of the attenuation constant, we see that scattering gives the following contribution to attenuation: $\alpha=n \sigma$. From here, using Eq. (3.41) to write $\alpha_{\mathrm{mol}}=\left(\varepsilon_{r}-1\right) / 4 \pi n$, and Eq. (45), we get

$$
\begin{equation*}
\alpha=\frac{k^{4}}{6 \pi n}\left(\varepsilon_{r}-1\right)^{2} . \tag{8.47}
\end{equation*}
$$

This is the famous Rayleigh scattering formula, which in particular explains the colors of blue sky and red sunsets. Indeed, through the visible light spectrum, $\omega$ changes almost two-fold; as a result, scattering of blue components of sunlight is an order of magnitude higher than that of its red components. More qualitatively, for air near the Earth surface, $\varepsilon_{r}-1 \approx 6 \times 10^{-4}$, and $n \sim 2.5 \times 10^{25} \mathrm{~m}^{-3}$ - see Sec. 3.3. Plugging these numbers into Eq. (47), we see that the characteristic length $\mathcal{L} \equiv 1 / \alpha$ of scattering is $\sim 30 \mathrm{~km}$ for blue light and $\sim 200 \mathrm{~km}$ for red light. ${ }^{18}$ The Earth atmosphere is thinner ( $h \sim 10$ km ), so that the Sun looks just a bit yellowish during most of the day. However, elementary geometry shows that on sunset, the light should pass length $l \sim\left(R_{\mathrm{E}} h\right)^{1 / 2} \approx 300 \mathrm{~km}$ to reach an Earth-surface observer; as a result, the blue components of Sun's light spectrum are almost completely scattered out, and even the red components are weakened considerably.

To conclude the discussion of Eq. (47), let me note that its comparison with the condition of the direct applicability of the Born approximation for a distributed object of size $a$ :

$$
\begin{equation*}
\alpha a \ll 1, \tag{8.48}
\end{equation*}
$$

[^365]implies, in particular, that if the electric polarizability of the material is small, $\varepsilon_{r} \rightarrow 1$, we may be able to use the approximation for an analysis of scattering by even relatively large objects, with size of the order of, or even larger than $\lambda$. However, for such extended objects, the phase difference factors (neglected above) step in, leading in particular to the important effects of interference and diffraction, to whose discussion we now proceed.

### 8.4. Interference and diffraction

These effects show up not as much in the total power of scattered radiation, as in its angular distribution. It is traditional to characterize this distribution by the differential cross-section defined as

$$
\begin{equation*}
\frac{d \sigma}{d \Omega} \equiv \frac{\bar{S}_{r} r^{2}}{\overline{S_{\text {incident }}}} \tag{8.49}
\end{equation*}
$$

Differential
crosssection: definition
where $r$ is the distance from the scatterer, at which the scattered wave is observed. Both the definition and notation become more clear if we notice that according to Eq. (26), at large distances ( $r \gg a$ ), the numerator in the right-hand part of Eq. (49), and hence the differential cross-section as the whole, does not depend on $r$, and that its integral over the total solid angle $\Omega=4 \pi$ coincides with the total crosssection defined by Eq. (39):

$$
\begin{equation*}
\oint_{4 \pi} \frac{d \sigma}{d \Omega} d \Omega=\frac{1}{\overline{S_{\text {incident }}}} r^{2} \oint_{4 \pi} \bar{S}_{r} d \Omega=\frac{1}{\overline{S_{\text {incident }}}} \oint_{r=\text { const }} \overline{S_{r}} d^{2} r=\frac{\overline{\mathcal{P}}}{\overline{S_{\text {incident }}}} \equiv \sigma . \tag{8.50}
\end{equation*}
$$

For example, according to Eq. (26), the angular distribution of radiation scattered by a point linear dipole, in the Born approximation, is rather broad; in particular, in the low-frequency limit (43),

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=k^{4} \alpha_{\mathrm{mol}}^{2} \sin ^{2} \theta \tag{8.51}
\end{equation*}
$$

If the wave is scattered by a small dielectric body, with a characteristic size $a \ll \lambda$ (i.e., $k a \ll 1$ ), then all its parts re-radiate the incident wave coherently. Hence, we can calculate it in the similar way, just replacing the molecular dipole moment (43) with the total dipole moment of the object - see Eq. (3.37):

$$
\begin{equation*}
\mathbf{p}=\mathbf{P} V=\left(\varepsilon_{r}-1\right) \varepsilon_{0} \mathbf{E} V, \tag{8.52}
\end{equation*}
$$

where $V \sim a^{3}$ is body's volume. As a result, the differential cross-section may be obtained from Eq. (51) with the replacement $\alpha_{\mathrm{mol}} \rightarrow V\left(\varepsilon_{r}-1\right) / 4 \pi$.

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\frac{k^{4} V^{2}}{(4 \pi)^{2}}\left(\varepsilon_{r}-1\right)^{2} \sin ^{2} \theta, \tag{8.53}
\end{equation*}
$$

i.e. follows the same $\sin ^{2} \theta$ law. The situation for extended objects, with at least one dimension of the order, or larger than the wavelength, is different: here we have to take into account that the phase shifts introduced by various parts of the body are different. Let us analyze this issue for an arbitrary collection of similar point scatterers located at points $\mathbf{r}_{j}$.

If wave vector of the incident plane wave is $\mathbf{k}_{0}$, the field the wave has the phase factor $\exp \left\{i \mathbf{k}_{0} \cdot \mathbf{r}\right\}$ - see Eq. (7.79). At the location of $j$-th scattering center, the factor equals to $\exp \left\{i \mathbf{k}_{0} \cdot \mathbf{r}_{j}\right\}$, so that the local polarization vector $\mathbf{p}$, and the scattered wave it creates, are proportional to this factor. On
its way to the observation point $\mathbf{r}$, the scattered wave, with wave vector $\mathbf{k}$ (with $k=k_{0}$ ), acquires an additional phase factor $\exp \left\{i \mathbf{k} \cdot\left(\mathbf{r}-\mathbf{r}_{j}\right)\right\}$, so that the scattered wave field is proportional to

$$
\begin{equation*}
\exp \left\{i \mathbf{k}_{0} \cdot \mathbf{r}_{j}+i \mathbf{k}\left(\mathbf{r}-\mathbf{r}_{j}\right)\right\}=\exp \left\{i\left(\mathbf{k}_{0}-\mathbf{k}\right) \cdot \mathbf{r}_{j}+i \mathbf{k} \cdot \mathbf{r}\right\}=e^{i \mathbf{k} \cdot \mathbf{r}} \exp \left\{-i\left(\mathbf{k}-\mathbf{k}_{0}\right) \cdot \mathbf{r}_{j}\right\} \tag{8.54}
\end{equation*}
$$

Since the first factor in the last expression does not depend on $\mathbf{r}_{j}$, in order to calculate the total scattering wave, it is sufficient to sum up the elementary phase factors $\exp \left\{-\mathrm{i} \mathbf{q} \cdot \mathbf{r}_{j}\right\}$, where vector

$$
\begin{equation*}
\mathbf{q} \equiv \mathbf{k}-\mathbf{k}_{0} \tag{8.55}
\end{equation*}
$$

has the physical sense of the wave vector change at scattering. ${ }^{19}$ It may look like the phase factor depends on the choice of origin. However, according to Eq. (7.42), the average intensity of the scattered wave is proportional to $E_{\omega} E_{\omega}{ }^{*}$, i.e. to the following real scalar function of vector $\mathbf{q}$ :

Scattering function

$$
\begin{equation*}
F(\mathbf{q})=\left(\sum_{j} \exp \left\{-i \mathbf{q} \cdot \mathbf{r}_{j}\right\}\right)\left(\sum_{j^{\prime}} \exp \left\{-i \mathbf{q} \cdot \mathbf{r}_{j^{\prime}}\right\}\right)^{*}=\sum_{j, j^{\prime}} \exp \left\{i \mathbf{q} \cdot\left(\mathbf{r}_{j}-\mathbf{r}_{j^{\prime}}\right)\right\} \equiv|I(\mathbf{q})|^{2} \tag{8.56}
\end{equation*}
$$

where the complex function

$$
\begin{equation*}
I(\mathbf{q}) \equiv \sum_{j} \exp \left\{-i \mathbf{q} \cdot \mathbf{r}_{j}\right\} \tag{8.57}
\end{equation*}
$$

is called the phase sum, may be calculated within any reference frame, without affecting the final result (56). The double-sum form of Eq. (56) is convenient to notice that for a system of many ( $N \gg 1$ ) of similar but randomly located scatterers, only the terms with $j=j$ ' accumulate at summation, so that $F(\mathbf{q})$ scales as $N$, rather than $N^{2}$ - thus justifying the above treatment of the Rayleigh scattering problem.

Let us start using Eq. (56) by applying it to the simplest problem of just two similar small scatterers, separated by a fixed distance $a$ :

$$
\begin{equation*}
F(\mathbf{q})=\sum_{j, j^{\prime}=1}^{2} \exp \left\{i \mathbf{q} \cdot\left(\mathbf{r}_{j}-\mathbf{r}_{j^{\prime}}\right)\right\}=2+\exp \left\{-i q_{a} a\right\}+\exp \left\{i q_{a} a\right\}=2\left(1+\cos q_{a} a\right)=4 \cos ^{2} \frac{q_{a} a}{2} \tag{8.58}
\end{equation*}
$$

where $q_{a} \equiv \mathbf{q} \cdot \mathbf{a} / a$ is the component of vector $\mathbf{q}$ along vector a connecting the scatterers. The apparent simplicity of this result may be a bit misleading, because the mutual plane of vectors $\mathbf{k}$ and $\mathbf{k}_{0}$ (and hence of vector $\mathbf{q}$ ) does not necessarily coincide with the mutual plane of vectors $\mathbf{k}_{0}$ and $\mathbf{E}_{\omega}$, so that the scattering angle $\alpha$ between vectors $\mathbf{k}$ and $\mathbf{k}_{0}$ is generally different from ( $\pi / 2-\theta$ ) - see Fig. 5.


Fig. 8.5. Angles important for the general scattering problem.

[^366]Moreover, vectors $\mathbf{q}$ and a may have another common plane, and angle between them is one more parameter that may be considered as independent from both $\alpha$ and $\theta$. As a result, the angular dependence of the scattered wave's intensity (and hence $d \sigma / d \Omega$ ), that depends on all three angles, may be rather complex.

This is why let me consider only the simple case when vectors $\mathbf{k}, \mathbf{k}_{0}$, and $\mathbf{a}$ are all in the same plane (Fig. 6a), with $\mathbf{k}_{0}$ perpendicular to a (leaving the general analysis for readers' exercise). Then, with our choice of coordinates, $q_{a}=q_{x}=k \sin \alpha$, and Eq. (58) is reduced to

$$
\begin{equation*}
F(\mathbf{q})=4 \cos ^{2} \frac{k a \sin \alpha}{2} \tag{8.59}
\end{equation*}
$$

This function always has two maxima, at $\alpha=0$ and $\alpha=\pi$, and possibly (if the product ka is large enough) other maxima at special angles $\alpha_{n}$ that satisfy the famous Bragg condition ${ }^{20}$

$$
\begin{equation*}
k a \sin \alpha_{n}=2 \pi n, \quad \text { i.e. } a \sin \alpha_{n}=n \lambda . \tag{8.60}
\end{equation*}
$$



Fig. 8.6. The simplest geometries for (a) interference and (b) diffraction.

As evident from Fig. 6a, this condition may be readily understood as the in-phase addition (frequently called the constructive interference) of two coherent waves scattered by the two points, when the difference between their paths toward the observer, $a \sin \alpha$, equals to an integer number of wavelengths. At each such maximum, $F=4$, due to the doubling of the wave amplitude and hence quadrupling its power.

If the distance between the point scatterers is large ( $k a \gg 1$ ), the first Bragg maxima correspond to small angles, $\alpha \ll 1$. For this region, Eq. (59) in reduced to a simple sinusoidal dependence of function $F$ on angle $\alpha$. Moreover, within the range of small $\alpha$, the polarization factor $\sin ^{2} \theta$ is virtually constant, so that the scattered wave intensity, and hence the differential cross-section

$$
\begin{equation*}
\frac{d \sigma}{d \Omega} \propto F(\mathbf{q})=4 \cos ^{2} \frac{k a \alpha}{2} \tag{8.61}
\end{equation*}
$$

Young's interference pattern

This is of course the well-known interference pattern, well known from the Young's two-slit experiment. ${ }^{21}$ (As will be discussed in the next section, theoretical description of the two-slit experiment

[^367]is more complex than that of the Born scattering, but is preferable experimentally, because at scattering, the wave of intensity (61) has to be observed on the backdrop of a stronger incident wave that propagates in almost the same direction, $\alpha=0$.)

The Bragg condition (60) does not change at scattering from $N>2$ similar, equidistant scatterers, located along the same straight line (because the condition is applicable to each pair of adjacent scatterers), but the interference pattern changes. Leaving the analysis of the case of arbitrary $N$ for reader's exercise, let me jump to the limit $N \rightarrow 0$, in which we may ignore the scatterer discreteness. The resulting pattern is similar to that at scattering by a continuous thin rod, so let us first discuss the Born scattering by an arbitrary distributed object - say an extended dielectric body with a constant value of $\varepsilon_{r}$. Transferring Eq. (56) from the sum to an integral, for the differential cross-section we get

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\frac{k^{4}}{(4 \pi)^{2}}\left(\varepsilon_{r}-1\right)^{2} F(\mathbf{q}) \sin ^{2} \theta=\frac{k^{4}}{(4 \pi)^{2}}\left(\varepsilon_{r}-1\right)^{2}|I(\mathbf{q})|^{2} \sin ^{2} \theta, \tag{8.62}
\end{equation*}
$$

where $I(\mathbf{q})$ now becomes the phase integral, ${ }^{22}$

> Phase integral

$$
\begin{equation*}
I(\mathbf{q})=\int_{V} \exp \left\{-i \mathbf{q} \cdot \mathbf{r}^{\prime}\right\} d^{3} r^{\prime} \tag{8.63}
\end{equation*}
$$

with the dimensionality of volume.
Now we may return to the particular case of a thin rod (with both dimensions of the crosssection's area much smaller than $\lambda$, but an arbitrary length $a$ ), otherwise keeping the same simple geometry as for two point scatterers - see Fig. 6b. In this case the phase integral is just

$$
\begin{equation*}
I(\mathbf{q})=A \int_{-a / 2}^{+a / 2} \exp \left\{-i q_{x} x^{\prime}\right) d x^{\prime}=A \frac{\exp \left\{-i q_{x} a / 2\right\}-\exp \left\{-i q_{x} a / 2\right\}}{-i q}=V \frac{\sin \xi}{\xi} \tag{8.64}
\end{equation*}
$$

where $V=A a$ is the volume of the rod, and $\xi$ is a dimensionless parameter defined as

$$
\begin{equation*}
\xi \equiv \frac{q_{x} a}{2}=\frac{k a \sin \alpha}{2} . \tag{8.65}
\end{equation*}
$$

The fraction participating in Eq. (64) is met in physics so frequently that is has deserved the special name sinc (not "sync", please!) function:

$$
\begin{equation*}
\operatorname{sinc} \xi \equiv \frac{\sin \xi}{\xi} \tag{8.66}
\end{equation*}
$$

Obviously, this function, plotted in Fig. 7, vanishes at all points $\xi_{n}=\pi n$, with integer $n$, besides point $n$ $=0: \operatorname{sinc} \xi_{0}=\operatorname{sinc} 0=1$.

[^368]

Fig. 8.7. Sinc function.

The function $F(\mathbf{q})=V^{2} \operatorname{sinc}^{2} \xi$, resulting from Eq. (64), is plotted by red line in Fig. 8, and is called the Fraunhofer diffraction pattern.


Fig. 8.8. The Fraunhofer diffraction pattern (solid red line) and its envelope $1 / \xi^{2}$ (dashed line). For comparison, the blue line shows the standard interference pattern $\cos ^{2} \xi$ - cf. Eq. (59).

Note that it oscillates with the same argument period $\Delta(k a \sin \alpha)=2 \pi / k a \ll 1$ as the interference pattern (59) from two point scatterers (shown with the blue line in Fig. 8). However, at the interference, the scattered wave intensity vanishes at angles $\alpha_{n}$ ' that satisfy condition

$$
\begin{equation*}
\frac{k a \sin \alpha_{n}^{\prime}}{2 \pi}=n+\frac{1}{2}, \tag{8.67}
\end{equation*}
$$

when the optical paths difference $a \sin \alpha$ equals to a semi-integer number of wavelengths $\lambda / 2=\pi / \mathrm{k}$, and hence the two waves from the scatterers arrive to the observer in anti-phase (the so-called destructive interference). On the other hand, for the diffraction from a continuous rod the minima occur at a different set of angles,

$$
\begin{equation*}
\frac{k a \sin \alpha_{n}}{2 \pi}=n \tag{8.68}
\end{equation*}
$$

i.e. exactly where the two-point interference pattern has its maxima. The reason for this relation is that the wave diffraction on the rod may be considered as a simultaneous interference of waves from all its fragments, and exactly at the observation angles when the rod edges give waves with phases shifted by $2 \pi n$, the interior point of the rod give waves with all possible phases, with their algebraic sum equal to
zero. Even more visibly in Fig. 8, at diffraction the intensity oscillations are limited by a rapidly decreasing envelope function $1 / \xi^{2}$. The reason for this fast decrease is that with each Fraunhofer diffraction period, a smaller and smaller fraction of the road gives an unbalanced contribution to the scattered wave.

If rod's length is small ( $k a \ll$ 1, i.e. $a \ll \lambda$ ), then sinc's argument $\xi$ is small at all scattering angles $\alpha$, so $I(\mathbf{q}) \approx V$, and Eq. (64) is reduced to Eq. (53). In the opposite limit, $a \gg \lambda$, the first zeros of function $I(\mathbf{q})$ correspond to very small angles $\alpha$, for which $\sin \theta \approx 1$, so that the differential crosssection is

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\frac{k^{4} V^{2}}{(4 \pi)^{2}}\left(\varepsilon_{r}-1\right)^{2} \operatorname{sinc}^{2} \frac{k a \alpha}{2}, \tag{8.69}
\end{equation*}
$$

i.e. Fig. 8 shows the scattering intensity as a function of the diffraction direction - if the pattern is observed within the plane containing the rod.

### 8.5. The Huygens principle

The Born approximation allows tracing the basic features of (and the difference between) the phenomena of interference and diffraction. Unfortunately, this approximation, based on the relative weakness of the scattered wave, cannot be used for more popular experimental implementations of these phenomena, for example, the Young's two-slit experiment, or diffraction on a single slit or orifice - see, e.g. Fig. 9. Indeed, at such experiments, the orifice size $a$ is typically much larger than light's wavelength, and as a result, no clear decomposition of the fields to the incident and "scattered" waves is possible.


Fig. 8.9. Typical geometry for the Huygens principle application.

However, for such experiments, another approximation, called the Huygens (or "HuygensFresnel") principle, ${ }^{23}$ is very instrumental: the passed wave may be presented as a linear superposition of spherical waves of the type (17), as if they were emitted by every point of the orifice (or more physically, by every point of the incident wave's front that has arrived at the orifice). This approximation is valid if the following strong conditions are satisfied:

[^369]\[

$$
\begin{equation*}
\lambda \ll a \ll r \tag{8.70}
\end{equation*}
$$

\]

where $r$ is the distance of the observation point from the orifice. In addition, as we have seen in the last section, at small $\lambda / a$ the diffraction phenomena are confined to angles $\alpha \sim 1 / k a \sim \lambda / a \ll 1$. For observation at such small angles, the mathematical expression of the Huygens principle, for a complex amplitude $f_{\omega}(\mathbf{r})$ of a monochromatic wave $f(\mathbf{r}, t)=\operatorname{Re}\left[f_{\omega} e^{-i \omega t}\right]$, is given by the following simple formula

$$
\begin{equation*}
f_{\omega}(\mathbf{r})=C \int_{\text {orifice }} f_{\omega}\left(\mathbf{r}^{\prime}\right) \frac{e^{i k R}}{R} d^{2} r^{\prime} \tag{8.71}
\end{equation*}
$$

Here $f$ is any transverse component of any of wave's fields (either $\mathbf{E}$ or $\mathbf{H}$ ), ${ }^{24} R$ is the distance between point $\mathbf{r}^{\prime}$ at the orifice and the observation point $\mathbf{r}$ (i.e. the magnitude of vector $\mathbf{R} \equiv \mathbf{r}-\mathbf{r}$ '), and $C$ is a complex constant.

Before describing the proof of Eq. (71), let me carry out its sanity check - which also will give us the constant $C$. Let us see what happens if the field under the integral is the usual plane wave $f_{\omega}(z)$ propagating along axis $z$ (i.e. there is no opaque screen at all), so we should take the whole $x-y$ plane, say with $z^{\prime}=0$, as the integration area (Fig. 10).


Fig. 8.10. The Huygens principle applied to a plane wave.

Then, for the observation point with coordinates $x=0, y=0$, and $z \gg \lambda$, Eq. (71) yields

$$
\begin{equation*}
f_{\omega}(z)=C f_{\omega}(0) \int d x^{\prime} \int d y^{\prime} \frac{\exp \left\{i k\left(x^{\prime 2}+y^{\prime 2}+z^{2}\right)^{1 / 2}\right\}}{\left(x^{\prime 2}+y^{\prime 2}+z^{2}\right)^{1 / 2}} \tag{8.72}
\end{equation*}
$$

Before specifying the integration limits, let us consider the range $\left|x^{\prime}\right|,\left|y^{\prime}\right| \ll z$. In this range the square root, met in Eq. (72) twice, may be approximated as

$$
\begin{equation*}
\left(x^{\prime 2}+y^{\prime 2}+z^{2}\right)^{1 / 2}=z\left(1+\frac{x^{\prime 2}+y^{\prime 2}}{z^{2}}\right)^{1 / 2} \approx z\left(1+\frac{x^{\prime 2}+y^{\prime 2}}{2 z}\right)=z+\frac{x^{\prime 2}+y^{\prime 2}}{2 z} \tag{8.73}
\end{equation*}
$$

The denominator of Eq. (72) is a much slower function of $x^{\prime}$ and $y^{\prime}$ than the exponent, and in it (as we will check a posteriori), it is sufficient to keep just the main, first term of expansion (73). With that, Eq. (72) becomes

[^370]\[

$$
\begin{equation*}
f_{\omega}(z)=C f_{\omega}(0) \frac{e^{i k z}}{z} \int d x^{\prime} \int d y^{\prime} \exp \frac{i k\left(x^{\prime 2}+y^{\prime 2}\right)}{2 z}=C f_{\omega}(0) \frac{e^{i k z}}{z} I_{x} I_{y} \tag{8.74}
\end{equation*}
$$

\]

where $I_{x}$ and $I_{y}$ are two similar integrals; for example,

$$
\begin{equation*}
I_{x}=\int \exp \frac{i k x^{\prime 2}}{2 z} d x^{\prime}=\left(\frac{2 z}{k}\right)^{1 / 2} \int \exp \left\{i \xi^{2}\right\} d \xi=\left(\frac{2 z}{k}\right)^{1 / 2}\left[\int \cos \left(\xi^{2}\right) d \xi+i \int \sin \left(\xi^{2}\right) d \xi\right] \tag{8.75}
\end{equation*}
$$

where $\xi \equiv(k / 2 z)^{1 / 2} x^{\prime}$. These are the so-called Fresnel integrals. I will discuss them in more detail in the next section, and right now, only one property of these integrals is important for us: if taken in symmetric limits $\left[-\xi_{0},+\xi_{0}\right]$, both of them rapidly converge to the same value, $(\pi / 2)^{1 / 2}$, as soon as $\xi_{0}$ becomes much larger than 1.25 This means that even if we do not impose any exact limits on the integration area in Eq. (72), this integral converges to value

$$
\begin{equation*}
f_{\omega}(z)=C f_{\omega}(0) \frac{e^{i k z}}{z}\left\{\left(\frac{2 z}{k}\right)^{1 / 2}\left[\left(\frac{\pi}{2}\right)^{1 / 2}+i\left(\frac{\pi}{2}\right)^{1 / 2}\right]\right\}^{2}=\left(C \frac{2 \pi i}{k}\right) f_{\omega}(0) e^{i k z} \tag{8.76}
\end{equation*}
$$

due to contributions from the central area with linear size of the order of $\Delta \xi \sim 1$, i.e.

$$
\begin{equation*}
\Delta x \sim \Delta y \sim\left(\frac{z}{k}\right)^{1 / 2} \sim(\lambda z)^{1 / 2} \tag{8.77}
\end{equation*}
$$

so that the contribution by front points $\mathbf{r}$ ' well beyond the range (77) is negligible. ${ }^{26}$ (Within our assumptions (70), which in particular require $\lambda$ to be much less than $z$, the diffraction angle $\Delta x / z \sim \Delta y / z$ $\sim(\lambda / z)^{1 / 2}$, corresponding to the important area of the front, is small.) In order to sustain the plane wave propagation, $f_{\omega}(\mathrm{z})=f_{\omega}(0) e^{i k z}$, constant $C$ in Eq. (76) has to be taken equal to $k / 2 \pi i$. Thus, the Huygens principle's prediction (71), in its final form, reads

Huygens principle's expression

$$
\begin{equation*}
f_{\omega}(\mathbf{r})=\frac{k}{2 \pi i} \int_{\text {orifice }} f_{\omega}\left(\mathbf{r}^{\prime}\right) \frac{e^{i k R}}{R} d^{2} r^{\prime} \tag{8.78}
\end{equation*}
$$

and describes, in particular, the straight propagation of the plane wave (in a uniform media).
Let me pause to emphasize how nontrivial this result is. It would be a natural corollary of Eq. (25) (and the linear superposition principle) if all points of the orifice were filled with point scatterers that re-emit all the incident waves into spherical waves. However, as it follows from the above proof, the Huygens principle is also valid if there is nothing in the orifice but the free space!

This is why it is important a proof of the principle, ${ }^{27}$ based on the Green's theorem (2.207). Let us apply this theorem to function $f=f_{\omega}$, where $f_{\omega}$ is the complex amplitude of a scalar component of one of wave's fields, which satisfies the Helmholtz equation (7.192),

[^371]\[

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) f_{\omega}(\mathbf{r})=0 \tag{8.79}
\end{equation*}
$$

\]

and function $g=g_{\omega}$, which is the time Fourier image of the corresponding Green's function. It may be defined, as usual, as the solution to the same equation with the added delta-functional right-hand part with an arbitrary coefficient, for example,

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=-4 \pi \delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \tag{8.80}
\end{equation*}
$$

With Eqs. (79) and (80) used to express the Laplace operators of functions $f_{\omega}$ and $g_{\omega}$, Eq. (2.207) becomes

$$
\begin{equation*}
\int_{V}\left\{f_{\omega}\left[-k^{2} g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)-4 \pi \delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right)\right]-g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)\left[-k^{2} f_{\omega}\right]\right\} d^{3} r=\oint_{S}\left[f_{\omega} \frac{\partial g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)}{\partial n}-g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \frac{\partial f_{\omega}}{\partial n}\right] d^{2} r, \tag{8.81}
\end{equation*}
$$

where $\mathbf{n}$ is the outward normal to the surface $S$ limiting volume $V$. Two terms in the left-hand side of this relation cancel, so that after swapping $\mathbf{r}$ and $\mathbf{r}$ ' we get

$$
\begin{equation*}
-4 \pi f_{\omega}(\mathbf{r})=\oint_{S}\left[f_{\omega}\left(\mathbf{r}^{\prime}\right) \frac{\partial g_{\omega}\left(\mathbf{r}^{\prime}, \mathbf{r}\right)}{\partial n^{\prime}}-g_{\omega}\left(\mathbf{r}^{\prime}, \mathbf{r}\right) \frac{\partial f_{\omega}\left(\mathbf{r}^{\prime}\right)}{\partial n^{\prime}}\right] d^{2} r^{\prime} . \tag{8.82}
\end{equation*}
$$

This relation is only correct if the selected volume $V$ includes point $\mathbf{r}$ (otherwise we would not get its left-hand part from the integration of the delta-function), but does not include the genuine source of the wave (otherwise Eq. (79) would have a nonvanishing right-hand part). Let $\mathbf{r}$ be the field observation point, $V$ all the source-free half-space (for example, the half-space right of the screen in Fig. 9), so that $S$ is the surface of the screen, including the orifice. Then the right-hand part of Eq. (82) describes the field in the observation point $\mathbf{r}$ induced by the wave passing through the orifice points $\mathbf{r}$ '. Since no waves are emitted by the opaque parts of the screen, we can limit the integration by the orifice area. ${ }^{28}$ Assuming also that the opaque parts of the screen do not re-emit waves "radiated" by the orifice, we can take the solution of Eq. (80) to be the retarded potential for the free space: ${ }^{29}$

$$
\begin{equation*}
g_{\omega}\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=\frac{e^{i k R}}{R} \tag{8.83}
\end{equation*}
$$

Plugging this expression into Eq. (82), we get

$$
\begin{equation*}
-4 \pi f_{\omega}(\mathbf{r})=\oint_{\text {orifice }}\left[f_{\omega}\left(\mathbf{r}^{\prime}\right) \frac{\partial}{\partial n^{\prime}}\left(\frac{e^{i k R}}{R}\right)-\left(\frac{e^{i k R}}{R}\right) \frac{\partial f_{\omega}\left(\mathbf{r}^{\prime}\right)}{\partial n^{\prime}}\right] d^{2} r^{\prime} \tag{8.84}
\end{equation*}
$$

This is the so-called Kirchhoff (or "Fresnel-Kirchhoff") integral. ${ }^{30}$ Now, let us make the two additional approximations. The first of them stems from Eq. (70): at $k a \gg 1$, the wave's spatial dependence in the orifice area may be presented as

[^372]\[

$$
\begin{equation*}
f_{\omega}\left(\mathbf{r}^{\prime}\right)=\left(\text { a slow function of } \mathbf{r}^{\prime}\right) \times \exp \left\{i \mathbf{k}_{0} \cdot \mathbf{r}^{\prime}\right\} \tag{8.85}
\end{equation*}
$$

\]

where "slow" means a function that changes on the scale of $a$ rather than $\lambda$. If, also, $k R \gg 1$, then the differentiation in Eq. (84) may be, in both instances, limited to the rapidly changing exponents, giving

$$
\begin{equation*}
-4 \pi f_{\omega}(\mathbf{r})=\oint_{A} i\left(\mathbf{k}+\mathbf{k}_{\mathbf{0}}\right) \cdot \mathbf{n}^{\prime} \frac{e^{i k R}}{R} f\left(\mathbf{r}^{\prime}\right) d^{2} r^{\prime}, \tag{8.86}
\end{equation*}
$$

Second, if all observation angles are small, we can take $\mathbf{k} \cdot \mathbf{n}^{\prime} \approx \mathbf{k}_{0} \cdot \mathbf{n}^{\prime} \approx-k$. With that, Eq. (86) is reduced to Eq. (78) expressing the Huygens principle.

It is clear that the principle immediately gives a very simple description of the interference of waves passing through two small holes in the screen. Indeed, if the hole size is negligible in comparison with distance $a$ between them (though still much larger than the wavelength!), Eq. (78) yields

$$
\begin{equation*}
f_{\omega}(\mathbf{r})=c_{1} e^{i k R_{1}}+c_{2} e^{i k R_{2}}, \quad \text { with } c_{1,2} \equiv \frac{k f_{1,2} A_{1,2}}{2 \pi i R_{1,2}} \tag{8.87}
\end{equation*}
$$

where $R_{1,2}$ are the distances between the holes and the observation point, and $A_{1,2}$ are the hole areas. For the interference wave intensity, Eq. (87) yields

$$
\begin{equation*}
\bar{S} \propto f_{\omega} f_{\omega}^{*}=\left|c_{1}\right|^{2}+\left|c_{2}\right|^{2}+2\left|c_{1}\right|\left|c_{2}\right| \cos \left[k\left(R_{1}-R_{2}\right)+\varphi\right], \quad \varphi \equiv \arg c_{1}-\arg c_{2} . \tag{8.88}
\end{equation*}
$$

The first two terms in this result clearly represent the intensities of partial waves passed through each hole, while the last one the result of their interference. The interference pattern's contrast ratio

$$
\begin{equation*}
R \equiv \frac{\bar{S}_{\max }}{\bar{S}_{\min }}=\left(\frac{\left|c_{1}\right|+\left|c_{2}\right|}{\left|c_{1}\right|-\left|c_{2}\right|}\right)^{2} \tag{8.89}
\end{equation*}
$$

is largest (infinite) when both waves have equal amplitudes.
The analysis of the interference pattern is simple if the line connecting the holes is perpendicular to wave vector $\mathbf{k} \approx \mathbf{k}_{0}-$ see Fig. 6a. Selecting the coordinate axes as shown in that figure, and using for distances $R_{1,2}$ the same expansion as in Eq. (73), for the interference term in Eq. (88) we get

$$
\begin{equation*}
\cos \left[k\left(R_{1}-R_{2}\right)+\varphi\right] \approx \cos \left(\frac{k x a}{z}+\varphi\right) . \tag{8.90}
\end{equation*}
$$

This means that the intensity does not depend on $y$, i.e. the interference pattern in the plane of constant $z$ presents straight, parallel strips, perpendicular to vector a, with the period given by Eq. (60), i.e. by the Bragg law. ${ }^{31}$ Note that this (somewhat counter-intuitive) result is strictly valid only at ( $x^{2}+y^{2}$ ) << z ${ }^{2}$; it is straightforward to use the next term in the Taylor expansion (73) to show that farther from the interference pattern center the strips start to diverge.

[^373]
### 8.6. Diffraction on a slit

Now let us use the Huygens principle to analyze a more complex problem: plane wave's diffraction on a long straight slit of constant width $a$ (Fig. 11).


Fig. 8.11. Diffraction on a slit.

According to Eq. (70), in order to use the Huygens principle for the problem analysis we need to have $\lambda \ll a \ll z$. Moreover, the simple formulation (78) of the principle is only valid for small observation angles, $|x| \ll z$. Note, however, that the relation between two small dimensionless numbers, $z / a$ and $a / \lambda$ is so far arbitrary; as we will see in a minute, this relation will determine the type of the observed diffraction pattern.

Let us apply Eq. (78) to our current problem (Fig. 11), for the sake of simplicity assuming the normal wave incidence, and taking $z=0$ at the screen plane:

$$
\begin{equation*}
f_{\omega}(x, z)=f_{0} \frac{k}{2 \pi i} \int_{-a}^{+a} d x^{\prime} \int_{-\infty}^{+\infty} d y^{\prime} \frac{\exp \left\{i k\left[\left(x-x^{\prime}\right)^{2}+y^{\prime 2}+z^{2}\right]^{1 / 2}\right\}}{\left[\left(x-x^{\prime}\right)^{2}+y^{\prime 2}+z^{2}\right]^{1 / 2}}, \tag{8.91}
\end{equation*}
$$

where $f_{0} \equiv f_{\omega}(x, 0)=$ const is the incident wave's amplitude. This is the same integral as in Eq. (72), except for the finite limits for $x^{\prime}$, and may be simplified similarly, using the small-angle condition ( $x-$ $\left.x^{\prime}\right)^{2}+y^{\prime 2} \ll z^{2}$ :

$$
\begin{equation*}
f(x, z) \approx f_{0} \frac{k}{2 \pi i} \frac{e^{i k z}}{z} \int_{-a / 2}^{+a / 2} d x^{\prime} \int_{-\infty}^{+\infty} d y^{\prime} \exp \frac{i k\left[\left(x-x^{\prime}\right)^{2}+y^{\prime 2}\right]}{2 z}=f_{0} \frac{k}{2 \pi i} \frac{e^{i k z}}{z} I_{x} I_{y} . \tag{8.92}
\end{equation*}
$$

The integral over $y$ is the same as in the last section:

$$
\begin{equation*}
I_{y} \equiv \int_{-\infty}^{+\infty} \exp \frac{i k y^{\prime 2}}{2 z} d y^{\prime}=\left(\frac{2 \pi i z}{k}\right)^{1 / 2} \tag{8.93}
\end{equation*}
$$

but the integral over $x$ is more complicated, because of its finite limits:

$$
\begin{equation*}
I_{x} \equiv \int_{-a / 2}^{+a / 2} \exp \frac{i k\left(x-x^{\prime}\right)^{2}}{2 z} d x^{\prime} \tag{8.94}
\end{equation*}
$$

It may be simplified in the following two (opposite) limits.
(i) Fraunhofer diffraction takes place when $z / a \gg a / \lambda$ - the relation which may be rewritten either as $a \ll(z \lambda)^{1 / 2}$, or as $k a^{2} \ll z$. In this limit the ratio $k x^{, 2} / z$ is negligibly small for all values of $x^{\prime}$ under the integral, and we can approximate it as

$$
\begin{align*}
I_{x} & =\int_{-a / 2}^{+a / 2} \exp \frac{i k\left(x^{2}-2 x x^{\prime}+x^{\prime 2}\right)}{2 z} d x^{\prime} \approx \int_{-a / 2}^{+a / 2} \exp \frac{i k\left(x^{2}-2 x x^{\prime}\right)}{2 z} d x^{\prime}  \tag{8.95}\\
& =\exp \frac{i k x^{2}}{2 z} \int_{-a / 2}^{+a / 2} \exp \left\{-\frac{i k x x^{\prime}}{z}\right\} d x^{\prime}=\frac{2 z}{k x} \exp \left\{\frac{i k x^{2}}{2 z}\right\} \sin \frac{k x a}{2 z},
\end{align*}
$$

so that Eq. (92) yields

$$
\begin{equation*}
f_{\omega}(x, z) \approx f_{0} \frac{k}{2 \pi i} \frac{e^{i k z}}{z} \frac{2 z}{k x}\left(\frac{2 \pi i z}{k}\right)^{1 / 2} \exp \left\{\frac{i k x^{2}}{2 z}\right\} \sin \frac{k x a}{2 z}, \tag{8.96}
\end{equation*}
$$

and hence the relative wave intensity is

Fraunhofer diffraction pattern

$$
\begin{equation*}
\frac{\bar{S}(x, z)}{S_{0}}=\left|\frac{f_{\omega}(x, z)}{f_{0}}\right|^{2}=\frac{8 z}{\pi k x^{2}} \sin ^{2} \frac{k x a}{2 z}=\frac{2}{\pi} \frac{k a^{2}}{z} \operatorname{sinc}^{2}\left(\frac{k a \alpha}{2}\right), \tag{8.97}
\end{equation*}
$$

where $S_{0}$ is the (average) intensity of the incident wave, and $\alpha \equiv x / z \ll 1$ is the scattering angle. Comparing this expression with Eq. (69), we see that this the diffraction pattern is exactly the same as that of a similar (uniform, 1D) object in the Born approximation - see the red line in Fig. 8. Note again that the angular width $\delta \alpha$ of the Fraunhofer pattern is of the order of $1 / k a$, so that its linear width $\delta x=$ $z \delta \alpha \sim z / k a \sim z \lambda / a .{ }^{32}$ Hence the condition of the Fraunhofer approximation validity may be also presented as $a \ll \delta x$.
(ii) Fresnel diffraction. In the opposite limit of a relatively wide slit, with $a \gg \delta x=z \delta \alpha \sim z / k a \sim$ $z \lambda / a$, i.e. $k a^{2} \gg z$, the diffraction patterns at two slit edges are well separated. Hence, near each edge (for example, near $x^{\prime}=-a / 2$ ) we may simplify Eq. (94) as

$$
\begin{equation*}
I_{x}(x) \approx \int_{-a / 2}^{+\infty} \exp \frac{i k\left(x-x^{\prime}\right)^{2}}{2 z} d x^{\prime}=\left(\frac{2 z}{k}\right)^{1 / 2} \int_{(k / 2 z)^{1 / 2}(x+a / 2)}^{+\infty} \exp \left\{i \zeta^{2}\right\} d \zeta \tag{8.98}
\end{equation*}
$$

and express it via the special functions called the Fresnel integrals: ${ }^{33}$

Fresnel
integrals

$$
\begin{equation*}
\ell(\xi) \equiv\left(\frac{2}{\pi}\right)^{1 / 2} \int_{0}^{\xi} \cos \left(\zeta^{2}\right) d \zeta, \quad S(\xi) \equiv\left(\frac{2}{\pi}\right)^{1 / 2} \int_{0}^{\xi} \sin \left(\zeta^{2}\right) d \zeta, \tag{8.99}
\end{equation*}
$$

whose plots are shown in Fig. 12. As was mentioned above, at large values of their argument ( $\xi$ ), both functions tend to $1 / 2$.

[^374]

Fig. 8. 12. Fresnel integrals.

Plugging this expression into Eq. (92) and (98), for the diffracted wave intensity, in the Fresnel limit (i.e. at $|x+a / 2| \ll a$ ), we get

$$
\begin{equation*}
\frac{\bar{S}(x, z)}{S_{0}}=\frac{1}{2}\left\{\left[C\left(\left(\frac{k}{2 z}\right)^{1 / 2}\left(x+\frac{a}{2}\right)\right)+\frac{1}{2}\right]^{2}+\left[S\left(\left(\frac{k}{2 z}\right)^{1 / 2}\left(x+\frac{a}{2}\right)\right)+\frac{1}{2}\right]^{2}\right\} \tag{8.100}
\end{equation*}
$$

A plot of this function (Fig. 13) shows that the diffraction pattern is very peculiar: while in the "shade" region $x<-a / 2$ the wave intensity fades monotonically, the transition to the "light" region within the gap ( $x>-a / 2$ ) is accompanied by intensity oscillations, just as at the Fraunhofer diffraction - cf. Fig. 8.


Fig. 8.13. Fresnel diffraction pattern.

This behavior, which is described by the following asymptotes,

$$
\frac{\bar{S}}{S_{0}} \rightarrow\left\{\begin{array}{cc}
1+\frac{1}{\sqrt{\pi}} \frac{\sin \left(\xi^{2}-\pi / 4\right)}{\xi}, & \text { for } \xi \equiv\left(\frac{k}{2 z}\right)^{1 / 2}\left(x+\frac{a}{2}\right) \rightarrow+\infty  \tag{8.101}\\
\frac{1}{4 \pi \xi^{2}}, & \text { for } \xi \rightarrow-\infty
\end{array}\right.
$$

is essentially an artifact of observing just the wave intensity (i.e. its real amplitude) rather than its phase as well. Indeed, as may be seen even more clearly from the parametric presentation of the Fresnel
integrals (Fig. 14), these functions oscillate similarly at large positive and negative values of their argument. Physically, this means that the wave diffraction by the slit edge leads to similar oscillations of its phase at $x<-a / 2$ and $x>-a / 2$; however, in the latter region (i.e. inside the slit) the diffracted wave overlaps the incident wave passing through the slit directly, and their interference reveals the phase oscillations, making them visible in the measured intensity as well.


Fig. 8.14. Parametric representation of the Fresnel integrals. This pattern is called either the Euler spiral or Cornu spiral.

Note that according to Eq. (100), the linear scale of the Fresnel diffraction pattern is $(2 z / k)^{1 / 2}$, i.e. is complied with estimate (77). If the slit is gradually narrowed, so that width $a$ becomes comparable to that scale, ${ }^{34}$ the Fresnel interference patterns from both edges start to "collide" (interfere). The resulting wave, fully described by Eq. (94), is just a sum of two contributions of the type (98) from the both edges of the slit. The resulting interference pattern is somewhat complicated, and only $a \ll \delta x$ it is reduced to the simple Fraunhofer pattern (97). Of course, this crossover from the Fresnel to Fraunhofer diffraction may be also observed, at fixed wavelength $\lambda$ and slit width $a$, by increasing $z$, i.e. by measuring the diffraction pattern farther and farther from the slit.

Note that the Fraunhofer limit is always valid if the diffraction measured as a function of the diffraction angle $\alpha$ alone, i.e. effectively at infinity, $z \rightarrow \infty$. This may be done, for example, by collecting the diffracted wave with a "positive" (converging) lense, and observing the diffraction pattern in its focal plane.

### 8.7. Geometrical optics placeholder

Behind all these details, I would not like the reader to miss the main feature of diffraction, that has an overwhelming practical significance. Namely, besides narrow diffraction "cones" (actually, parabolic-shaped regions) with lateral scale $\Delta x \sim(\lambda z)^{1 / 2}$, the wave far behind a slit of width $a \gg \lambda$ repeats the field just behind the slit, i.e. reproduces the unperturbed incident wave inside the slit, and has negligible intensity in the shade regions outside it. An evident generalization of this fact is that when a plane wave (in particular an electromagnetic wave) passes any opaque object of large size $a \gg \lambda$, it propagates around it, by distances $z$ up to $\sim a^{2} / \lambda$, along straight lines, with virtually negligible diffraction

[^375]effects. This fact gives the strict foundation for the very notion of the wave ray (or beam), as the line perpendicular to the local front of a quasi-plane wave. In a uniform media such ray is a straight line, but changes in accordance with the Snell law at the interface of two media with different wave speed $v$, i.e. different values of the refraction index. The notion of rays enables the whole field of geometric optics, devoted mostly to ray tracing in various (sometimes very complex) systems.

This is why, at this point, an E\&M course that followed the scientific logic more faithfully than this one, would give an extended discussion of the geometric and quasi-geometric optics, including (as a minimum ${ }^{35}$ ) such vital topics as

- the so-called lensmaker's equation expressing the focus length $f$ of a lens via the curvature radii of its spherical surfaces and the refraction index of the lens material,
- the thin lens formula relating the image distance from the lens via $f$ and the source distance,
- the concepts of basic optical instruments such as telescopes and microscopes,
- the concepts of the spherical, angular, and chromatic aberrations (image distortions);
- wave effects in optical instruments, including the so-called Abbe limit ${ }^{36}$ on the focal spot size. ${ }^{37}$

However, since I have made a (possibly, wrong) decision to follow the common tradition in selecting the main topics for this course, I do not have time left for such discussion. Still, I am placing this "placeholder" pseudo-section to relay my conviction that any educated physicist has to know the geometric optics basics. If the reader has not had an exposure to this subject during his or her undergraduate studies, I highly recommend at least browsing one of available textbooks. ${ }^{38}$

### 8.8. Fraunhofer diffraction from more complex scatterers

So far, our discussion of diffraction has been limited to a very simple geometry - a single slit in an otherwise opaque screen (Fig. 11). However, in the most important Fraunhofer limit, $z \gg k a^{2}$, it is easy to get a very simple expression for the plane wave diffraction/interference by a plane orifice (with linear size $\sim a$ ) of an arbitrary shape. Indeed, the evident 2D generalization of approximation (93)-(94) is

$$
\begin{align*}
I_{x} I_{y} & =\int_{\text {orifice }} \exp \frac{i k\left[\left(x-x^{\prime}\right)^{2}+\left(y-y^{\prime}\right)^{2}\right]}{2 z} d x^{\prime} d y^{\prime} \\
& \approx \exp \left\{\frac{i k\left(x^{2}+y^{2}\right)}{2 z}\right\} \int_{\text {orifice }} \exp \left\{-i \frac{k x x^{\prime}}{z}-i \frac{k y y^{\prime}}{z}\right\} d x^{\prime} d y^{\prime} \tag{8.102}
\end{align*}
$$

${ }^{35}$ Admittedly, even this list leaves aside several spectacular effects due to crystal anisotropy, including such a beauty as conical refraction in biaxial crystals - see, e.g., Chapter 15 of the classical textbook by M. Born and E. Wolf, cited in the end of Sec. 7.1.
${ }^{36}$ Reportedly, due to not only E. Abbe (1873), but also to H. von Helmholtz (1874).
${ }^{37}$ In contrast to other topics of this list, whose study may be based on the ray approach, i.e. on purely geometric optics, the description of these effects requires at least an approximate account of wave properties of light. Such account may be based either on the Huygens principle or on the so-called paraxial equation

$$
\partial a / \partial z=(1 / 2 i k) \nabla_{x, y}^{2} a,
$$

for the complex amplitude $a(\mathbf{r})$ of the field represented in the form $f(\mathbf{r})=a(\mathbf{r}) e^{i k z}$. The paraxial approximation follows from the Helmholtz equation (7.192) in essentially the same limit $(|\nabla a| \ll k ;|x|,|y| \ll z)$ as Eq. (78).
${ }^{38}$ My top recommendation for that purpose would be Chapters 3-6 and Sec. 8.6 in Born and Wolf. A simpler alternative is Chapter 10 in G. R. Fowles, Introduction to Modern Optics, $2^{\text {nd }}$ ed., Dover, 1989.
so that besides the inconsequential total phase factor, Eq. (92) is reduced to

$$
\begin{equation*}
f(\boldsymbol{\rho}) \propto f_{0} \int_{\text {orifice }} \exp \left\{-\mathbf{i} \mathbf{\kappa} \cdot \boldsymbol{\rho}^{\prime}\right\} d^{2} \rho^{\prime}=f_{0} \int_{\text {screen }} T\left(\boldsymbol{\rho}^{\prime}\right) \exp \left\{-\mathbf{i} \mathbf{\kappa} \cdot \boldsymbol{\rho}^{\prime}\right\} d^{2} \rho^{\prime} \tag{8.103}
\end{equation*}
$$

where the 2 D vector $\kappa$ (not to be confused with wave vector $\mathbf{k}$ that is virtually perpendicular to $\kappa!$ ) is defined as

$$
\begin{equation*}
\boldsymbol{\kappa} \equiv k \frac{\mathbf{\rho}}{Z} \approx \mathbf{q} \equiv \mathbf{k}-\mathbf{k}_{0}, \tag{8.104}
\end{equation*}
$$

$\rho=\{x, y\}$ and $\rho^{\prime}=\left\{x^{\prime}, y^{\prime}\right\}$ are 2D radius-vectors in, respectively, the observation and screen planes (both nearly normal to vectors $\mathbf{k}$ and $\mathbf{k}_{0}$ ), function $T\left(\rho^{\prime}\right)$ describes screen's transparency at point $\rho^{\prime}$, and the last integral in Eq. (103) is over the whole screen plane $z^{\prime}=0$. (Though the strict equivalence of the two forms of Eq. (103) is only valid if $T\left(\rho^{\prime}\right)$ equals to either 1 or 0 , its last form may be readily obtained from Eq. (78) with $f\left(\mathbf{r}^{\prime}\right)=T\left(\rho^{\prime}\right) f_{0}$ for any transparency profile, provided that $T\left(\rho^{\prime}\right)$ is an arbitrary function but changes only at distances much larger than $\lambda \equiv 2 \pi / k$.)

From the mathematical point of view, the last form of Eq. (103) is the 2D spatial Fourier transform of function $T\left(\rho^{\prime}\right)$, with the reciprocal variable $\kappa$ revealed by the observation point position: $\rho$ $=(z / k) \kappa=(z \lambda / 2 \pi) \kappa$. This interpretation is useful because of the experience we all have with the Fourier transform, mostly in the context of its time/frequency applications. For example, if the orifice is a single small hole, $T(\rho$ ') may be approximated by a delta-function, so that Eq. (103) yields $f(\rho) \approx$ const. This corresponds (at least for the small diffraction angles $\alpha \equiv \rho / z$, for which the Huygens approximation is valid) to a spherical wave spreading from the point-like orifice. Next, for two small holes, Eq. (103) immediately gives the Young interference pattern (90). Let me now use Eq. (103) to analyze the simplest (and most important) 1D transparency profiles, leaving 2D cases for reader's exercise.
(i) A single slit of width $a$ (Fig. 11) may be described by transparency

$$
T\left(\boldsymbol{\rho}^{\prime}\right)=\left\{\begin{array}{lr}
1, & \text { for }\left|x^{\prime}\right|<a / 2  \tag{8.105}\\
0, & \text { otherwise }
\end{array}\right.
$$

Its substitution into Eq. (103) yields

$$
\begin{equation*}
f(\boldsymbol{\rho}) \propto f_{0} \int_{-a / 2}^{+a / 2} \exp \left\{-i \kappa_{x} x^{\prime}\right\} d x^{\prime}=f_{0} \frac{\exp \left\{-i \kappa_{x} a / 2\right\}-\exp \left\{i \kappa_{x} a / 2\right\}}{-i \kappa_{x}} \propto \operatorname{sinc}\left(\frac{\kappa_{x} a}{2}\right)=\operatorname{sinc}\left(\frac{k x a}{2 z}\right), \tag{8.106}
\end{equation*}
$$

naturally returning us to Eqs. (64) and (97), and hence to the red lines in Fig. 8 for the wave intensity. (Please note again that Eq. (103) describes only the Fraunhofer, but not the Fresnel diffraction!)
(ii) Two narrow similar, parallel slits with a much larger distance $a$ between them, may be described by taking

$$
\begin{equation*}
T\left(\boldsymbol{\rho}^{\prime}\right) \propto \delta\left(x^{\prime}-a / 2\right)+\delta\left(x^{\prime}+a / 2\right) \tag{8.107}
\end{equation*}
$$

so that Eq. (103) yields the generic interference pattern,

$$
\begin{equation*}
f(\boldsymbol{\rho}) \propto f_{0}\left[\exp \left\{-\frac{i \kappa_{x} a}{2}\right\}+\exp \left\{\frac{i \kappa_{x} a}{2}\right\}\right] \propto \cos \frac{\kappa_{x} a}{2}=\cos \frac{k x a}{2 z}, \tag{8.108}
\end{equation*}
$$

whose intensity is shown with the blue line in Fig. 8.
(iii) In a more realistic Young-type two-slit experiment, each slit has width (say, w) which is much larger than light wavelength $\lambda$, but still much smaller than slit spacing $a$. This situation may be described by the following transparency function

$$
T\left(\boldsymbol{\rho}^{\prime}\right)=\sum_{ \pm}\left\{\begin{array}{lr}
1, & \text { for }\left|x^{\prime} \pm a / 2\right|<w / 2  \tag{8.109}\\
0, & \text { otherwise },
\end{array}\right.
$$

for which Eq. (103) yields a natural combination of results (106) (with a replaced with $w$ ) and (108):

$$
\begin{equation*}
f(\mathbf{r}) \propto \operatorname{sinc}\left(\frac{k x w}{2 z}\right) \cos \left(\frac{k x a}{2 z}\right) . \tag{8.110}
\end{equation*}
$$

This is the usual interference pattern modulated by a Fraunhofer-diffraction envelope (shown with the dashed blue line Fig. 15). Since function $\operatorname{sinc}^{2} \xi$ decreases very fast beyond its first zeros at $\xi= \pm \pi$, the practical number of observable interference fringes is close to $2 a / w$.


Fig. 8.15. Young's double-slit interference pattern for a finite slit width.
(iv) A structure very useful for experimental and engineering practice is a set of many parallel slits, called the diffraction grating. ${ }^{39}$ Indeed, if the slit width is much less than the grating period $d$, then the transparency function may be approximated as

$$
\begin{equation*}
T\left(\boldsymbol{\rho}^{\prime}\right) \propto \sum_{n=-\infty}^{+\infty} \delta\left(x^{\prime}-n d\right) \tag{8.111}
\end{equation*}
$$

and Eq. (103) yields

$$
\begin{equation*}
f(\boldsymbol{\rho}) \propto \sum_{n=-\infty}^{n=+\infty} \exp \left\{-i n \kappa_{x} d\right\}=\sum_{n=-\infty}^{n=+\infty} \exp \left\{-i \frac{n k x d}{z}\right\} . \tag{8.112}
\end{equation*}
$$

This sum vanishes for all values of $\kappa_{x} d$ that are not multiples of $2 \pi$, so that the result describes sharp intensity peaks at diffraction angles

[^376]\[

$$
\begin{equation*}
\alpha_{m} \equiv\left(\frac{x}{z}\right)_{m}=\left(\frac{\kappa_{x}}{k}\right)_{m}=\frac{2 \pi}{k d} m=\frac{\lambda}{d} m . \tag{8.113}
\end{equation*}
$$

\]

Taking into account that this result is only valid for small angles $\left|\alpha_{m}\right| \ll 1$, it may be interpreted exactly as Eq. (59) - see Fig. 6a. However, in contrast with the interference (108) from two slits, the destructive interference from many slits kills the net wave as soon as the angle is even slightly different from each Bragg angle (60). This is very convenient for spectroscopic purposes, because the diffraction lines produced by multi-frequency waves do not overlap even if the frequencies of their adjacent components are very close.

Two features of practical diffraction gratings make their properties different from this simple picture. First, the finite number $N$ of slits, which may be described by limiting sum (112) to interval $n=$ $[-N / 2,+N / 2]$, results in the finite spread, $\delta \alpha / \alpha \sim 1 / N$, of each diffraction peak, and hence in the reduction of grating's spectral resolution. (Unintentional variations of the inter-slit distance $d$ have a similar effect, so that before the advent of high-resolution photolithography, special high-precision mechanical tools have been used for grating fabrication.)

Second, the finite slit width $w$ leads to the diffraction peak pattern modulation by a $\operatorname{sinc}^{2}(k w \alpha / 2)$ envelope, similarly to pattern shown in Fig. 15. Actually, for spectroscopic purposes such modulation is a plus, because only one diffraction peak (say, with $m= \pm 1$ ) is practically used, and if the frequency spectrum of the analyzed wave is very broad (cover more than one octave), the higher peaks produce undesirable hindrance. Because of this reason, $w$ is frequently selected to be equal exactly to $d / 2$, thus suppressing each other diffraction maximum. Moreover, sometimes semi-transparent films are used to make the transparency function $T\left(\mathbf{r}^{\prime}\right)$ continuous and close to the sinusoidal one:

$$
\begin{equation*}
T\left(\boldsymbol{\rho}^{\prime}\right) \approx T_{0}+T_{1} \cos \frac{2 \pi x^{\prime}}{d}=T_{0}+\frac{T_{1}}{2}\left(\exp \left\{i \frac{2 \pi x^{\prime}}{d}\right\}+\exp \left\{-i \frac{2 \pi x^{\prime}}{d}\right\}\right) \tag{8.114}
\end{equation*}
$$

Plugging the last expression into Eq. (103) and integrating, we see that the output wave consists of just 3 components: the direct-passing wave (proportional to $T_{0}$ ) and two diffracted waves (proportional to $T_{1}$ ) propagating in the directions of the two lowest Bragg angles, $\alpha_{ \pm 1}= \pm \lambda / d$.

Relation (103) may be also readily used to obtain one more general (and rather curious) result called the Babinet principle. Consider two experiments with diffraction of similar plane waves on two "complementary" screens who together would cover the whole plane, without a hole or an overlap. (Think, for example, about an opaque disk of radius $R$ and a large opaque screen with a round orifice of the same radius.) Then, according to the Babinet principle, the diffracted wave patterns produced by these two screens in all directions with $\alpha \neq 0$ are identical. The proof of this principle is straightforward: since the transparency functions produced by the screens are complementary in the following sense:

$$
\begin{equation*}
T\left(\boldsymbol{\rho}^{\prime}\right) \equiv T_{1}\left(\boldsymbol{\rho}^{\prime}\right)+T_{2}\left(\boldsymbol{\rho}^{\prime}\right)=1, \tag{8.115}
\end{equation*}
$$

and (in the Fraunhofer approximation (103) only!) the diffracted wave is a linear Fourier transform of $T\left(\rho^{\prime}\right)$, we get

$$
\begin{equation*}
f_{1}(\boldsymbol{\rho})+f_{2}(\boldsymbol{\rho})=f_{0}(\boldsymbol{p}) \tag{8.116}
\end{equation*}
$$

where $f_{0}$ is the wave "scattered" by the composite screen with $T_{0}(\rho$ ' $) \equiv 1$, i.e. the unperturbed initial wave propagating in the initial direction $(\alpha=0)$. In all other directions, $f_{1}=-f_{2}$, i.e. the diffracted waves
are indeed similar besides the difference in sign - which is equivalent to a phase shift by $\pm \pi$. However, it is important to remember that the Babinet principle notwithstanding, in real experiments the diffracted waves may interfere with the unperturbed plane wave $f_{0}(\rho)$, leading to different diffraction pattern in cases 1 and $2-$ see, e.g., Fig. 13 and its discussion.

### 8.9. Magnetic dipole and electric quadrupole radiation

Throughout this chapter, we have seen how many important results may be obtained from Eq. (26) for the electric dipole radiation by a small-size source (Fig. 1). Only in rare cases when such radiation is absent, for example if the dipole moment $\mathbf{p}$ of the source equals zero (or does not change at time - either at all, or at the frequency of our interest), higher-order effects may be important. I will discuss the main two of them, the quadrupole electric and dipole magnetic radiation - mostly for reference purposes, because we would not have much time to discuss their applications.

In Sec. 2 above, the electric dipole radiation was calculated by plugging the first, leading term of expansion (19) into the exact formula (17b) for the retarded vector-potential $\mathbf{A}(\mathbf{r}, t)$. Let us make a more exact calculation, by keeping the second term of that expansion as well:

$$
\begin{equation*}
\mathbf{j}\left(\mathbf{r}^{\prime}, t-\frac{R}{v}\right) \approx \mathbf{j}\left(\mathbf{r}^{\prime}, t-\frac{r}{v}+\frac{\mathbf{r}^{\prime} \cdot \mathbf{n}}{v}\right)=\mathbf{j}\left(\mathbf{r}^{\prime}, t^{\prime}+\frac{\mathbf{r}^{\prime} \cdot \mathbf{n}}{v}\right), \quad \text { where } \quad t^{\prime} \equiv t-\frac{r}{v} . \tag{8.117}
\end{equation*}
$$

Since this expansion is only valid if the last term in the second argument is relatively small, in the Taylor expansion of $\mathbf{j}$ with respect to that argument we may keep just the first two leading terms:

$$
\begin{equation*}
\mathbf{j}\left(\mathbf{r}^{\prime}, t^{\prime}+\frac{\mathbf{r}^{\prime} \cdot \mathbf{n}}{v}\right) \approx \mathbf{j}\left(\mathbf{r}^{\prime}, t^{\prime}\right)+\frac{1}{v} \frac{\partial}{\partial t^{\prime}} \mathbf{j}\left(\mathbf{r}^{\prime}, t^{\prime}\right)\left(\mathbf{r}^{\prime} \cdot \mathbf{n}\right) \tag{8.118}
\end{equation*}
$$

so that Eq. (17b) yields $\mathbf{A}=\mathbf{A}_{e}+\mathbf{A}^{\prime}$, where $\mathbf{A}_{e}$ is the electric dipole contribution as given by Eq. (23), and $\mathbf{A}^{\prime}$ is the new term of the next order in small parameter $r^{\prime} \ll r$ :

$$
\begin{equation*}
\mathbf{A}^{\prime}(\mathbf{r}, t)=\frac{\mu}{4 \pi r v} \frac{\partial}{\partial t^{\prime}} \int \mathbf{j}\left(\mathbf{r}^{\prime}, t^{\prime}\right)\left(\mathbf{r}^{\prime} \cdot \mathbf{n}\right) d^{3} r^{\prime} \tag{8.119}
\end{equation*}
$$

Just as was done in Sec. 2, let us evaluate this term for a system of non-relativistic particles with electric charges $q_{k}$ and radius-vectors $\mathbf{r}_{k}(t)$ :

$$
\begin{equation*}
\mathbf{A}^{\prime}(\mathbf{r}, t)=\frac{\mu}{4 \pi r v}\left[\frac{d}{d t} \sum_{k} q_{k} \dot{\mathbf{r}}_{k}\left(\mathbf{r}_{k} \cdot \mathbf{n}\right)\right]_{t=t^{\prime}} \tag{8.120}
\end{equation*}
$$

Using the "bac minus cab" identity of the vector algebra again, ${ }^{40}$ Eq. (120) may be rewritten as

$$
\begin{align*}
\dot{\mathbf{r}}_{k}\left(\mathbf{r}_{k} \cdot \mathbf{n}\right) & =\frac{1}{2} \dot{\mathbf{r}}_{k}\left(\mathbf{r}_{k} \cdot \mathbf{n}\right)+\frac{1}{2} \dot{\mathbf{r}}_{k}\left(\mathbf{n} \cdot \mathbf{r}_{k}\right)=\frac{1}{2}\left(\mathbf{r}_{k} \times \dot{\mathbf{r}}_{k}\right) \times \mathbf{n}+\frac{1}{2} \mathbf{r}_{k}\left(\mathbf{n} \cdot \dot{\mathbf{r}}_{k}\right)+\frac{1}{2} \dot{\mathbf{r}}_{k}\left(\mathbf{n} \cdot \mathbf{r}_{k}\right) \\
& =\frac{1}{2}\left(\mathbf{r}_{k} \times \dot{\mathbf{r}}_{k}\right) \times \mathbf{n}+\frac{1}{2} \frac{d}{d t}\left[\mathbf{r}_{k}\left(\mathbf{n} \cdot \mathbf{r}_{k}\right)\right], \tag{8.121}
\end{align*}
$$

so that the right-hand part of Eq. (120) may be presented as a sum of two terms, $\mathbf{A}^{\prime}=\mathbf{A}_{m}+\mathbf{A}_{q}$, where

[^377]\[

$$
\begin{gather*}
\mathbf{A}_{m}(\mathbf{r}, t)=\frac{\mu}{4 \pi r v} \dot{\mathbf{m}}\left(t^{\prime}\right) \times \mathbf{n}=\frac{\mu}{4 \pi r v} \dot{\mathbf{m}}\left(t-\frac{r}{v}\right) \times \mathbf{n}, \quad \text { with } \mathbf{m}(t) \equiv \frac{1}{2} \sum_{k} \mathbf{r}_{k}(t) \times q_{k} \dot{\mathbf{r}}_{k}(t),  \tag{8.122}\\
\mathbf{A}_{q}(\mathbf{r}, t)=\frac{\mu}{8 \pi r v}\left[\frac{d^{2}}{d t^{2}} \sum_{k} q_{k} \mathbf{r}_{k}\left(\mathbf{n} \cdot \mathbf{r}_{k}\right)\right]_{t=t^{\prime}} \tag{8.123}
\end{gather*}
$$
\]

Comparing the second of Eqs. (122) with Eq. (5.91), we see that $\mathbf{m}$ is just the magnetic moment of the source. On the other hand, the first of Eqs. (122) is absolutely similar in structure to Eq. (23), with $\mathbf{p}$ replaced by $(\mathbf{m} \times \mathbf{n}) / v$, so that for the corresponding component of the magnetic field it gives (in the same approximation $r \gg \lambda$ ) the result similar to Eq. (24):

$$
\begin{equation*}
\mathbf{B}_{m}(\mathbf{r}, t)=\frac{\mu}{4 \pi r v} \nabla \times\left[\dot{\mathbf{m}}\left(t-\frac{r}{v}\right) \times \mathbf{n}\right]=-\frac{\mu}{4 \pi r v^{2}} \mathbf{n} \times\left[\ddot{\mathbf{m}}\left(t-\frac{r}{v}\right) \times \mathbf{n}\right] . \tag{8.124}
\end{equation*}
$$

According to this expression, just as at the electric dipole radiation, vector $\mathbf{B}$ is perpendicular to vector $\mathbf{n}$, and its magnitude is also proportional to the $\sin \theta$, where $\theta$ is now the angle between the direction toward the observation point and the second time derivative of vector $\mathbf{m}$ rather than $\mathbf{p}$ :

$$
\begin{equation*}
B_{m}=\frac{\mu}{4 \pi r v^{2}} \ddot{m}\left(t-\frac{r}{v}\right) \sin \theta . \tag{8.125}
\end{equation*}
$$

As the result, the intensity of this magnetic dipole radiation has the similar angular distribution:

$$
\begin{equation*}
S_{r}=Z H^{2}=\frac{Z}{\left(4 \pi v^{2} r\right)^{2}}\left[\ddot{m}\left(t-\frac{r}{v}\right)\right]^{2} \sin ^{2} \theta \tag{8.126}
\end{equation*}
$$

- cf. Eq. (26). Note, however, that this radiation is usually much weaker than its electric counterpart. For example, for a non-relativistic particle with electric charge $q$, moving on a trajectory with of size $\sim a$, the electric dipole moment is of the order of $q a$, while its magnetic moment scales as $q a^{2} \omega$, where $\omega$ is the motion frequency. As a result, the ratio of the magnetic and electric dipole radiation intensities is of the order of $(a \omega / v)^{2}$, i.e. the squared ratio of particle's speed to the speed of emitted waves - that has to be much smaller than 1 for our non-relativistic estimate to be valid.

The angular distribution of the electric quadrupole radiation, described by Eq. (123), is more complicated. In order to show this, we may add to $\mathbf{A}_{q}$ a vector parallel to $\mathbf{n}$ (i.e. along the wave propagation), getting

$$
\begin{equation*}
\mathbf{A}_{q}(\mathbf{r}, t) \rightarrow \frac{\mu}{24 \pi r v} \ddot{\mathbf{Q}}\left(t-\frac{r}{v}\right), \quad \text { where } \mathbf{Q} \equiv \sum_{k} q_{k}\left\{3 \mathbf{r}_{k}\left(\mathbf{n} \cdot \mathbf{r}_{k}\right)-\mathbf{n} r_{k}^{2}\right\}, \tag{8.127}
\end{equation*}
$$

because this addition does not give any contribution to the transverse component of the electric and magnetic fields, i.e. to the radiated wave. According to the above definition of vector $\mathbf{Q}$, its Cartesian components may be presented as ${ }^{41}$

[^378]\[

$$
\begin{equation*}
Q_{j}=\sum_{j^{\prime}=1}^{3} Q_{i j}, n_{j^{\prime}} \tag{8.128}
\end{equation*}
$$

\]

where $Q_{i j}$, are elements of the so-called electric quadrupole tensor $\mathcal{Q}$ of the system:42

$$
\begin{equation*}
\mathcal{Q}_{j j^{\prime}}=\sum_{k} q_{k}\left(3 r_{j} r_{j^{\prime}}-r^{2} \delta_{j j^{\prime}}\right)_{k} . \tag{8.129a}
\end{equation*}
$$

For clarity, let me spell out the tensor in its matrix form:

$$
Q=\sum_{k} q_{k}\left(\begin{array}{ccc}
2 x^{2}-y^{2}-z^{2} & 3 x y & 3 x z  \tag{8.129b}\\
3 x y & 2 y^{2}-x^{2}-z^{2} & 3 y z \\
3 x z & 3 y z & 2 z^{2}-x^{2}-y^{2}
\end{array}\right)_{k}
$$

Differentiating the first of Eqs. (127) at $r \gg \lambda$, we get

$$
\begin{equation*}
\mathbf{B}_{q}(\mathbf{r}, t)=-\frac{\mu}{24 \pi r v^{2}} \mathbf{n} \times \dddot{\mathbf{Q}}\left(t-\frac{r}{v}\right) . \tag{8.130}
\end{equation*}
$$

Superficially, this expression is similar to Eqs. (24) or (124), but according to Eqs. (127) and (129), components of vector $\mathbf{Q}$ depend on the direction of vector $\mathbf{n}$, leading to a different angular dependence of $S_{r}$.

As the simplest example, let us consider a system of two equal point electric charges moving at equal distances $d(t) \ll \lambda$ from a stationary center (Fig. 16).


Fig. 8.16. The simplest system emitting electric quadrupole radiation.

Due to the symmetry of the system, its dipole moments $\mathbf{p}$ and $\mathbf{m}$ (and hence its electric and magnetic dipole radiation) vanish, but the quadrupole tensor (129) still has nonvanishing components. With the coordinate choice shown in Fig. 16, these components are diagonal:

$$
\begin{equation*}
Q_{x x}=Q_{y y}=-2 q d^{2}, \quad Q_{z z}=4 q d^{2} . \tag{8.131}
\end{equation*}
$$

With axis $x$ in the plane of the direction $\mathbf{n}$ toward the source (Fig. 16), so that $n_{x}=\sin \theta, n_{y}=0, n_{z}=\cos$ $\theta$, Eq. (128) yields

$$
\begin{equation*}
Q_{x}=-2 q d^{2} \sin \theta, \quad Q_{y}=0, \quad Q_{z}=4 q d^{2} \cos \theta \tag{8.132}
\end{equation*}
$$

[^379]Electric quadrupole
radiation field
so that the vector product in Eq. (130) has only one nonvanishing Cartesian component:

$$
\begin{equation*}
(\mathbf{n} \times \dddot{\mathbf{Q}})_{y}=n_{z} \dddot{Q}_{x}-n_{x} \dddot{Q}_{z}=-6 q \sin \theta \cos \theta \frac{d^{3}}{d t^{3}}\left[d^{2}(t)\right] . \tag{8.133}
\end{equation*}
$$

As a result, the radiation intensity is proportional to $\sin ^{2} \theta \cos ^{2} \theta$, i.e. vanishes not only along the symmetry axis (as the dipole radiation does), but also in all directions perpendicular to this axis, reaching its maximum at $\theta=\pi / 4$.

For more complex systems, the angular distribution of the electric quadrupole radiation may be different, but its total power may be always presented in a simple form

$$
\begin{equation*}
P_{q}=\frac{Z}{1440 \pi v^{4}} \sum_{j, j^{\prime}=1}^{3}\left(\dddot{Q}_{j j^{\prime}}\right)^{2} \tag{8.134}
\end{equation*}
$$

Let me finish this section by giving, without proof, one more fact important for applications: due to their different spatial structure, the magnetic dipole and electric quadrupole radiation fields do not interfere, i.e. the total power of radiation (neglecting higher multipole terms) may be found as the sum of these components, calculated independently.

### 8.10. Exercise problems

8.1.* In the electric dipole approximation, calculate the angular distribution and total power of electromagnetic radiation by the following classical model of the hydrogen atom: an electron rotating, at a constant distance $r$, about a much heavier proton. Use the latter result to evaluate the classical lifetime of the atom, borrowing the initial value of $R$ from quantum mechanics: $R(0)=r_{\mathrm{B}} \approx 0.53 \times 10^{-10} \mathrm{~m}$.
8.2. A non-relativistic particle of mass $m$ with the electric charge $q$ is placed into a uniform magnetic field $\mathbf{B}$. Derive the law of decrease of particle's kinetic energy due to its electromagnetic radiation at the cyclotron frequency $\omega_{c}=q B / m$. Evaluate the rate of such radiation cooling for electrons in a magnetic field of 1 T , and estimate the electron energy interval in which this result is qualitatively correct.

Hint: The cyclotron motion will be discussed in detail (for arbitrary particle velocities $v \sim c$ ) in Sec. 9.6 below, but I hope that the reader knows that in the non-relativistic case ( $v \ll c$ ) the above formula for $\omega_{c}$ may be readily obtained by combining the $2^{\text {nd }}$ Newton law $m v_{\perp}{ }^{2} / R=q v_{\perp} B$ for the circular motion of the particle under the effect of the magnetic component of the Lorentz force (5.10), and the geometric relation $v_{\perp}=R \omega_{c}$. (Here $\mathbf{v}_{\perp}$ is particle's velocity within the plane normal to vector $\mathbf{B}$.)
8.3. Solve the dipole antenna radiation problem discussed in Sec. 2 (see Fig. 3) for the optimal length $l=\lambda / 2$, assuming ${ }^{43}$ that the current distribution in each of its arms is sinusoidal:

$$
I(z, t)=I_{0} \cos \frac{\pi z}{l} \cos \omega t
$$

[^380]8.4. Use the harmonic oscillator model of a bound charge, given by Eq. (7.30), to explore the transition between two scattering limits discussed in Sec. 3, in particular the resonant scattering taking place at $\omega \approx \omega_{0}$. In this context, discuss the contribution of scattering into oscillator's damping.
8.5. ${ }^{*}$ A sphere of radius $R$, made of a material with constant permanent electric polarization $P_{0}$ and mass density $\rho$, is free to rotate about its center of mass. Calculate the total cross-section of scattering, by the sphere, of a linearly polarized electromagnetic wave of frequency $\omega \ll R / c$, propagating in free space, in the limit of small wave amplitude, assuming that the initial orientation of the polarization vector $\mathbf{P}_{0}$ is random.
8.6. Use the Born approximation to analyze the interference pattern produced by plane wave's scattering on a set of $N$ similar, equidistant points on a straight line normal to the direction of the incident wave's propagation - see Fig. on the right. Discuss the trend(s) of the pattern in the limit $N \rightarrow \infty$.

8.7. Use the Born approximation to calculate the differential cross-section of plane wave scattering by a dielectric cube of side $a$, with $\varepsilon \approx \varepsilon_{0}$. In the limits $k a \ll 1$ and $k a \gg 1$ (where $k$ is the wave vector), analyze the angular dependence of the differential cross-section. Calculate the full crosssection for the simplest case when the incident wave vector is parallel to one of cube's sides.
8.8. Use the Born approximation to calculate the differential cross-section of plane wave scattering by a nonmagnetic, uniform dielectric sphere with $\varepsilon \approx \varepsilon_{0}$, of an arbitrary radius $R$. In the limits $k R \ll 1$ and $1 \ll k R$ (where $k$ is the wave number), analyze the angular dependence of the differential cross-section, and calculate the full cross-section.
8.9. A sphere of radius $R$ is made of a uniform, nonmagnetic, linear dielectric material. Calculate its full cross-section of scattering of a low-frequency monochromatic wave, with $k \ll 1 / R$, for an arbitrary dielectric constant, and compare the result with the solution of the previous problem.
8.10. Solve the previous problem, also in the low-frequency limit $k R \ll 1$, for the case when the sphere's material has a frequency-independent Ohmic conductivity, and $\varepsilon_{\mathrm{opt}}=\varepsilon_{0}$, and a relatively large skin depth $\left(\delta_{s} \gg R\right)$, and compare the results.
8.11. Use the Born approximation to calculate the differential cross-section of plane wave scattering on a right, circular cylinder of length $l$ and radius $R$, for arbitrary incidence.
8.12. Formulate the quantitative condition of the Born approximation validity for a uniform linear-dielectric scatterer with all linear dimensions of the order of $a$.
8.13. Use the Huygens principle to calculate wave's intensity on the symmetry plane of the slit diffraction experiment (i.e. at $x=0$ in Fig. 11), for arbitrary ratio $z / k a^{2}$.
8.14. A plane wave with wavelength $\lambda$ is normally incident on an opaque, plane screen, with a round orifice of radius $R \gg \lambda$. Use the Huygens principle to calculate passed wave's intensity distribution along system's symmetry axis, at distances $z \gg R$ from the screen (see Fig. on the right), and analyze the result.

8.15. A plane monochromatic wave is normally incident on an opaque circular disk of radius $R \gg \lambda$. Use the Huygens principle to calculate wave's intensity at distance $z \gg R$ behind the disk center (see Fig. on the right). Discuss the result.

8.16. Use the Huygens principle to analyze the Fraunhofer diffraction of a plane wave normally incident on a square-shape hole, of size $a \times a$, in an opaque screen. Sketch the diffraction pattern you would observe at a sufficiently large distance, and quantify expression "sufficiently large" for this case.
8.17. Within the Fraunhofer approximation, analyze the pattern produced by a 1 D diffraction grating with the periodic transparency profile shown in Fig. on the right, for the normal incidence of a plane, monochromatic wave.

8.18. $N$ equal point charges are attached, at equal intervals, to a circle rotating with a constant angular velocity about its center - see Fig. on the right. For what values of $N$ does the system emit:
(i) the electric dipole radiation?
(ii) the magnetic dipole radiation?
(iii) the electric quadrupole radiation?

8.19. The orientation of a magnetic dipole $\mathbf{m}$, of a fixed magnitude, is rotating about a certain axis with angular velocity $\omega$, with angle $\theta$ between them staying constant. Calculate the angular distribution and the average power of its radiation (into free space).
8.20. Complete the solution of the problem started in Sec. 9, by calculating the full power of radiation of the system of two charges oscillating in antiphase along the same straight line - see Fig. 6. Also, calculate the average radiation power for the case of harmonic oscillations, $d(t)=a \cos \omega t$, compare it with the case of a single charge performing similar oscillations, and interpret the difference.

## This page is

## Chapter 9. Special Relativity

This chapter starts with a brief review of the special relativity's basics. This background is used, later in the chapter, for the analysis of the relation between electromagnetic field values measured in different reference frames moving relative to each other, and discussions of relativistic particle dynamics in the electric and magnetic fields, and of analytical mechanics of electromagnetism.

### 9.1. Einstein postulates and the Lorentz transform

As was emphasized at the derivation of expressions for the dipole and quadrupole radiation in the last chapter, they are only valid for systems of non-relativistic particles. Thus, these results cannot be used for description of such important phenomena as the Cherenkov radiation or synchrotron radiation, in which relativistic effects are essential. Moreover, analysis of motion of charged relativistic particles in electric and magnetic fields is also a natural part of electrodynamics. This is why I will follow the tradition of using this course for a (by necessity, brief) introduction to special relativity theory. This theory is based on the idea that measurements of all physical variables (including spatial and even temporal intervals between two events) may give different results in different reference frames, in particular two frames moving relative to each other translationally (i.e. without rotation), with a certain constant velocity $\mathbf{v}$ (Fig. 1).


Fig. 9.1. Translational, uniform motion of two reference frames.

In the non-relativistic (Newtonian) mechanics the problem of transfer between such reference frames has a simple solution at least in the limit $v \ll c$, because the basic equation of particle dynamics (the $2^{\text {nd }}$ Newton law) ${ }^{1}$

$$
\begin{equation*}
m_{k} \ddot{\mathbf{r}}_{k}=-\nabla_{k} \sum_{k^{\prime}} U\left(\mathbf{r}_{k}-\mathbf{r}_{k^{\prime}}\right), \tag{9.1}
\end{equation*}
$$

where $U$, the potential energy of inter-particle interactions, is invariant with respect to the so-called Galilean transform (or "transformation"). ${ }^{2}$ Choosing the coordinate axes of both frames so that axes $x$ and $x^{\prime}$ are parallel to vector $\mathbf{v}$ (Fig. 1), the transform ${ }^{3}$ may be presented as

Galilean transform

$$
\begin{equation*}
x=x^{\prime}+v t^{\prime}, \quad y=y^{\prime}, \quad z=z^{\prime}, \quad t=t^{\prime} \tag{9.2a}
\end{equation*}
$$

[^381]and plugging Eq. (2a) into Eq. (1), we get an absolutely similarly looking equation of motion in the "moving" reference frame 0'. Since the reciprocal transform,
\[

$$
\begin{equation*}
x^{\prime}=x-v t, \quad y=y^{\prime}, \quad z^{\prime}=z, \quad t^{\prime}=t \tag{9.2b}
\end{equation*}
$$

\]

is similar to the direct one, with the replacement of $(+v)$ with $(-v)$, we may say that the Galilean invariance means that there is no any "master" (absolute) spatial reference frame in classical mechanics, although the spatial and temporal intervals between different events are absolute (reference-frame invariant).

However, it is straightforward to use Eq. (2) to check that the form of the wave equation

$$
\begin{equation*}
\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial z^{2}}-\frac{1}{c^{2}} \frac{\partial^{2}}{\partial t^{2}}\right) f=0 \tag{9.3}
\end{equation*}
$$

describing in particular the electromagnetic wave propagation in free space, ${ }^{4}$ is not Galilean-invariant. ${ }^{5}$ For the "usual" (say, elastic) waves, which obey a similar equation albeit with a different speed, ${ }^{6}$ this lack of Galilean invariance is natural and is compatible with the invariance of Eq. (1), from which the wave equation originates. This is because the elastic waves are essentially the oscillations of interacting particles of a certain medium (e.g., an elastic solid), which makes the reference frame connected to this medium, special. So, if the electromagnetic waves were oscillations of a certain special medium (that was first called the "luminiferous aether" ${ }^{7}$ and later just ether), similar arguments might be applicable to reconcile Eqs. (2) and (3).

The detection of such a medium was the goal of the Michelson-Morley measurements (carried out between 1881 and 1887 with better and better precision), that are sometimes called "the most famous failed experiment in physics". Figure 2 shows a crude scheme of their experiments.


[^382]A nearly-monochromatic wave is split in two parts (nominally, of equal intensity), using a semitransparent mirror tilted by $45^{\circ}$ to the incident wave direction. These two partial waves are reflected back by two genuine mirrors, and arrive at the same semi-transparent mirror again. Here a half of each wave is returned to the light source area (where they vanish without affecting the source), but another half passes toward the detector, forming, with its counterpart, an interference pattern similar to that in the Young experiment. Thus each of the interfering waves has traveled twice (back and forth) each of two mutually perpendicular "arms" of the interferometer. Assuming that the ether, in which light propagates with speed $c$, moves with speed $v<c$ along one of the arms, of length $l_{l}$, it is straightforward (and hence left for reader's exercise :-) to get the following expression for the difference between light roundtrip times:

$$
\begin{equation*}
\Delta t=\frac{2}{c}\left(\frac{l_{t}}{\left(1-v^{2} / c^{2}\right)^{1 / 2}}-\frac{l_{l}}{1-v^{2} / c^{2}}\right) \approx \frac{l}{c}\left(\frac{v}{c}\right)^{2} \tag{9.4}
\end{equation*}
$$

where $l_{t}$ is the length of the second, "transverse" arm of the interferometer (perpendicular to $\mathbf{v}$ ), and the last, approximate expression is valid at $l_{t} \approx l_{l}$ and $v \ll c$.

Since Earth moves around the Sun with speed $v_{\mathrm{E}} \approx 30 \mathrm{~km} / \mathrm{s} \approx 10^{-4} c$, the arm positions relative to this motion alternate, due to Earth rotation about its axis, each 6 hours - see the right panel of Fig. 2. Hence if we assume that the ether rests in Sun's reference frame, $\Delta t$ (and the corresponding shift of interference fringes), has to alternate with this half-period as well. The same alternation may be achieved, at a smaller time scale, by a deliberate rotation of the instrument by $\pi / 2$. In the most precise version of the Michelson-Morley experiment (1887), this shift was expected to be close to 0.4 of the fringe pattern period. The result was negative, with the error bar about 0.01 of the fringe period. ${ }^{8}$

The most prominent immediate explanation of this zero result ${ }^{9}$ was suggested in 1889 by G. FitzGerald and (independently and more qualitatively) by H. Lorentz in 1892: as evident from Eq. (4), if the longitudinal arm of the interferometer itself experiences the so-called length contraction,

$$
\begin{equation*}
l_{l}(v)=l_{l}(0)\left(1-\frac{v^{2}}{c^{2}}\right)^{1 / 2} \tag{9.5}
\end{equation*}
$$

while the transverse arm's length is not affected by the motion relative to the ether, this kills $\Delta t$. This, extremely radical, idea received a strong support from the proof, in 1887-1905, that the Maxwell equations, and hence the wave equation (3), are form-invariant under the so-called Lorentz transform. ${ }^{10}$ For the choice of coordinates shown in Fig. 1, the transform reads

[^383]\[

$$
\begin{equation*}
x=\frac{x^{\prime}+v t^{\prime}}{\left(1-v^{2} / c^{2}\right)^{1 / 2}}, \quad y=y^{\prime}, \quad z=z^{\prime}, \quad t=\frac{t^{\prime}+\left(v / c^{2}\right) x^{\prime}}{\left(1-v^{2} / c^{2}\right)^{1 / 2}} . \tag{9.6a}
\end{equation*}
$$

\]

It is elementary to solve these equations for the primed coordinates to get the reciprocal transform

$$
\begin{equation*}
x^{\prime}=\frac{x-v t}{\left(1-v^{2} / c^{2}\right)^{1 / 2}}, \quad y^{\prime}=y, \quad z^{\prime}=z, \quad t^{\prime}=\frac{t-\left(v / c^{2}\right) x}{\left(1-v^{2} / c^{2}\right)^{1 / 2}} . \tag{9.6b}
\end{equation*}
$$

(I will soon present Eqs. (6) in a more elegant form.)
The Lorentz transform relations (6) are evidently reduced to the Galilean transform formulas (2) at $v^{2} \ll c^{2}$. As will be proved in the next section, Eqs. (6) also yield the Lorentz length contraction (5). However, all attempts to give a reasonable interpretation of these equations while keeping the notion of the ether have failed, in particular because of the restrictions imposed by results of earlier experiments carried out in 1851 and 1853 by H. Fizeau - that were repeated with higher accuracy by the same Michelson and Morley in 1886. These experiments have shown that if one sticks to the ether concept, this hypothetical medium should be partially "dragged" by any moving dielectric media with a speed proportional to $\left(\varepsilon_{r}-1\right)$. Careful reasoning shows that such local drag is irreconcilable with the assumed continuity of the ether.

In his famous 1905 paper, Albert Einstein has suggested a bold resolution of this contradiction, essentially removing the concept of the ether altogether. Moreover, he argued that the Lorentz transform is the general property of time and space, rather than of the electromagnetic field alone. He has started with two postulates, the first one essentially repeating the principle of relativity, formulated earlier (1904) by H. Poincaré in the following form:
"...the laws of physical phenomena should be the same, whether for an observer fixed, or for an observer carried along in a uniform movement of translation; so that we have not and could not have any means of discerning whether or not we are carried along in such a motion." ${ }^{11}$

The second Einstein's postulate was that the speed of light $c$, in free space, should be constant in all reference frames. (This is essentially a denial of ether's existence.)

Then, Einstein showed how naturally do the Lorenz transform relations (6) follow from his postulates, with a few (very natural) additional assumptions. Let a point source emit a short flash of light, at the moment $t=t^{\prime}=0$ when origins of the reference frames shown in Fig. 1 coincide. Then, according to the second of Einstein's postulates, in each of the frames the spherical wave propagates with the same speed $c$, i.e. coordinates of points of its front, measured in the two frames, have to obey equations

$$
\begin{align*}
& (c t)^{2}-\left(x^{2}+y^{2}+z^{2}\right)=0, \\
& \left(c t^{\prime}\right)^{2}-\left(x^{\prime 2}+y^{\prime 2}+z^{\prime 2}\right)=0 . \tag{9.7}
\end{align*}
$$

What may be the general relation between the combinations in the left-hand side of these equations - not for this selected pair of events, the light flash and its detection, but in general? A very natural (essentially, the only justifiable) choice is

[^384]\[

$$
\begin{equation*}
\left[(c t)^{2}-\left(x^{2}+y^{2}+z^{2}\right)\right]=f\left(v^{2}\right)\left[\left(c t^{\prime}\right)^{2}-\left(x^{\prime 2}+y^{\prime 2}+z^{\prime 2}\right)\right] . \tag{9.8}
\end{equation*}
$$

\]

Now, according to the first postulate, the same relation should be valid if we swap the reference frames ( $x \leftrightarrow x^{\prime}$, etc.) and replace $v$ with $(-v)$. This is only possible if $f^{2}=1$, so that excluding option $f=-1$ (which is incompatible with the Galilean transform in the limit $v / c \rightarrow 0$ ), we get

$$
\begin{equation*}
(c t)^{2}-\left(x^{2}+y^{2}+z^{2}\right)=\left(c t^{\prime}\right)^{2}-\left(x^{\prime 2}+y^{\prime 2}+z^{\prime 2}\right) . \tag{9.9}
\end{equation*}
$$

For the line $y=y^{\prime}=0, z=z^{\prime}=0$, Eq. (9) is reduced to

$$
\begin{equation*}
(c t)^{2}-x^{2}=\left(c t^{\prime}\right)^{2}-x^{\prime 2} . \tag{9.10}
\end{equation*}
$$

It is very illuminating to interpret this relation as the one resulting from a mutual rotation of the reference frames (that now have to include clocks to measure time) on the plane of coordinate $x$ and the so-called Euclidian time $\tau \equiv i c t-$ see Fig. 3.


Fig. 9.3. The Lorentz transform as a mutual rotation of reference frames on the $[x, \tau]$ plane.

Indeed, rewriting Eq. (10) as

$$
\begin{equation*}
\tau^{2}+x^{2}=\tau^{\prime 2}+x^{\prime 2} \tag{9.11}
\end{equation*}
$$

we may consider it as the invariance of the squared radius at the rotation that is shown in Fig. 3 and described by the evident geometric relations

$$
\begin{align*}
& x=x^{\prime} \cos \psi-\tau^{\prime} \sin \psi,  \tag{9.12a}\\
& \tau=x^{\prime} \sin \psi+\tau^{\prime} \cos \psi,
\end{align*}
$$

with the reciprocal relations

$$
\begin{align*}
& x^{\prime}=x \cos \psi+\tau \sin \psi, \\
& \tau^{\prime}=-x \sin \psi+\tau \cos \psi . \tag{9.12b}
\end{align*}
$$

So far, angle $\psi$ has been arbitrary. In the spirit of Eq. (8), a natural choice is $\psi=\psi(v)$, with the requirement $\psi(0)=0$. In order to find this function, let us write the definition of velocity $v$ of frame $0^{\prime}$, as measured in reference frame 0 : for $x^{\prime}=0, x=v t$. In variables $x$ and $\tau$, this means

$$
\begin{equation*}
\left.\left.\frac{x}{\tau}\right|_{x^{\prime}=0} \equiv \frac{x}{i c t}\right|_{x^{\prime}=0}=\frac{v}{i c} . \tag{9.13}
\end{equation*}
$$

On the other hand, for the same point $x^{\prime}=0$, Eqs. (12a) yield

$$
\begin{equation*}
\left.\frac{x}{\tau}\right|_{x^{\prime}=0}=-\tan \psi \tag{9.14}
\end{equation*}
$$

These two expressions are compatible only if

$$
\begin{equation*}
\tan \psi=\frac{i v}{c} \tag{9.15}
\end{equation*}
$$

so that

$$
\begin{equation*}
\sin \psi \equiv \frac{\tan \psi}{\left(1+\tan ^{2} \psi\right)^{1 / 2}}=\frac{i v / c}{\left(1-v^{2} / c^{2}\right)^{1 / 2}} \equiv i \beta \gamma, \quad \cos \psi \equiv \frac{1}{\left(1+\tan ^{2} \psi\right)^{1 / 2}}=\frac{1}{\left(1-v^{2} / c^{2}\right)^{1 / 2}} \equiv \gamma \tag{9.16}
\end{equation*}
$$

where $\beta$ and $\gamma$ are two very convenient and commonly used dimensionless parameters defined as

$$
\begin{equation*}
\boldsymbol{\beta} \equiv \frac{\mathbf{v}}{c}, \quad \gamma \equiv \frac{1}{\left(1-v^{2} / c^{2}\right)^{1 / 2}}=\frac{1}{\left(1-\beta^{2}\right)^{1 / 2}} . \tag{9.17}
\end{equation*}
$$

(Vector $\beta$ is called the normalized velocity, while scalar $\gamma$, the Lorentz factor.) ${ }^{12}$
Using the relations for $\psi$, Eqs. (12) become

$$
\begin{array}{ll}
x=\gamma\left(x^{\prime}-i \beta \tau^{\prime}\right), & \tau=\gamma\left(i \beta x^{\prime}+\tau^{\prime}\right), \\
x^{\prime}=\gamma(x+i \beta \tau), & \tau^{\prime}=\gamma(-i \beta x+\tau) . \tag{9.18b}
\end{array}
$$

Now returning to the real variables $[x, c t]$, we get the Lorentz transform relations (6) in a more compact form: ${ }^{13}$

$$
\begin{array}{llll}
x=\gamma\left(x^{\prime}+\beta c t^{\prime}\right), & y=y^{\prime}, & z=z^{\prime}, & c t=\gamma\left(c t^{\prime}+\beta x^{\prime}\right), \\
x^{\prime}=\gamma(x-\beta c t), & y^{\prime}=y, & z^{\prime}=z, & c t^{\prime}=\gamma(c t-\beta x) . \tag{9.19b}
\end{array}
$$

An immediate corollary of Eqs. (6) is that for $\gamma$ to stay real, we need $v^{2} \leq c^{2}$, i.e. that the speed of any physical body (to which we could connect a reference frame) cannot exceed the speed of light, as measured in any physically meaningful reference frame. ${ }^{14}$

### 9.2. Relativistic kinematic effects

In order to discuss other corollaries of Eqs. (19), we need to spend a few minutes to discuss what do these relations actually mean. Evidently, they are trying to tell us that the spatial and temporal intervals are not absolute (as they are in the Newtonian space), but do depend on the reference frame they are measured in. So, we have to understand very clearly what exactly may be measured - and thus may be discussed in a physics theory. Recognizing this necessity, A. Einstein has introduced the notion of numerous imaginary observers that may be distributed all over each reference frame. Each observer has a clock and may use it to measure the instants of local events. He also conjectured that:
(i) all observers within the same reference frame may agree on a common length measure ("a scale"), i.e. on their relative positions in that frame, and synchronize their clocks, ${ }^{15}$ and

[^385](ii) observers belonging to different reference frames may agree on the nomenclature of world events (e.g., short flashes of light) to which their respective measurements belong.

Actually, these additional postulates have been already implied in our "derivation" of the Lorentz transform in Sec. 1. For example, by $\{x, y, z$, and $t\}$ we mean the results of space and time measurements of a certain world event, about that all observers belonging to frame 0 agree. Similarly, all observers of frame 0 ' have to agree about results $\left\{x^{\prime}, y^{\prime}, z^{\prime}, t^{\prime}\right\}$. Finally, when the origin of frame $0^{\prime}$ passes by some sequential points $x_{k}$ of frame 0 , observers in that frame may measure its passage times $t_{k}$ without a fundamental error, and know that all these times belong to $x^{\prime}=0$.

Now we can analyze the major corollaries of the Lorentz transform, which are rather striking from the point of view of our everyday (rather non-relativistic :-) experience.
(i) Length contraction. Let us consider a rigid rod, stretched along axis $x$, with length $l=x_{2}-x_{1}$, where $x_{1,2}$ are the coordinates of rod's ends, as measured in its rest frame 0 , at any instant $t$ (Fig. 4). What would be the rod's length $l$ ' measured by the Einstein observers in the moving frame 0 '?


Fig. 9.4. Relativistic length contraction.

At a time instant $t$ ' agreed upon in advance, the observers who find themselves exactly at the rod's ends, may register that fact, and then subtract their coordinates $x^{\prime}{ }_{1,2}$ to calculate the apparent rod length $l^{\prime}=x_{2}{ }^{\prime}-x_{1}{ }^{\prime}$ in the moving frame. According to Eq. (19a), $l$ may be expressed via $l^{\prime}$ as

$$
\begin{equation*}
l \equiv x_{2}-x_{1}=\gamma\left(x_{2}^{\prime}+\beta c t^{\prime}\right)-\gamma\left(x_{1}^{\prime}+\beta c t^{\prime}\right)=\gamma\left(x_{2}^{\prime}-x_{1}^{\prime}\right)=\gamma l^{\prime}>l^{\prime} . \tag{9.20a}
\end{equation*}
$$

Hence, the rod's length, as measured in the moving reference frame is

Length contraction

$$
\begin{equation*}
l^{\prime}=\frac{l}{\gamma}=l\left(1-\frac{v^{2}}{c^{2}}\right)^{1 / 2} \leq l \tag{9.20b}
\end{equation*}
$$

in accordance with the FitzGerald-Lorentz hypothesis (5). This is the relativistic length contraction effect: an object is always the longest (has the so-called proper length l) if measured in its rest frame. Note that according to Eq. (19), the length contraction takes place only in the direction of the relative motion of two reference frames. As has been noted in Sec. 1, this result immediately explains the zero result of the Michelson-Morley-type experiments, so that they give a convincing evidence (if not an irrefutable proof) of Eq. (20).

[^386](ii) Time dilation. Now let us use Eqs. (19a) to find the time interval $\Delta t$, as measured in frame 0, between two world events - say, two ticks of a clock moving with frame 0 ' (Fig. 5), i.e. having constant values of $x^{\prime}, y^{\prime}$, and $z^{\prime}$.


Fig. 9.5. Relativistic time dilation.

Let the time interval between these two events, measured in clock's rest frame $0^{\prime}$, be $\Delta t^{\prime} \equiv t_{2}{ }^{\prime}-$ $t_{1}$ '. At these two moments, the clock would fly by certain two Einstein's observers at rest in frame 0 , so that they can record the corresponding moments $t_{1,2}$ shown by their clocks, and then calculate $\Delta t$ as their difference. According to the second of Eqs. (19a),

$$
\begin{equation*}
\Delta t \equiv t_{2}-t_{1}=\frac{\gamma}{c}\left[\left(c t_{2}^{\prime}+\beta x^{\prime}\right)-\left(c t_{1}^{\prime}+\beta x^{\prime}\right)\right]=\gamma \Delta t^{\prime} \tag{9.21a}
\end{equation*}
$$

so that, finally,

$$
\begin{equation*}
\Delta t=\gamma \Delta t^{\prime} \equiv \frac{\Delta t^{\prime}}{\left(1-v^{2} / c^{2}\right)^{1 / 2}} \geq \Delta t^{\prime} \tag{9.21b}
\end{equation*}
$$

This is the famous relativistic time dilation (or "dilatation") effect: a time interval is longer if measured in a frame (in our case, frame 0) moving relatively to the clock, while that in the rest frame is the shortest - the so-called proper time interval.

This counter-intuitive effect is the everyday reality at experiments with high-energy elementary particles. For example, in a typical (by no means record-breaking) experiment carried out in Fermilab, a beam of charged 200 GeV pions with $\gamma \approx 1,400$ passed distance $l=300 \mathrm{~m}$ distance with the measured loss of only $3 \%$ of the initial beam intensity due to the pion decay (mostly, into muon-neutrino pairs) with proper lifetime $t_{0} \approx 2.56 \times 10^{-8} \mathrm{~s}$. Without the time dilation, only an $\exp \left\{-1 / c t_{0}\right\} \sim 10^{-17}$ part of the initial pions would survive, while the relativity-corrected number $\exp \{-l / c t\}=\exp \left\{-l / c \gamma t_{0}\right\} \approx 0.97$ was in a full accordance with experimental measurements. As another example, the global positioning system (GPS) is designed with the account of the time dilation due to the velocity of its satellites (and also some gravity-induced, i.e. general-relativity corrections that I do not have time to discuss) and would give large errors without such corrections. So, there is no doubt that time dilation (21) is a reality, though the precision of its experimental tests I am aware of has been limited by a few percent, because of almost unavoidable involvement of gravity effects. ${ }^{16}$

Before the first reliable observation of the time dilation (by B. Rossi and D. Hall in 1940), there had been serious doubts in the reality of this effect, the most famous being the twin paradox first posed (together with an immediate suggestion of its resolution) by P. Langevin in 1911. Let us send one of two twins on a long star journey with a speed $v$ approaching $c$. Upon his return to Earth, who of the twins

[^387]would be older? The naïve approach is to say that due to the relativity principle, not one can be (and hence there is no time dilation), because each twin could claim that his counterpart, rather than himself, was moving, with the same speed $v$, just in the opposite direction. The resolution of the paradox in the general theory of relativity (which can handle gravity and acceleration effects) is that one of the twins had to be accelerated to be brought back, and hence the reference frames have to be dissimilar: only one of them may stay inertial all the time. Because of that, the twin who had been accelerated ("actually traveling") would be younger than his sibling when they meet.
(iii) Velocity transformation. Now let us calculate velocity $\mathbf{u}$ of a particle, as observed in reference frame 0, provided that its velocity, as measured in frame 0 ', is u' (Fig. 6).


Fig. 9.6. Relativistic velocity addition.

Keeping the usual definition of velocity, but with due attention to the relativity of not only spatial but also temporal intervals, we may write

$$
\begin{equation*}
\mathbf{u} \equiv \frac{d \mathbf{r}}{d t}, \quad \mathbf{u}^{\prime} \equiv \frac{d \mathbf{r}^{\prime}}{d t^{\prime}} . \tag{9.21}
\end{equation*}
$$

Plugging in the differentials of the Lorentz transform relations (6a), we get

$$
\begin{equation*}
u_{x}=\frac{d x}{d t}=\frac{d x^{\prime}+v d t^{\prime}}{d t^{\prime}+v d x^{\prime} / c^{2}}=\frac{u_{x}^{\prime}+v}{1+u_{x}^{\prime} v / c^{2}}, \quad u_{y}=\frac{d y}{d t}=\frac{1}{\gamma} \frac{d y^{\prime}}{d t^{\prime}+v d x^{\prime} / c^{2}}=\frac{1}{\gamma} \frac{u_{y}^{\prime}}{1+u_{x}^{\prime} v / c^{2}}, \tag{9.22}
\end{equation*}
$$

and the similar formula for $u_{z}$. In the classical limit $v / c \rightarrow 0$, these relations are reduced to

$$
\begin{equation*}
u_{x}=u_{x}^{\prime}+v, \quad u_{y}=u_{y}^{\prime}, \quad u_{z}=u_{z}^{\prime} \tag{9.23}
\end{equation*}
$$

and may be merged into the familiar Galilean vector form

$$
\begin{equation*}
\mathbf{u}=\mathbf{u}^{\prime}+\mathbf{v}, \text { for } v \ll c \tag{9.24}
\end{equation*}
$$

In order to see how strange the full relativistic rules (22) are, let us first consider a purely longitudinal motion, $u_{y}=u_{z}=0$; then ${ }^{17}$

$$
\begin{equation*}
u=\frac{u^{\prime}+v}{1+u^{\prime} v / c^{2}} \tag{9.25}
\end{equation*}
$$

where $u \equiv u_{x}$ and $u^{\prime} \equiv u^{\prime}{ }_{x}$. Figure 7 shows $u$ as the function of $u^{\prime}$, given by this formula, for several values of the reference frames' relative velocity $v$.

[^388]

Fig. 9.7. Longitudinal velocity addition.

The first sanity check is that if $v=0$, i.e. the reference frames are at rest relative to each other, then $u=u^{\prime}$, as it should be - see the diagonal straight line. Next, if magnitudes of $u$ ' and $v$ are both below $c$, so is the magnitude of $u$. (Also good, because otherwise ordinary particles in one frame would be tachyons in the other one, and the theory would be in a big trouble.) Now strange things start: even as $u$ ' and $v$ are both approaching $c$, then $u$ is also close to $c$, but does not exceed it. As an example, if we fired ahead a bullet with speed $0.9 c$ from a spaceship moving from the Earth also at $0.9 c$, Eq. (25) predicts the speed of the bullet relative to Earth to be just $[(0.9+0.9) /(1+0.9 \times 0.9)] c \approx 0.994 c<c$, rather than $(0.9+0.9) c=1.8 c>c$ as in the Galilean kinematics. We certainly should accept this strangeness of relativity, because it is necessary to fulfill the $2^{\text {nd }}$ Einstein's postulate: the independence of the speed of light in any reference frame. Indeed, for $u^{\prime}= \pm c$, Eq. (25) yields $u= \pm c$, regardless of $v$.

In the opposite case of transverse motion, when a particle moves across the relative motion of the frames (for example, at our choice of coordinates, $u^{\prime}{ }_{x}=u^{\prime}{ }_{z}=0$ ), Eqs. (22) yield a less spectacular result

$$
\begin{equation*}
u_{y}=\frac{u_{y}^{\prime}}{\gamma} \leq u_{y}^{\prime} . \tag{9.26}
\end{equation*}
$$

This effect comes purely from the time dilation, because the transverse coordinates are Lorentzinvariant.

In the case when both $u_{x}$ ' and $u_{y}$ ' are substantial (but $u_{z}{ }^{\prime}$ is still zero), we may divide expressions (22) by each other to relate angles $\theta$ of particle propagation, as observed in the two reference frames:

$$
\begin{equation*}
\tan \theta \equiv \frac{u_{y}}{u_{x}}=\frac{u^{\prime}{ }_{y}}{\gamma\left(u_{x}^{\prime}+v\right)}=\frac{\sin \theta^{\prime}}{\gamma\left(\cos \theta^{\prime}+v / u^{\prime}\right)} . \tag{9.27}
\end{equation*}
$$

This expression describes, in particular, the so-called stellar aberration effect, the dependence of the observed direction $\theta$ toward a star on the speed $v$ of the telescope motion relative to the star - see Fig. 8. (The effect is readily observable experimentally as the annual aberration due to the periodic change of speed $v$ by $2 \nu_{\mathrm{E}} \approx 60 \mathrm{~km} / \mathrm{s}$ because of Earth's rotation about the Sun. Since the aberration's main part
is of the first order in $v_{\mathrm{E}} / C \sim 10^{-4}$, the effect is very significant and has been known since the early 1700s.)


Fig. 9.8. Stellar aberration.

For the analysis of this effect, it is sufficient to take, in Eq. (27), $u^{\prime}=c$, i.e. $v / u^{\prime}=\beta$, and interpret $\theta$ ' as the "proper" direction to the star, that would be measured at $v=0 .{ }^{18}$ At $\beta \ll 1$, both Eq. (27) and the Galilean result (which the reader is invited to derive directly from Fig. 8),

$$
\begin{equation*}
\tan \theta=\frac{\sin \theta^{\prime}}{\cos \theta^{\prime}+\beta}, \tag{9.28}
\end{equation*}
$$

may be well approximated by the first-order term

$$
\begin{equation*}
\Delta \theta \equiv \theta^{\prime}-\theta \approx \beta \sin \theta \tag{9.29}
\end{equation*}
$$

Unfortunately, it is not easy to use the difference between Eqs. (27) and (28), of the second order in $\beta$, for the special relativity confirmation, because other components of Earth's motion, such as its rotation, nutation and torque-induced precession, ${ }^{19}$ give masking first-order contributions to the aberration.

Finally, at a completely arbitrary direction of vector u', Eqs. (22) may be readily used to calculate the velocity magnitude. The most popular form of the resulting expression is for the square of relative velocity (or rather relative reduced velocity $\boldsymbol{\beta}$ ) of two particles,

$$
\begin{equation*}
\beta^{2}=\frac{\left(\boldsymbol{\beta}_{1}-\boldsymbol{\beta}_{2}\right)^{2}-\left|\boldsymbol{\beta}_{1} \cdot \boldsymbol{\beta}_{2}\right|}{\left(1-\boldsymbol{\beta}_{1} \cdot \boldsymbol{\beta}_{2}\right)^{2}} \leq 1 \tag{9.30}
\end{equation*}
$$

where $\boldsymbol{\beta}_{1,2} \equiv \mathbf{v}_{1,2} / c$ are their normalized velocities as measured in the same reference frame.
(iv) The Doppler effect. Now let us consider a plane, monochromatic wave moving along axis $x$ :

$$
\begin{equation*}
f=\operatorname{Re}\left[f_{\omega} \exp \{i(k x-\omega t\}]=\left|f_{\omega}\right| \cos \left(k x-\omega t+\arg f_{\omega}\right) .\right. \tag{9.31}
\end{equation*}
$$

[^389]Its total phase, $\Psi \equiv k x-\omega t+\arg f_{\omega}$ (in contrast to amplitude $\left|f_{\omega}\right|$ !) cannot depend on the observer's reference frame, because all fields of a traveling wave vanish simultaneously at $\Psi=2 \pi n$, (for all integer $n$ ) and such "world events" should take place in all reference frames. The only way to keep $\Psi=\Psi$ ' at all times is to have ${ }^{20}$

$$
\begin{equation*}
k x-\omega t=k^{\prime} x^{\prime}-\omega^{\prime} t^{\prime} . \tag{9.32}
\end{equation*}
$$

First, let us consider the Doppler effect describing usual non-relativistic waves, e.g., oscillations of particles of a certain medium. Using the Galilean transform (2), we may rewrite Eq. (32) as

$$
\begin{equation*}
k\left(x^{\prime}+v t\right)-\omega t=k^{\prime} x^{\prime}-\omega^{\prime} t . \tag{9.33}
\end{equation*}
$$

Since this transform leaves all space intervals (including wavelength $\lambda=2 \pi / k$ ) intact, we can take $k=k$, so that Eq. (33) yields

$$
\begin{equation*}
\omega^{\prime}=\omega-k v . \tag{9.34}
\end{equation*}
$$

For a dispersion-free medium, the wave number $k$ is the ratio of its frequency $\omega$, as measured in the reference frame bound to the medium, and the wave velocity $v_{w}$. In particular, if the wave source rests in the medium, we can bind frame 0 to the medium as well, and frame 0 ' to wave's receiver (so that $v=v_{r}$ ), so that

$$
\begin{equation*}
k=\frac{\omega}{v_{w}}, \tag{9.35}
\end{equation*}
$$

and for the frequency perceived by the receiver, Eq. (34) yields

$$
\begin{equation*}
\omega^{\prime}=\omega \frac{v_{w}-v_{r}}{v_{w}} \tag{9.36}
\end{equation*}
$$

On the other hand, if the receiver and the medium are at rest in reference frame 0 ', while the wave source is bound to frame 0 (so that $v=-v_{s}$ ), Eq. (35) should be replaced with

$$
\begin{equation*}
k=k^{\prime}=\frac{\omega^{\prime}}{v_{w}} \tag{9.37}
\end{equation*}
$$

and Eq. (34) yields a different result:

$$
\begin{equation*}
\omega^{\prime}=\omega \frac{v_{w}}{v_{w}-v_{s}} \tag{9.38}
\end{equation*}
$$

Finally, if both the source and detector are moving, it is straightforward to combine these two results to get the general relation

$$
\begin{equation*}
\omega^{\prime}=\omega \frac{v_{w}-v_{r}}{v_{w}-v_{s}} . \tag{9.39}
\end{equation*}
$$

At low speeds of both the source and receiver, this result simplifies,

[^390]\[

$$
\begin{equation*}
\omega^{\prime} \approx \omega(1-\beta), \quad \beta \equiv \frac{v_{r}-v_{s}}{v_{w}}, \tag{9.40}
\end{equation*}
$$

\]

but at speeds comparable to $v_{w}$ we have to use the more general Eq. (39). Thus, the usual Doppler effect is affected not only by the relative speed ( $v_{r}-v_{s}$ ) of wave's source and detector, but also of their speeds relative to the medium in which waves propagate.

Somewhat counter-intuitively, for the electromagnetic waves the calculations are simpler, because for them the propagation medium (ether) does not exist, wave velocity equals $\pm c$ in any reference frame, and there are no two separate cases: we can always take $k= \pm \omega / c, k^{\prime}= \pm \omega^{\prime} / c$. Plugging these relations, together with the Lorentz transform (19a), into the phase-invariance equation (32), we get

$$
\begin{equation*}
\pm \frac{\omega}{c} \gamma\left(x^{\prime}+\beta c t^{\prime}\right)-\omega \gamma \frac{c t^{\prime}+\beta x^{\prime}}{c}= \pm \frac{\omega^{\prime}}{c} x^{\prime}-\omega^{\prime} t^{\prime} . \tag{9.41}
\end{equation*}
$$

This relation has to hold for any $x^{\prime}$ and $t^{\prime}$, so we may require the net coefficients before these variables to vanish. These two requirements yield the same condition:

$$
\begin{equation*}
\omega^{\prime}=\omega \gamma(1 \mp \beta) \tag{9.42}
\end{equation*}
$$

This result is already quite simple, but may be transformed further to be even more illuminating:

$$
\begin{equation*}
\omega^{\prime}=\omega \frac{1 \mp \beta}{\left(1-\beta^{2}\right)^{1 / 2}}=\omega\left[\frac{(1 \mp \beta)(1 \mp \beta)}{(1+\beta)(1-\beta)}\right]^{1 / 2} . \tag{9.43}
\end{equation*}
$$

At any sign before $\beta$, one pair of parentheses cancel, so that

$$
\begin{equation*}
\omega^{\prime}=\omega\left(\frac{1 \mp \beta}{1 \pm \beta}\right)^{1 / 2} \tag{9.44}
\end{equation*}
$$

(It may look like the reciprocal expression of $\omega$ via $\omega^{\prime}$ is different, violating the relativity principle. However, in this case we have to change the sign of $\beta$, because the relative velocity of the system is opposite, so we come down to Eq. (44) again.)

Thus the Doppler effect for electromagnetic waves depends only on the relative velocity $v=\beta c$ between the wave source and detector - as it should be, given the absence of the ether. At velocities much below $c$, Eq. (43) may be crudely approximated as

$$
\begin{equation*}
\omega^{\prime} \approx \omega \frac{1 \mp \beta / 2}{1 \pm \beta / 2} \approx \omega(1 \mp \beta) \tag{9.45}
\end{equation*}
$$

i.e. in the first approximation in $\beta \equiv v / c$ it coincides with the corresponding limit (38) of the usual Doppler effect. However, even at $v \ll c$ there is still a difference of the order of $(v / c)^{2}$ between the Galilean and Lorentzian relations.

If the wave vector $\mathbf{k}$ is tilted by angle $\theta$ to vector $\mathbf{v}$ (as measured in frame 0 ), then we have to repeat the calculations, with $k$ replaced by $k_{x}$, and components $k_{y}$ and $k_{z}$ left intact at the Lorentz transform. As a result, Eq. (42) is generalized as

$$
\begin{equation*}
\omega^{\prime}=\omega \gamma(1-\beta \cos \theta) . \tag{9.46}
\end{equation*}
$$

For the cases $\cos \theta= \pm 1$, Eq. (44) reduces to our previous result. However, at $\theta=\pi / 2$ (i.e. $\cos \theta=0$ ), the relation is rather different:

$$
\begin{equation*}
\omega^{\prime}=\gamma \omega=\frac{\omega}{\left(1-\beta^{2}\right)^{1 / 2}} . \tag{9.47}
\end{equation*}
$$

This is the transverse Doppler effect - which is completely absent in the non-relativistic physics. Its first experimental evidence was obtained using electron beams (as suggested in 1906 by J. Stark), by H. Ives and G. Stilwell in 1938 and 1941. Later, similar experiments were repeated several times, but the first unambiguous measurement were performed only in 1979 by D. Hasselkamp et al. who confirmed Eq. (47) with a relative accuracy about $10 \%$. This precision may not look too spectacular, but besides the special tests discussed above, the Lorentz transform formulas have been also confirmed, less directly, by a huge body of other experimental data, especially in high energy physics, being in agreement with calculations incorporating the transform as their part. This is why, with every respect to the challenging authority spirit, I should warn the reader: you decide to challenge the relativity theory (that is called "theory" by tradition only), you would also need to explain all these data. ${ }^{21}$ Best luck with that!

### 9.3. 4-vectors, momentum, mass, and energy

Before proceeding to relativistic dynamics, let us discuss a mathematical language that makes all the calculations more compact - and more beautiful. We have already seen that spatial coordinates $\{x, y$, $z\}$ and product $c t$ are Lorentz-transformed similarly - see Eqs. (19). So it is natural to consider them as components of a 4-component vector (or, for short, 4-vector),

$$
\begin{equation*}
\left\{x_{0}, x_{1}, x_{2}, x_{3}\right\}=\{c t, \mathbf{r}\}, \tag{9.48}
\end{equation*}
$$

with components

$$
\begin{equation*}
x_{0}=c t, \quad x_{1}=x, \quad x_{2}=y, \quad x_{3}=z . \tag{9.49}
\end{equation*}
$$

According to Eqs. (19), its components are Lorentz-transformed as

$$
\begin{equation*}
x_{j}=\sum_{j^{\prime}=0}^{3} L_{j j^{\prime}, X^{\prime}}{ }_{j^{\prime}}, \tag{9.50}
\end{equation*}
$$

[^391]mentioned in Sec. 8.9, the usual (3D) vector is not just any ordered set (string) of three scalars $\left\{A_{x}, A_{y}\right.$, $\left.A_{z}\right\}$; if we want it to represent a reference-frame-independent physical variable, vector components have to obey certain rules at transfer from one reference frame to another. In particular, vector's 3D norm (magnitude squared),
\[

$$
\begin{equation*}
A^{2}=A_{x}^{2}+A_{y}^{2}+A_{z}^{2}, \tag{9.52}
\end{equation*}
$$

\]

should be an invariant at the Galilean transform (2). However, a naïve extension of this formula to 4vectors would not work, because, according to the calculations of Sec. 1, the Lorentz transform keeps intact combinations of the type (7), with one sign negative, rather than the sum of all components squared. Hence for the 4 -vector all the rules of the game have to be reviewed and adjusted - or rather redefined from the very beginning.

Arbitrary 4 -vector is a string of 4 scalars,

General 4 -vector

$$
\begin{equation*}
\left\{A_{0}, A_{1}, A_{2}, A_{3}\right\} \tag{9.53}
\end{equation*}
$$

defined in 4D Minkowski space, ${ }^{22}$ whose components $A_{j}$, as measured in systems 0 and 0 ', shown in Fig. 1, obey the Lorentz transform similar to Eq. (50):

General 4-vector's Lorentz transform

Lorentz invariance

$$
\begin{equation*}
A_{j}=\sum_{j^{\prime}=0}^{3} L_{i j^{\prime}} A_{j^{\prime}}^{\prime} \tag{9.54}
\end{equation*}
$$

As we have already seen on the example of the space-time 4-vector (48), this means in particular that
$\square$

$$
\begin{equation*}
A_{0}^{2}-\sum_{j=1}^{3} A_{j}^{2}=\left(A_{0}^{\prime}\right)^{2}-\sum_{j=1}^{3}\left(A_{j}^{\prime}\right)^{2} \tag{9.55}
\end{equation*}
$$

This is the so-called Lorentz invariance condition of the norm of the 4 -vector. (The difference between this relation and Eq. (52), pertaining to the Euclidian geometry, is the reason why the Minkowski space is called pseudo-Euclidian.) It is also straightforward to use Eqs. (51) and (54) to check that an evident generalization of the norm, the scalar product of two arbitrary 4 -vectors,

Scalar 4-product

$$
\begin{equation*}
A_{0} B_{0}-\sum_{j=1}^{3} A_{j} B_{j} \tag{9.56}
\end{equation*}
$$

is also Lorentz-invariant.
Now consider the 4 -vector corresponding to a infinitesimal interval between two close world events:

$$
\begin{equation*}
\left\{d x_{0}, d x_{1}, d x_{2}, d x_{3}\right\}=\{c d t, d \mathbf{r}\} \tag{9.57}
\end{equation*}
$$

its norm,

Interval between two close events

$$
\begin{equation*}
(d s)^{2} \equiv d x_{0}^{2}-\sum_{j=1}^{3} d x_{j}^{2}=c^{2}(d t)^{2}-(d r)^{2} \tag{9.58}
\end{equation*}
$$

[^392]is of course also Lorentz-invariant. Since the speed of any particle (or signal) cannot be larger than $c$, for any pair of world events that are in a causal relation with each other, $d r$ cannot be larger than $c d t$, i.e. such time-like interval $(d s)^{2}$ cannot be negative. The 4D surface separating such intervals from spacelike intervals (ds) ${ }^{2}<0$ is called the light cone (Fig. 9).


Fig. 9.9. $2+1$ dimensional image of the light cone (which is actually $3+1$ dimensional).

Now let us assume that these two close world events happen with the same particle that moves with velocity $\mathbf{u}$. Then in the frame moving with a particle $(\mathbf{v}=\mathbf{u})$, the last term in the right-hand part of Eq. (58) equals zero, so that

$$
\begin{equation*}
d s=c d \tau \tag{9.59}
\end{equation*}
$$

where $d \tau$ is the proper time interval. But according to Eq. (21), this means that we can write

$$
\begin{equation*}
d \tau=\frac{d t}{\gamma} \tag{9.60}
\end{equation*}
$$

where $d t$ is the time interval in an arbitrary (besides being inertial) reference frame, while

$$
\begin{equation*}
\boldsymbol{\beta} \equiv \frac{\mathbf{u}}{c} \quad \text { and } \gamma \equiv \frac{1}{\left(1-\beta^{2}\right)^{1 / 2}}=\frac{1}{\left(1-u^{2} / c^{2}\right)^{1 / 2}} \tag{9.61}
\end{equation*}
$$

are the parameters (17) corresponding to particle's velocity ( $\mathbf{u}$ ) in that frame, so that $d s=c d t / \gamma^{23}$
Now, let us explore whether a 4 -vector can be formed using spatial components of particle's velocity

$$
\begin{equation*}
\mathbf{u}=\left\{\frac{d x}{d t}, \frac{d y}{d t}, \frac{d z}{d t}\right\} . \tag{9.62}
\end{equation*}
$$

Here we have a slight problem: as Eqs. (22) show, these components do not obey the Lorentz transform. However, let us use $d \tau \equiv d t / \gamma$, the proper time interval of the particle, to form the following string:

[^393]\[

$$
\begin{equation*}
\left\{\frac{d x_{0}}{d \tau}, \frac{d x_{1}}{d \tau}, \frac{d x_{2}}{d \tau}, \frac{d x_{3}}{d \tau}\right\}=\gamma\left\{c, \frac{d x}{d t}, \frac{d y}{d t}, \frac{d z}{d t}\right\}=\gamma\{c, \mathbf{u}\} . \tag{9.63}
\end{equation*}
$$

\]

As follows from comparison of the first form of this expression with Eq. (48), since the time-space vector obeys the Lorentz transform, and $\tau$ is Lorentz-invariant, string (63) is a legitimate 4 -vector. It is called the 4-velocity of the particle.

Now we are properly equipped to proceed to dynamics. Let us start with such basic notions of momentum $\mathbf{p}$ and energy $\varepsilon$ - so far, for a free particle. ${ }^{24}$ Perhaps the most elegant way to "derive" (or rather guess ${ }^{25}$ ) expressions for $\mathbf{p}$ and $\varepsilon$ as functions of particle's velocity $\mathbf{u}$ is based on analytical mechanics. Due to the conservation of $\mathbf{v}$, the trajectory of a free particle in the 4D Minkowski space is always a straight line. Hence, from the Hamilton principle of minimum action, ${ }^{26}$ we may expect its action $S$, between points 1 and 2 , to be a linear function of the space-time interval (59):

Free
particle's action

$$
\begin{equation*}
\mathcal{S}=\alpha \int_{1}^{2} d s=\alpha c \int_{1}^{2} d \tau=\alpha c \int_{t_{1}}^{t_{2}} \frac{d t}{\gamma} \tag{9.64}
\end{equation*}
$$

where $\alpha$ is some constant. On the other hand, in analytical mechanics the action is defined as

$$
\begin{equation*}
\mathcal{S}=\int_{t_{1}}^{t_{2}} \mathcal{L} d t \tag{9.65}
\end{equation*}
$$

where $\mathcal{L}$ is particle's Lagrangian function. ${ }^{27}$ Comparing these two expressions, we get

$$
\begin{equation*}
\mathcal{L}=\frac{\alpha c}{\gamma}=\alpha c\left(1-\frac{u^{2}}{c^{2}}\right)^{1 / 2} . \tag{9.66}
\end{equation*}
$$

In the non-relativistic limit $(u \ll c)$, this function tends to

$$
\begin{equation*}
\mathcal{L} \approx \alpha c\left(1-\frac{u^{2}}{2 c^{2}}\right)=\alpha c-\frac{\alpha u^{2}}{2 c} . \tag{9.67}
\end{equation*}
$$

In order to correspond to the Newtonian mechanics, the last (velocity-dependent) term should equal $m u^{2} / 2$. From here we find $\alpha=-m c$, so that, finally,

Free particle's Lagrangian function

$$
\begin{equation*}
\mathcal{L}=-m c^{2}\left(1-\frac{u^{2}}{c^{2}}\right)^{1 / 2} \tag{9.68}
\end{equation*}
$$

[^394]Now we can find Cartesian components $p_{j}$ of particle's momentum, as the generalized momenta corresponding to components $r_{j}(j=1,2,3)$ of the 3D radius-vector $\mathbf{r}$ : ${ }^{28}$

$$
\begin{equation*}
p_{j}=\frac{\partial \mathcal{L}}{\partial \dot{r}_{j}}=\frac{\partial \mathscr{L}}{\partial u_{j}}=-m c^{2} \frac{\partial}{\partial u_{j}}\left(1-\frac{u_{1}^{2}+u_{2}^{2}+u_{3}^{2}}{c^{2}}\right)^{1 / 2}=\frac{m u_{j}}{\left(1-u^{2} / c^{2}\right)^{1 / 2}}=m \gamma u_{j} . \tag{9.69}
\end{equation*}
$$

Thus for the 3D vector of momentum, we can write the result in the same form as in non-relativistic mechanics,

$$
\begin{equation*}
\mathbf{p}=m \gamma \mathbf{u}=M \mathbf{u} \tag{9.70}
\end{equation*}
$$

if we introduce the reference-frame-dependent scalar $M$ (called the relativistic mass) defined as

$$
\begin{equation*}
M \equiv m \gamma=\frac{m}{\left(1-u^{2} / c^{2}\right)^{1 / 2}} \geq m \tag{9.71}
\end{equation*}
$$

$m$ being the non-relativistic mass of the particle. (It is also called the rest mass, because in the reference frame in that the particle rests, Eq. (71) yields $M=m$.)

Next, let us return to analytical mechanics to calculate particle's energy $\varepsilon$ (which for a free particle coincides with the Hamiltonian function $\not \not F):{ }^{27}$

$$
\begin{equation*}
\varepsilon=\not \mathcal{H}=\sum_{j=1}^{3} p_{j} u_{j}-\mathcal{L}=\mathbf{p} \cdot \mathbf{u}-\mathcal{L}=\frac{m u^{2}}{\left(1-u^{2} / c^{2}\right)^{1 / 2}}+m c^{2}\left(1-\frac{u^{2}}{c^{2}}\right)=\frac{m c^{2}}{\left(1-u^{2} / c^{2}\right)^{1 / 2}} . \tag{9.72}
\end{equation*}
$$

Thus, we have arrived at the most famous of Einstein's formulas (and probably the most famous formula of physics as a whole),

$$
\begin{equation*}
\varepsilon=m \gamma c^{2}=M c^{2} \tag{9.73}
\end{equation*}
$$

that expresses the relation between particle's mass and energy. ${ }^{29}$ In the non-relativistic limit, it reduces to

$$
\begin{equation*}
\varepsilon=\frac{m c^{2}}{\left(1-u^{2} / c^{2}\right)^{1 / 2}} \approx m c^{2}\left(1+\frac{u^{2}}{2 c^{2}}\right)=m c^{2}+\frac{m u^{2}}{2} \tag{9.74}
\end{equation*}
$$

the first term $m c^{2}$ being called the rest energy of a particle.
Now let us consider the following string of 4 scalars:

$$
\begin{equation*}
\left\{\frac{\varepsilon}{c}, p_{1}, p_{2}, p_{3}\right\}=\left\{\frac{\varepsilon}{c}, \mathbf{p}\right\} . \tag{9.75}
\end{equation*}
$$

Using Eqs. (70) and (73) to present this expression as

[^395]\[

$$
\begin{equation*}
\left\{\frac{\varepsilon}{c}, \mathbf{p}\right\}=m \gamma\{c, \mathbf{u}\} \tag{9.76}
\end{equation*}
$$

\]

and comparing the result with Eq. (63), we immediately see that, since $m$ is Lorentz-invariant, this string is a legitimate 4 -vector of energy-momentum. As a result, its norm,

$$
\begin{equation*}
\left(\frac{\varepsilon}{c}\right)^{2}-p^{2} \tag{9.77}
\end{equation*}
$$

is Lorentz-invariant, and in particular has to be equal to the norm in the particle rest frame. But in that frame, $p=0$, and $\varepsilon=m c^{2}$, so that in an arbitrary frame

$$
\begin{equation*}
\left(\frac{\varepsilon}{c}\right)^{2}-p^{2}=(m c)^{2} \tag{9.78a}
\end{equation*}
$$

This very important relation ${ }^{30}$ between the relativistic energy and momentum (valid for free particles only!) is usually presented in the form ${ }^{31}$

$$
\begin{equation*}
\varepsilon^{2}=\left(m c^{2}\right)^{2}+(p c)^{2} \tag{9.78b}
\end{equation*}
$$

According to Eq. (70), in the ultra-relativistic limit $u \rightarrow c, p$ tends to infinity while $m c^{2}$ stays constant, so that $p c \gg m c^{2}$. As follows from Eq. (78), in this limit $\varepsilon \approx p c$. Though the above discussion was for particles with finite $m$, the 4 -vector formalism allows us to consider particles with zero rest mass as ultra-relativistic particles for which the above energy-to-moment relation,

$$
\begin{equation*}
\varepsilon=p c, \quad \text { for } m=0 \tag{9.79}
\end{equation*}
$$

is exact. Quantum electrodynamics ${ }^{32}$ tells us that under certain conditions, electromagnetic field quanta (photons) may be also considered as such massless particles, with momentum $\mathbf{p}=\hbar \mathbf{k}$. Plugging (the modulus of) the last relation into Eq. (78), for photon's energy we get $\varepsilon=p c=\hbar k c=\hbar \omega$. Please note that according to Eq. (73), the relativistic mass of a photon is finite: $M=\varepsilon / c^{2}=\hbar \omega / c^{2}$, so that the term "massless particle" has a limited meaning: $m=0$. For example, the mass of an optical phonon is of the order of $10^{-36} \mathrm{~kg}$. This is not too much, but still a noticeable (approximately one-millionth) part of the rest mass $m_{e}$ of an electron.

The fundamental relations (70) and (73) have been repeatedly verified in numerous particle collision experiments, in which the total energy and momentum of a system of particles are conserved at the same conditions at in the non-relativistic dynamics. (For momentum, this is the absence of external forces, and for energy, the elasticity of particle interactions - in other words, the absence of alternative channels of energy escape.) Of course, generally, the total energy of the system is conserved, including the potential energy of particle interactions. However, at typical particle collisions, the

[^396]potential energy vanishes so rapidly with the distance between them that we can use the momentum and energy conservation using Eq. (73).

As an example, let us calculate the minimum energy $\mathcal{\varepsilon}_{\text {min }}$ of a proton $\left(\mathrm{p}_{a}\right)$, necessary for the well-known high-energy reaction that generates a new proton-antiproton pair, $\mathrm{p}_{a}+\mathrm{p}_{b} \rightarrow \mathrm{p}+\mathrm{p}+\mathrm{p}+\bar{p}$, provided that before the collision, proton $\mathrm{p}_{b}$ has been at rest in the lab frame. This minimum evidently corresponds to the vanishing relative velocity of the reaction products, i.e. their motion with virtually the same velocity $\left(\mathbf{u}_{\text {fin }}\right)$, as seen from the lab frame - see Fig. 10.


Fig. 9.10. High-energy proton reaction at $\varepsilon \approx \varepsilon_{\text {min }}$ - schematically.

Due to the momentum conservation, this velocity should have the same direction as the initial velocity ( $\mathbf{u}_{\text {min }}$ ) of proton $p_{a}$. This is why two scalar equations: of for the energy conservation,

$$
\begin{equation*}
\frac{m c^{2}}{\left(1-u_{\min }^{2} / c^{2}\right)^{1 / 2}}+m c^{2}=\frac{4 m c^{2}}{\left(1-u_{\mathrm{fin}}^{2} / c^{2}\right)^{1 / 2}}, \tag{9.80a}
\end{equation*}
$$

and momentum conservation,

$$
\begin{equation*}
\frac{m u}{\left(1-u_{\min }^{2} / c^{2}\right)^{1 / 2}}+0=\frac{4 m u_{\mathrm{fin}}}{\left(1-u_{\mathrm{fin}}^{2} / c^{2}\right)^{1 / 2}}, \tag{9.80b}
\end{equation*}
$$

are sufficient to find both $u_{\text {min }}$ and $u_{\text {fin }}$. After a conceptually simple but rather tedious solution of this system of two nonlinear equations, we get

$$
\begin{equation*}
u_{\min }=\frac{4 \sqrt{3}}{7} c, \quad u_{\text {fin }}=\frac{\sqrt{3}}{2} c . \tag{9.81}
\end{equation*}
$$

Finally, we can use Eq. (73) to calculate the required energy: $\varepsilon_{\min }=7 \mathrm{mc}^{2}$. (Note that of the acceleration energy $6 m c^{2}$, only $2 m c^{2}$ go into the "useful" proton-antiproton pair production.) Proton's rest mass, $m_{p} \approx$ $1.67 \times 10^{-27} \mathrm{~kg}$, corresponds to the rest energy $m c^{2} \approx 1.502 \times 10^{-10} \mathrm{~J} \approx 0.938 \mathrm{GeV}$, so that $\varepsilon_{\min } \approx 6.57 \mathrm{GeV}$.

The second, more intelligent way to solve the same problem is to use the center-of-mass (c.o.m.) reference frame that, in relativity, is defined as the frame in which the total momentum of the system vanishes. ${ }^{33}$ In this frame, at $\varepsilon=\varepsilon_{\text {min }}$, the velocity and momenta of all reaction products are equal to zero, while velocities of protons $\mathrm{p}_{a}$ and $\mathrm{p}_{b}$ before the collision are equal and opposite, with some magnitude $u$ '. Hence the energy conservation law becomes

$$
\begin{equation*}
\frac{2 m c^{2}}{\left(1-u^{\prime 2} / c^{2}\right)^{1 / 2}}=4 m c^{2} \tag{9.82}
\end{equation*}
$$

[^397]readily giving $u^{\prime}=(\sqrt{3} / 2) c$. This is of course the same result as Eq. (81) gives for $u_{\text {fin }}$. Now we can use the fact that the velocity of proton $\mathrm{p}_{b}$ in the c.o.m. frame is $\left(-u^{\prime}\right)$, and hence the speed of proton $\mathrm{p}_{a}$ is $(+u ')$. Hence we may find the lab-frame speed of proton $p_{a}$ using the velocity transform formula (25):
\[

$$
\begin{equation*}
u_{\min }=\frac{2 u^{\prime}}{1+u^{\prime 2} / c^{2}} \tag{9.83}
\end{equation*}
$$

\]

This relation gives the same result as the first method, $u_{\min }=(4 \sqrt{ } 3 / 7) c$, but in a much simpler way.

### 9.4. More on 4-vectors and 4-tensors

This is a good moment to describe a formalism that will allow us, in particular, to solve the same proton collision problem in one more (and arguably, the most elegant) way. More importantly, this formalism will be virtually necessary for the description of the Lorentz transform of the electromagnetic field, and its interaction with relativistic particles - otherwise the formulas would be too cumbersome. Let us call the 4 -vectors we have used before,

$$
\begin{equation*}
A^{\alpha} \equiv\left\{A_{0}, \mathbf{A}\right\}, \tag{9.84}
\end{equation*}
$$

contravariant, and denote them with the top index, and introduce also covariant vectors,

$$
\begin{equation*}
A_{\alpha} \equiv\left\{A_{0},-\mathbf{A}\right\} \tag{9.85}
\end{equation*}
$$

marked by the lower index. Now if we form a scalar product of these vectors using the standard (3Dlike) rule, just as a sum of the products of the corresponding components, we immediately get

$$
\begin{equation*}
A_{\alpha} A^{\alpha} \equiv A^{\alpha} A_{\alpha} \equiv A_{0}^{2}-A^{2} \tag{9.86}
\end{equation*}
$$

Here and below the sign of sum of four components of the product has been dropped. ${ }^{34}$
The scalar product (86) is just the norm of the 4 -vector in our former definition, and as we already know, is Lorentz-invariant. Moreover, the scalar product of two different vectors (also a Lorentz invariant), may be written in any of two similar forms: ${ }^{35}$

## Scalar product <br> forms

$$
\begin{equation*}
A_{0} B_{0}-\mathbf{A} \cdot \mathbf{B} \equiv A_{\alpha} B^{\alpha}=A^{\alpha} B_{\alpha} \tag{9.87}
\end{equation*}
$$

again, the only caveat is to take one vector in the covariant, and another in the contravariant form.
Now let us return to our sample problem (Fig. 10). Since all components ( $\mathcal{L} / \mathrm{c}$ and $\mathbf{p}$ ) of the total 4-momentum of our system are conserved at the collision, its norm is conserved as well:

$$
\begin{equation*}
\left(p_{a}+p_{b}\right)_{\alpha}\left(p_{a}+p_{b}\right)^{\alpha}=(4 p)_{\alpha}(4 p)^{\alpha} . \tag{9.88}
\end{equation*}
$$

Since now the vector product is the usual math construct, we know that the parentheses in the left-hand part of this equation may be multiplied as usual. We may also swap the operands and move constant factors around as convenient. As a result, we get

[^398]\[

$$
\begin{equation*}
\left(p_{a}\right)_{\alpha}\left(p_{a}\right)^{\alpha}+\left(p_{b}\right)_{\alpha}\left(p_{b}\right)^{\alpha}+2\left(p_{a}\right)_{\alpha}\left(p_{b}\right)^{\alpha}=16 p_{\alpha} p^{\alpha} . \tag{9.89}
\end{equation*}
$$

\]

Thanks to the Lorentz-invariance of each of the terms, we can calculate each of them in the reference frame we like. For the first two terms in left-hand part, as well as for the right-hand part term, it is beneficial to use the frames in which that particular proton is at rest; as a result, each of the lefthand part terms equals $(m c)^{2}$, while the right-hand part equals $16(m c)^{2}$. On the contrary, the last term of the left-hand part is better evaluated in the lab frame, because in that frame the three spatial components of the 4 -momentum $p_{b}$ vanish, and the scalar product is the just the product of scalars $\varepsilon / c$ for protons $a$ and $b$. For the latter proton this is just $m c$, so that we get a simple equation,

$$
\begin{equation*}
(m c)^{2}+(m c)^{2}+2 \frac{\varepsilon_{\min }}{c} m c=16(m c)^{2}, \tag{9.90}
\end{equation*}
$$

immediately giving the final result: $\varepsilon_{\min }=7 m c^{2}$ we have already had.
Let me hope that this example was a convincing demonstration of the convenience of presenting 4 -vectors in the contravariant (84) and covariant (85) forms, ${ }^{36}$ with Lorentz-invariant norms (86). To be useful for more complex tasks, the formalism should be developed a little bit further. In particular, it is crucial to know how do the 4 -vectors change under the Lorentz transform. For contravariant vectors, we already know the answer (54), but let us rewrite it in the new notation:

$$
\begin{equation*}
A^{\alpha}=L_{\beta}^{\alpha} A^{\prime \beta} \tag{9.91}
\end{equation*}
$$

where $L_{\beta}^{\alpha}$ is the mixed Lorentz tensor (51):37

$$
L_{\beta}^{\alpha}=\left(\begin{array}{cccc}
\gamma & \beta \gamma & 0 & 0  \tag{9.92}\\
\beta \gamma & \gamma & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right)
$$

Note that though the position of indices $\alpha$ and $\beta$ in the Lorentz tensor notation is not crucial, because it is symmetric, it is convenient to place them using the general index balance rule: the difference of the numbers of the upper and lower indices should be the same in both parts of any 4 -vector/tensor equality, with the top index in the denominator of a fraction counted as a bottom index in the numerator, and vice versa. (Check yourself that all our formulas above do satisfy this rule.)

In order to rewrite Eq. (91) in a more general form that would not depend on the particular orientation of the coordinate axes (Fig. 1), let us use the contravariant and covariant forms of the 4vector of the time-space interval (57),

[^399]\[

$$
\begin{equation*}
d x^{\alpha}=\{c d t, d \mathbf{r}\}, \quad d x_{\alpha}=\{c d t,-d \mathbf{r}\} ; \tag{9.93}
\end{equation*}
$$

\]

then its norm (58) may be presented as ${ }^{38}$

$$
\begin{equation*}
(d s)^{2} \equiv(c d t)^{2}-(d r)^{2}=d x^{\alpha} d x_{\alpha}=d x_{\alpha} d x^{\alpha} \tag{9.94}
\end{equation*}
$$

Applying Eq. (91) to the contravariant form of vector (93), we get

$$
\begin{equation*}
d x^{\alpha}=L_{\beta}^{\alpha} d x^{\prime \beta} . \tag{9.95}
\end{equation*}
$$

But, with our new shorthand notation, we can also write the usual rule of differentiation of each component $x^{\alpha}$, considering it as a (in our case, linear) function of $4 \operatorname{arguments} x^{, \beta}$, as follows:

$$
\begin{equation*}
d x^{\alpha}=\frac{\partial x^{\alpha}}{\partial x^{\prime \beta}} d x^{\prime \beta} . \tag{9.96}
\end{equation*}
$$

Comparing Eqs. (95) and (96), we can rewrite the general Lorentz transform rule (92) in the new form,

$$
\begin{equation*}
A^{\alpha}=\frac{\partial x^{\alpha}}{\partial x^{\prime \beta}} A^{\prime \beta} \tag{9.97a}
\end{equation*}
$$

which evidently does not depend on the coordinate axes orientation.
It is straightforward to verify that the reciprocal transform may be presented as

Reciprocal
Lorentz transform

$$
\begin{equation*}
A^{\prime \alpha}=\frac{\partial x^{\prime \alpha}}{\partial x^{\beta}} A^{\beta} \tag{9.97b}
\end{equation*}
$$

However, the reciprocal transform differs from the direct one only by the sign of the relative velocity of the frames, so that for the coordinate choice shown in Fig. 1, the matrix is

$$
\frac{\partial x^{\prime \alpha}}{\partial x^{\beta}}=\left(\begin{array}{cccc}
\gamma & -\beta \gamma & 0 & 0  \tag{9.98}\\
-\beta \gamma & \gamma & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right),
$$

Since, according to Eqs. (84)-(85), covariant 4-vectors differ from the contravariant ones by the sign of the spatial components, their direct transform is given by matrix (98). Hence their direct and reciprocal transforms may be represented, respectively, as
${ }^{38}$ Another way to write this relation is $(d s)^{2}=g_{\alpha \beta} d x^{\alpha} d x^{\beta}=g^{\alpha \beta} d x_{\alpha} d x_{\beta}$, where double summation over indices $\alpha$ and $\beta$ is implied, and $g$ is the so-called metric tensor,

$$
g^{\alpha \beta} \equiv g_{\alpha \beta} \equiv\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{array}\right)
$$

that may be used, in particular, to a transfer a covariant vector into the corresponding contravariant one and back: $A^{\alpha}=g^{\alpha \beta} A_{\beta}, A_{\alpha}=g_{\alpha \beta} A^{\beta}$. The metric tensor plays a key role in general relativity, in which it is affected by gravity - "curved" by particle masses.

$$
\begin{equation*}
A_{\alpha}=\frac{\partial x^{\prime \beta}}{\partial x^{\alpha}} A_{\beta}^{\prime}, \quad A_{\alpha}^{\prime}=\frac{\partial x^{\beta}}{\partial x^{\prime \alpha}} A_{\beta} \tag{9.99}
\end{equation*}
$$

evidently satisfying the index balance rule. (Note that primed quantities are now multiplied, rather than divided as in the contravariant case.) As a sanity check, let us apply this formalism to the scalar product $A_{\alpha} A^{\alpha}$. As Eq. (96) shows, the implicit summation notation allows us to multiply and divide any equality by the same partial differential of a coordinate, so that we can write:

$$
\begin{equation*}
A_{\alpha} A^{\alpha}=\frac{\partial x^{\prime \beta}}{\partial x^{\alpha}} \frac{\partial x^{\alpha}}{\partial x^{\prime \gamma}} A_{\beta}^{\prime} A^{\prime \gamma}=\frac{\partial x^{\beta}}{\partial x^{\prime \gamma}} A_{\beta}^{\prime} A^{\prime \gamma}=\delta_{\beta \gamma} A_{\beta}^{\prime} A^{\prime \gamma}=A_{\gamma}^{\prime} A^{\prime \gamma}, \tag{9.100}
\end{equation*}
$$

i.e. the scalar product $A_{\alpha} A^{\alpha}$ (as well as $A^{\alpha} A_{\alpha}$ ) is Lorentz-invariant, as it should be.

Now, let us consider the 4 -vectors of derivatives. Here we should be very careful. Consider, for example, the following vector operator

$$
\begin{equation*}
\frac{\partial}{\partial x^{\alpha}} \equiv\left\{\frac{\partial}{\partial(c t)}, \nabla\right\} \tag{9.101}
\end{equation*}
$$

As was discussed above, the operator is not changed by its multiplication and division by another differential, e.g., $\partial x^{, \beta}$ (with the corresponding implied summation over $\beta$ ), so that

$$
\begin{equation*}
\frac{\partial}{\partial x^{\alpha}}=\frac{\partial x^{\prime \beta}}{\partial x^{\alpha}} \frac{\partial}{\partial x^{\prime \beta}} . \tag{9.102}
\end{equation*}
$$

But, according to the first of Eqs. (99), this is exactly how the covariant vectors are Lorentztransformed! Hence, we have to consider the derivative over a contravariant space-time interval as a covariant 4 -vector, and vice versa. ${ }^{39}$ (This result might be also expected from the index balance rule.) In particular, this means that the scalar product

$$
\begin{equation*}
\frac{\partial}{\partial x^{\alpha}} A^{\alpha} \equiv \frac{\partial A_{0}}{\partial(c t)}+\nabla \cdot \mathbf{A} \tag{9.103}
\end{equation*}
$$

should be Lorentz-invariant for any legitimate 4 -vector. A convenient shorthand for the covariant derivative, which complies with the index balance rule, is

$$
\begin{equation*}
\frac{\partial}{\partial x^{\alpha}} \equiv \partial_{\alpha} \tag{9.104}
\end{equation*}
$$

so that the invariant scalar product may be written just as $\partial_{a} A^{\alpha}$. A similar definition of the contravariant derivative,

$$
\begin{equation*}
\partial^{\alpha} \equiv \frac{\partial}{\partial x_{\alpha}}=\left\{\frac{\partial}{\partial(c t)},-\nabla\right\}, \tag{9.105}
\end{equation*}
$$

allows us to write the Lorentz-invariant scalar product (103) in any of two forms:

$$
\begin{equation*}
\frac{\partial A_{0}}{\partial(c t)}+\nabla \cdot \mathbf{A}=\partial^{\alpha} A_{\alpha}=\partial_{\alpha} A^{\alpha} . \tag{9.106}
\end{equation*}
$$

[^400]Finally, let us see how does the general Lorentz transform changes 4 -tensors. A second-rank $4 \times 4$ matrix is a legitimate 4 -tensor if both 4 -vectors it relates obey the Lorentz transform. For example, if two legitimate 4 -vectors are related as

$$
\begin{equation*}
A^{\alpha}=T^{\alpha \beta} B_{\beta} \tag{9.107}
\end{equation*}
$$

we should require that

$$
\begin{equation*}
A^{\prime \alpha}=T^{\prime \alpha \beta} B_{\beta}^{\prime}, \tag{9.108}
\end{equation*}
$$

where $A^{\alpha}$ and $A^{\prime \alpha}$ are related by Eqs. (97), while $B_{\beta}$ and $B^{\prime}{ }_{\beta}$, by Eqs. (99). This requirement immediately yields

Lorentz transform of 4-tensors

$$
\begin{equation*}
T^{\alpha \beta}=\frac{\partial x^{\alpha}}{\partial x^{\prime \gamma}} \frac{\partial x^{\beta}}{\partial x^{\prime \delta}} T^{\gamma \delta}, \quad T^{\prime \alpha \beta}=\frac{\partial x^{\prime \alpha}}{\partial x^{\gamma}} \frac{\partial x^{\prime \beta}}{\partial x^{\delta}} T^{\gamma \delta} \tag{9.109}
\end{equation*}
$$

with the implied summation over two indices, $\gamma$ and $\delta$. The rules for covariant and mixed tensors are similar. ${ }^{40}$

### 9.5. Maxwell equations in the 4 -form

This 4-vector formalism background is already sufficient to analyze the Lorentz transform of the electromagnetic field. Just to warm up, let us consider the continuity equation (4.5),

$$
\begin{equation*}
\frac{\partial \rho}{\partial t}+\nabla \cdot \mathbf{j}=0 \tag{9.110}
\end{equation*}
$$

which expresses the electric charge conservation, and, as we already know, is compatible with the Maxwell equations. If we now define the contravariant and covariant 4-vectors of electric current as

4-vector of electric current

Continuity equation in 4-form

$$
\begin{equation*}
j^{\alpha}=\{\rho c, \mathbf{j}\}, \quad j_{\alpha}=\{\rho c,-\mathbf{j}\} \tag{9.111}
\end{equation*}
$$

then Eq. (110) may be presented in the form

$$
\begin{equation*}
\partial^{\alpha} j_{\alpha}=\partial_{\alpha} j^{\alpha}=0 \tag{9.112}
\end{equation*}
$$

showing that the continuity equation is form-invariant ${ }^{41}$ with respect to the Lorentz transform.
Of course, such equation form invariance does not mean that all component values of the 4vectors participating in the equation are the same in both frames! For example, let us have some static charge density $\rho$ in frame 0 ; then Eq. (97b), applied to the contravariant form of 4 -vector (111), reads

$$
\begin{equation*}
j^{\prime \alpha}=\frac{\partial x^{\prime \alpha}}{\partial x^{\beta}} j^{\beta}, \quad j^{\beta}=\{\rho c, 0,0,0\} . \tag{9.113}
\end{equation*}
$$

[^401]Using the explicit form (98) of the reciprocal Lorentz matrix for the coordinate choice shown in Fig. 1, we see that this relation yields

$$
\begin{equation*}
\rho^{\prime}=\gamma \rho, \quad j_{x}^{\prime}=-\gamma \beta \rho c=-\gamma \rho \rho, \quad j_{y}^{\prime}=j_{z}^{\prime}=0 . \tag{9.114}
\end{equation*}
$$

Since the charge velocity, as observed from frame 0 ', is $(-\mathbf{v})$, the non-relativistic result would be $\mathbf{j}=-\mathbf{v} \rho$. The additional $\gamma$ factor in the relativistic results for both charge density and current is caused by the length contraction: $d x^{\prime}=d x / \gamma$, so that in order to keep the total charge $d Q=\rho d^{3} r=\rho d x d y d z$ inside the elementary volume $d^{3} r=d x d y d z$ intact, $\rho$ (and hence $j_{x}$ ) should increase proportionally.

Next, in the end of Chapter 6 we have seen that Maxwell equations for potentials $\phi$ and $\mathbf{A}$ may be presented in a similar form (6.109), under the Lorenz (again, not "Lorentz" please!) gauge condition (6.108). For the free space, this condition takes the form

$$
\begin{equation*}
\nabla \cdot \mathbf{A}+\frac{1}{c^{2}} \frac{\partial \phi}{\partial t}=0 \tag{9.115}
\end{equation*}
$$

This expression gives us a hint how to form the 4-vector of potentials: 42

$$
\begin{equation*}
A^{\alpha}=\left\{\frac{\phi}{c}, \mathbf{A}\right\}, \quad A_{\alpha}=\left\{\frac{\phi}{c},-\mathbf{A}\right\} ; \tag{9.116}
\end{equation*}
$$

indeed, these vectors satisfy Eq. (115) in its 4-vector form:

$$
\begin{equation*}
\partial^{\alpha} A_{\alpha}=\partial_{\alpha} A^{\alpha}=0 . \tag{9.117}
\end{equation*}
$$

Since this scalar product is Lorentz-invariant, and derivatives (104)-(105) are legitimate 4vectors, this implies that 4 -vector (116) is also legitimate, i.e. obeys the Lorentz transform formulas (97), (99). A more convincing evidence of this fact may be obtained from Maxwell equations (6.109) for the potentials. In free space, they may be rewritten as

$$
\begin{equation*}
\left[\frac{\partial^{2}}{\partial(c t)^{2}}-\nabla^{2}\right] \frac{\phi}{c}=\frac{(\rho c)}{\varepsilon_{0} c^{2}} \equiv \mu_{0}(\rho c), \quad\left[\frac{\partial^{2}}{\partial(c t)^{2}}-\nabla^{2}\right] \mathbf{A}=\mu_{0} \mathbf{j} . \tag{9.118}
\end{equation*}
$$

Using definition (116), these equations may be merged to one: ${ }^{43}$

$$
\begin{equation*}
\square A^{\alpha}=\mu_{0} j^{\alpha}, \tag{9.119}
\end{equation*}
$$

where $\square$ is the d'Alembert operator ${ }^{44}$ that may be presented as either of two scalar products,

$$
\begin{equation*}
\square \equiv \frac{\partial^{2}}{\partial(c t)^{2}}-\nabla^{2}=\partial^{\beta} \partial_{\beta}=\partial_{\beta} \partial^{\beta} \tag{9.120}
\end{equation*}
$$

and hence is Lorentz-invariant. Because of that, and the fact that the Lorentz transform changes both 4vectors $A^{\alpha}$ and $j^{\alpha}$ in a similar way, Eq. (119) does not depend on the reference frame choice. Thus we

[^402]have arrived at a key point of this chapter: we see that Maxwell equations are indeed form-invariant with respect to the Lorentz transform. As a by-product, the 4 -vector form (119) of these equations (for potentials) is extremely simple - and beautiful.

However, as we have seen in Chapter 7, for many applications the Maxwell equations for field vectors are more convenient; so let us present them in the 4 -form. For that, we may express the Cartesian components of the usual (3D) field vector vectors

$$
\begin{equation*}
\mathbf{E}=-\nabla \phi-\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B}=\nabla \times \mathbf{A} \tag{9.121}
\end{equation*}
$$

via those of the potential 4-vector $A^{\alpha}$. For example,

$$
\begin{gather*}
E_{x}=-\frac{\partial \phi}{\partial x}-\frac{\partial A_{x}}{\partial t}=-c\left(\frac{\partial}{\partial x} \frac{\phi}{c}+\frac{\partial A_{x}}{\partial(c t)}\right) \equiv-c\left(\partial^{0} A^{1}-\partial^{1} A^{0}\right),  \tag{9.122}\\
B_{x}=\frac{\partial A_{z}}{\partial y}-\frac{\partial A_{y}}{\partial z} \equiv-\left(\partial^{2} A^{3}-\partial^{3} A^{2}\right) . \tag{9.123}
\end{gather*}
$$

Completing similar calculations for other field components, we find that the following asymmetric, contravariant field-strength tensor,

$$
\begin{equation*}
F^{\alpha \beta} \equiv \partial^{\alpha} A^{\beta}-\partial^{\beta} A^{\alpha}, \tag{9.124}
\end{equation*}
$$

may be expressed via the field components as follows: ${ }^{45}$

Fieldstrength tensors

$$
F^{\alpha \beta}=\left(\begin{array}{cccc}
0 & -E_{x} / c & -E_{y} / c & -E_{z} / c  \tag{9.125a}\\
E_{x} / c & 0 & -B_{z} & B_{y} \\
E_{y} / c & B_{z} & 0 & -B_{x} \\
E_{z} / c & -B_{y} & B_{x} & 0
\end{array}\right),
$$

so that the covariant form of the tensor is

$$
F_{\alpha \beta} \equiv g_{\alpha \gamma} F^{\gamma \delta} g_{\delta \beta}=\left(\begin{array}{cccc}
0 & E_{x} / c & E_{y} / c & E_{z} / c  \tag{9.125b}\\
-E_{x} / c & 0 & -B_{z} & B_{y} \\
-E_{y} / c & B_{z} & 0 & -B_{x} \\
-E_{z} / c & -B_{y} & B_{x} & 0
\end{array}\right) .
$$

If this expression looks a bit too bulky, note that as a reward, the pair of inhomogeneous Maxwell equations, i.e. the two first equations of the system (6.93), which in free space ( $\mathbf{D}=\varepsilon_{0} \mathbf{E}, \mathbf{B}=$ $\left.\mu_{0} \mathbf{H}\right)$ may be rewritten as

$$
\begin{equation*}
\nabla \cdot \frac{\mathbf{E}}{c}=\mu_{0} c \rho, \quad \nabla \times \mathbf{B}-\frac{\partial}{\partial(c t)} \frac{\mathbf{E}}{c}=\mu_{0} \mathbf{j}, \tag{9.126}
\end{equation*}
$$

may be now rewritten in a very simple (and manifestly form-invariant) way,
${ }^{45}$ In Gaussian units, this formula, as well as Eq. (131) for $G^{\alpha \beta}$, does not have factors $c$ in all the denominators.

$$
\begin{equation*}
\partial_{\alpha} F^{\alpha \beta}=\mu_{0} j^{\beta} \tag{9.127}
\end{equation*}
$$

which is comparable with Eq. (119) in its beauty and simplicity. Somewhat counter-intuitively, the pair of homogeneous Maxwell equations,

$$
\begin{equation*}
\nabla \times \mathbf{E}+\frac{\partial \mathbf{B}}{\partial t}=0, \quad \nabla \cdot \mathbf{B}=0 \tag{9.128}
\end{equation*}
$$

look, in the 4-vector notation, a bit more complicated:46

$$
\begin{equation*}
\partial_{\alpha} F_{\beta \gamma}+\partial_{\beta} F_{\gamma \alpha}+\partial_{\gamma} F_{\alpha \beta}=0 . \tag{9.129}
\end{equation*}
$$

Note, however, that Eq. (128) may be also represented in a much simpler form,

$$
\begin{equation*}
\partial_{\alpha} G^{\alpha \beta}=0 \tag{9.130}
\end{equation*}
$$

using the so-called dual (and also asymmetric) tensor

$$
G^{\alpha \beta}=\left(\begin{array}{cccc}
0 & B_{x} & B_{y} & B_{z}  \tag{9.131}\\
-B_{x} & 0 & -E_{z} / c & E_{y} / c \\
-B_{y} & E_{z} / c & 0 & -E_{x} / c \\
-B_{z} & -E_{y} / c & E_{x} / c & 0
\end{array}\right)
$$

which may be obtained from $F^{\alpha \beta}$, given by Eq. (125), by the following replacements:

$$
\begin{equation*}
\frac{\mathbf{E}}{c} \rightarrow-\mathbf{B}, \quad \mathbf{B} \rightarrow \frac{\mathbf{E}}{c} \tag{9.132}
\end{equation*}
$$

Besides the proof of the form-invariance of the Maxwell equations, the 4 -vector formalism allows us to achieve our initial goal: find out how do the electric and magnetic field component change at the transfer between reference frames. Let us apply to tensor $F^{\alpha \beta}$ the reciprocal Lorentz transform given by the second of Eqs. (109). Generally, it gives, for each field component, a sum of 16 terms, but since (for our choice of coordinates, shown in Fig. 1) there are many zeros in the Lorentz transform matrix, and diagonal components of $F^{\gamma \delta}$ equal zero as well, the calculations are rather doable. Let us calculate, for example, $E_{x}^{\prime} \equiv-c F^{, 01}$. The only nonvanishing terms in the right-hand part are

$$
\begin{equation*}
E_{x}^{\prime}=-c F^{01}=-c\left(\frac{\partial x^{\prime 0}}{\partial x^{1}} \frac{\partial x^{\prime 1}}{\partial x^{0}} F^{10}+\frac{\partial x^{\prime 0}}{\partial x^{0}} \frac{\partial x^{\prime 1}}{\partial x^{1}} F^{01}\right)=-c \gamma^{2}\left(\beta^{2}-1\right) \frac{E_{x}}{c}=E_{x} . \tag{9.133}
\end{equation*}
$$

Repeating the calculation for other 5 components of the fields, we get very important relations

$$
\begin{array}{ll}
E_{x}^{\prime}=E_{x}, & B_{x}^{\prime}=B_{x}, \\
E_{y}^{\prime}=\gamma\left(E_{y}-v B_{z}\right), & B_{y}^{\prime}=\gamma\left(B_{y}+v E_{z} / c^{2}\right),  \tag{9.134}\\
E_{z}^{\prime}=\gamma\left(E_{z}+v B_{y}\right), & B_{z}^{\prime}=\gamma\left(B_{z}-v E_{y} / c^{2}\right),
\end{array}
$$

whose more compact "semi-vector" form is

[^403]Lorentz transform of components

$$
\begin{array}{ll}
\mathbf{E}_{\|}^{\prime}=\mathbf{E}_{\|}, & \mathbf{B}_{\|}^{\prime}=\mathbf{B}_{\|},  \tag{9.135}\\
\mathbf{E}_{\perp}^{\prime}=\gamma(\mathbf{E}+\mathbf{v} \times \mathbf{B})_{\perp}, & \mathbf{B}_{\perp}^{\prime}=\gamma\left(\mathbf{B}-\mathbf{v} \times \mathbf{E} / c^{2}\right)_{\perp},
\end{array}
$$

where indices $\|$ and $\perp$ stand, respectively, for the field components parallel and perpendicular to the relative velocity $\mathbf{v}$ of the two reference frames. In the non-relativistic limit, the Lorentz factor $\gamma$ tends to 1, and Eqs. (135) acquire an even simpler form

$$
\begin{equation*}
\mathbf{E}^{\prime} \rightarrow \mathbf{E}+\mathbf{v} \times \mathbf{B}, \quad \mathbf{B}^{\prime} \rightarrow \mathbf{B}-\frac{1}{c^{2}} \mathbf{v} \times \mathbf{E} . \tag{9.136}
\end{equation*}
$$

Thus we see that the electric and magnetic fields actually transform to each other even in the first order of the $v / c$ ratio. For example, if we fly across the field lines of a uniform, static, purely electric field $\mathbf{E}$ (e.g., the one in a plane capacitor) we will see not only the electric field re-normalization (in the second order of the $v / c$ ratio), but also a nonvanishing dc magnetic field $\mathbf{B}$ ' perpendicular to both vector $\mathbf{E}$ and vector $\mathbf{v}$, the direction of our motion. This is of course what might be expected from the relativity principle: from the point of view of the moving observer (which is as legitimate as that of a stationary observer), the surface charges of capacitor plates, that create field $\mathbf{E}$, move back creating dc currents (114) which induce the apparent magnetic field. Similarly, motion across a magnetic field creates, from the point of view of the moving observer, an electric field.

This fact is very important philosophically. One can say there is no such thing in Mother Nature as an electric field (or a magnetic field) all by itself. Not only can the electric field induce the magnetic field (and vice versa) in dynamics, but even in an apparently static configuration, what exactly we measure depends on our speed relative to the field sources - hence the very appropriate term for the whole field we are studying: the electromagnetism.

Another simple but very important application of Eqs. (134)-(135) is the calculation of the fields created by a charged particle moving in free space by inertia, i.e. along a straight line with constant velocity $\mathbf{u}$, at the impact parameter ${ }^{47}$ (the closest distance) $b$ from the observer. Selecting frame 0 ' to move with the particle in its origin, and frame 0 to reside in the "lab" (in that fields $\mathbf{E}$ and $\mathbf{B}$ are measured), we can take $\mathbf{v}=\mathbf{u}$. In this case fields $\mathbf{E}^{\prime}$ and $\mathbf{B}$ ' may be calculated from, respectively, electro- and magnetostatics, because in frame 0 ' the particle does not move:

$$
\begin{equation*}
\mathbf{E}^{\prime}=\frac{q}{4 \pi \varepsilon_{0}} \frac{\mathbf{r}^{\prime}}{r^{\prime 3}}, \quad \mathbf{B}^{\prime}=0 . \tag{9.137}
\end{equation*}
$$

Selecting the coordinate axes so that at the measurement point $x=0, y=b, z=0$ (Fig. 11a), we may write $x^{\prime}=-u t^{\prime}, y^{\prime}=b, z^{\prime}=0$, so that $r^{\prime}=\left(u^{2} t^{\prime 2}+b^{2}\right)^{1 / 2}$, and the field components are as follows:

$$
\begin{equation*}
E_{x}^{\prime}=-\frac{q}{4 \pi \varepsilon_{0}} \frac{u t^{\prime}}{\left(u^{2} t^{\prime 2}+b^{2}\right)^{3 / 2}}, \quad E_{y}^{\prime}=\frac{q}{4 \pi \varepsilon_{0}} \frac{b}{\left(u^{2} t^{\prime 2}+b^{2}\right)^{3 / 2}}, \quad E_{z}^{\prime}=0, \quad B_{x}^{\prime}=B_{y}^{\prime}=B_{z}^{\prime}=0 . \tag{9.138}
\end{equation*}
$$

Now using the last of Eq. (19b), with $x=0$, for the time transform, and the equations reciprocal to Eqs. (134) for the field transform (it is evident that they are similar to the direct transform with $v$ replaced with $-v=-u$ ), in the lab frame we get

[^404]\[

$$
\begin{gather*}
E_{x}=E_{x}^{\prime}=-\frac{q}{4 \pi \varepsilon_{0}} \frac{u \gamma t}{\left(u^{2} \gamma^{2} t^{2}+b^{2}\right)^{3 / 2}}, \quad E_{y}=\gamma E_{y}^{\prime}=\frac{q}{4 \pi \varepsilon_{0}} \frac{\gamma b}{\left(u^{2} \gamma^{2} t^{2}+b^{2}\right)^{3 / 2}}, \quad E_{z}=0,  \tag{9.139}\\
B_{x}=0, \quad B_{y}=0, \quad B_{z}=\frac{\gamma u}{c^{2}} E_{y}^{\prime}=\frac{u}{c^{2}} \frac{q}{4 \pi \varepsilon_{0}} \frac{\gamma b}{\left(u^{2} \gamma^{2} t^{2}+b^{2}\right)^{3 / 2}}=\frac{u}{c^{2}} E_{y} . \tag{9.140}
\end{gather*}
$$
\]


(b)

Fig. 9.11. Field pulses induced by a uniformly moving charge.

These results, ${ }^{48}$ plotted in Fig. 11b, reveal two major effects. First, the charge passage by the observer generates not only an electric field pulse, but also a magnetic field pulse. This is natural, because, as was repeatedly discussed in Chapter 5, charge motion is essentially an electric current. ${ }^{49}$ Second, Eqs. (139)-(140) show that the pulse duration scale is

$$
\begin{equation*}
\Delta t=\frac{b}{\gamma u}=\frac{b}{u}\left(1-\frac{u^{2}}{c^{2}}\right)^{1 / 2}, \tag{9.141}
\end{equation*}
$$

i.e. shrinks to zero as the charge velocity $u$ approaches the speed of light. This is of course a direct corollary of the relativistic length contraction: in the frame 0 ' moving with the charge, the longitudinal spread of its electric field at distance $b$ from the motion line is of the order of $\Delta x^{\prime}=b$. When observed from the lab frame 0, this interval, in accordance with Eq. (20), shrinks to $\Delta x=\Delta x^{\prime} / \gamma=b / \gamma$, and so does the pulse duration scale $\Delta t=\Delta x / u=b / \gamma u$.

### 9.6. Relativistic particles in electric and magnetic fields

Now let us analyze dynamics of charged particles in electric and magnetic fields. Inspired by "our" success of forming the 4 -vector (75) of energy-momentum,

$$
\begin{equation*}
p^{\alpha}=\left\{\frac{\varepsilon}{c}, \mathbf{p}\right\}=\gamma\{m c, \mathbf{p}\}=m \frac{d x^{\alpha}}{d \tau} \equiv m u^{\alpha} \tag{9.142}
\end{equation*}
$$

where $u^{\alpha}$ is the contravariant form of the 4-velocity (63) of the particle,

[^405]\[

$$
\begin{equation*}
u^{\alpha} \equiv \frac{d x^{\alpha}}{d \tau}, \quad u_{\alpha} \equiv \frac{d x_{\alpha}}{d \tau} \tag{9.143}
\end{equation*}
$$

\]

we may notice that the non-relativistic equation of motion, resulting from the Lorentz-force formula (5.10) for the three spatial components of $p^{\alpha}$, at charged particle's motion in electromagnetic field,

Particle's dynamics in 4-form
is fully consistent with the following 4-vector equality (which is evidently form-invariant):

$$
\begin{equation*}
\frac{d p^{\alpha}}{d \tau}=q F^{\alpha \beta} u_{\beta} \tag{9.145}
\end{equation*}
$$

For example, the $\alpha=1$ component of this equation reads

$$
\begin{equation*}
\frac{d p^{1}}{d \tau}=q F^{1 \beta} u_{\beta}=q\left[\frac{E_{x}}{c} \gamma c+0 \cdot\left(-\gamma u_{x}\right)+\left(-B_{z}\right)\left(-\gamma u_{y}\right)+B_{y}\left(-\gamma u_{z}\right)\right]=q \gamma[\mathbf{E}+\mathbf{u} \times \mathbf{B}]_{x}, \tag{9.146}
\end{equation*}
$$

and similarly for two other spatial components ( $\alpha=2$ and $\alpha=3$ ). We see that these expressions differ from the Newton law (144) by the extra factor $\gamma$. However, plugging into Eq. (146) the definition of the proper time interval, $d \tau=d t / \gamma$, and canceling $\gamma$ in both parts, we recover Eq. (144) exactly - for any velocity of the particle! The only caveat is that if $u$ is comparable with $c, \mathbf{p}$ in Eq. (144) has to be understood as the relativistic momentum (70) proportional to the velocity-dependent mass $M=\gamma m \geq m$ rather than to the rest mass $m$.

The only remaining task is to examine the meaning of the $0^{\text {th }}$ component of Eq. (145). Let us spell it out:

$$
\begin{equation*}
\frac{d p^{0}}{d \tau}=q F^{0 \beta} u_{\beta}=q\left[0 \cdot \gamma c+\left(-\frac{E_{x}}{c}\right)\left(-u_{x}\right)+\left(-\frac{E_{y}}{c}\right)\left(-\mu_{y}\right)+\left(-\frac{E_{z}}{c}\right)\left(-\gamma u_{z}\right)\right]=q \gamma \frac{\mathbf{E}}{c} \cdot \mathbf{u} . \tag{9.147}
\end{equation*}
$$

Recalling that $p^{0}=\varepsilon / c$, and using $d \tau=d t / \gamma$ again, we see that Eq. (147) looks exactly as the nonrelativistic relation for the kinetic energy change, ${ }^{50}$

Particle's energy evolution

$$
\begin{equation*}
\frac{d \varepsilon}{d t}=q \mathbf{E} \cdot \mathbf{u} \tag{9.148}
\end{equation*}
$$

besides that in the relativistic case the energy has to be taken in the general form (73).
No question, the 4 -component equation (145) of relativistic dynamics is beautiful in its simplicity. However, for the solution of particular problems, Eqs. (144) and (148) are frequently preferable. As an illustration of this point, let us now use these equations to explore the relativistic effects at charged particle motion in uniform, time-independent electric and magnetic fields. In doing that, we will, for the time being, neglect the contributions into the field by the particle itself. ${ }^{51}$

[^406](i) Uniform magnetic field. Let the magnetic field be constant and uniform in the "lab" reference frame 0. Then in this frame, Eqs. (144) and (148) yield
\[

$$
\begin{equation*}
\frac{d \mathbf{p}}{d t}=q \mathbf{u} \times \mathbf{B}, \quad \frac{d \varepsilon}{d t}=0 . \tag{9.149}
\end{equation*}
$$

\]

From the second equation, $\varepsilon=$ const, we get $u=$ const, $\beta \equiv u / c=$ const, $\gamma \equiv\left(1-\beta^{2}\right)^{-1 / 2}=$ const, and $M \equiv$ $\gamma m=$ const, so that the first of Eqs. (149) may be rewritten as

$$
\begin{equation*}
\frac{d \mathbf{u}}{d t}=\mathbf{u} \times \boldsymbol{\omega}_{c} \tag{9.150}
\end{equation*}
$$

where $\omega_{c}$ is the vector directed along the magnetic field $\mathbf{B}$, with the magnitude equal to the cyclotron frequency (sometimes called "gyrofrequency")

$$
\begin{equation*}
\omega_{c} \equiv \frac{q B}{M}=\frac{q B}{\gamma m}=\frac{q c^{2} B}{\varepsilon} . \tag{9.151}
\end{equation*}
$$

If particle's initial velocity $\mathbf{u}_{0}$ is perpendicular to the magnetic field, Eq. (150) describes its circular motion, with a constant speed $u=u_{0}$, in a plane perpendicular to $\mathbf{B}$, and frequency (151). In the non-relativistic limit $u \ll c$, when $\gamma \rightarrow 1$, i.e. $M \rightarrow m$, the cyclotron frequency is independent on the speed, but as the kinetic energy is increased to comparable to the rest energy of the particle, the frequency decreases, and in the ultra-relativistic limit,

$$
\begin{equation*}
\omega_{c} \approx q c \frac{B}{p}, \quad \text { at } u \approx c . \tag{9.152}
\end{equation*}
$$

The cyclotron motion radius may be calculated as $R=u / \omega_{c}$; in the non-relativistic limit it is proportional to particle's speed, i.e. to the square root of its kinetic energy. However, in the general case the radius is proportional to particle's relativistic momentum rather than its speed:

$$
\begin{equation*}
R=\frac{u}{\omega_{c}}=\frac{M u}{q B}=\frac{m \gamma u}{q B}=\frac{1}{q} \frac{p}{B}, \tag{9.153}
\end{equation*}
$$

Cyclotron radius
so that in the ultra-relativistic limit, when $p \approx \varepsilon / c, R$ is proportional to the kinetic energy.
This dependence of $\omega_{c}$ and $R$ on energy are the major factors in design of circular accelerators of charged particles. In the simplest of these machines (the cyclotron, invented in 1929 by E. Lawrence), frequency $\omega$ of the accelerating ac electric field is constant, so that even it is tuned to $\omega_{c}$ of the initially injected particles, the drop of the cyclotron frequency with energy eventually violates this tuning. Due to this reason, the maximum particle speed is limited to just $\sim 0.1 c$ (for protons, corresponding to the kinetic energy of just $\sim 15 \mathrm{MeV}$ ). This problem may be addressed in several ways. In particular, in synchrotrons (such as Fermilab's Tevatron and CERN's LHC) the magnetic field is gradually increased in time to compensate the momentum increase $(B \propto p)$, so that both $R(148)$ and $\omega_{c}(147)$ stay constant, enabling proton acceleration to energies as high as $\sim 7 \mathrm{TeV}$, i.e. $\sim 2,000 \mathrm{mc}^{2} .{ }^{52}$

[^407]Returning to our initial problem, if particle's initial velocity has a component $u_{\|}$along the magnetic field, it is conserved in time, so that the trajectory is a spiral around the magnetic field lines. As Eqs. (149) show, in this case Eq. (150) remains valid, but in Eqs. (151) and (153) the full speed and momentum have to be replaced with magnitudes of their (also time-conserved) components, $u_{\perp}$ and $p_{\perp}$, normal to $\mathbf{B}$, while the Lorentz factor $\gamma$ in those formulas still requires the full speed of the particle.

Finally, in the special case when particle's initial velocity is directed exactly along the magnetic field's direction, it continues to move by straight line along vector B. In this case, the cyclotron frequency (151) remains finite, but does not correspond to any real motion, because $R=0$.
(ii) Uniform electric field. This problem is (technically) more complex than the previous one, because in the electric field, particle's kinetic energy may change. Directing axis $z$ along the field, from Eq. (144) we get

$$
\begin{equation*}
\frac{d p_{z}}{d t}=q E, \quad \frac{d \mathbf{p}_{\perp}}{d t}=0 . \tag{9.154}
\end{equation*}
$$

If the field does not change in time, the first integration of these equations is trivial,

$$
\begin{equation*}
p_{z}(t)=p_{z}(0)+q E t, \quad \mathbf{p}_{\perp}(t)=\text { const }=\mathbf{p}_{\perp}(0), \tag{9.155}
\end{equation*}
$$

but the further integration requires care, because the effective mass $M=\gamma m$ of the particle depends on its full speed:

$$
\begin{equation*}
u^{2}=u_{z}^{2}+u_{\perp}^{2}, \tag{9.156}
\end{equation*}
$$

making the two motions, along and across the field, mutually dependent.
If the initial velocity is perpendicular to field $\mathbf{E}$, i.e. if $p_{z}(0)=0, p_{\perp}(0)=p(0) \equiv p_{0}$, the easiest way to proceed is to calculate the kinetic energy first:

$$
\begin{equation*}
\mathcal{\varepsilon}^{2}=\left(m c^{2}\right)^{2}+c^{2} p^{2}(t)=\varepsilon_{0}^{2}+c^{2}(q E t)^{2}, \quad \text { where } \varepsilon_{0} \equiv\left[\left(m c^{2}\right)^{2}+c^{2} p_{0}^{2}\right]^{1 / 2} \tag{9.157}
\end{equation*}
$$

On the other hand, we can calculate the same energy by integrating Eq. (148),

$$
\begin{equation*}
\frac{d \varepsilon}{d t}=q \mathbf{E} \cdot \mathbf{u}=q E \frac{d z}{d t}, \tag{9.158}
\end{equation*}
$$

over time, with a simple result:

$$
\begin{equation*}
\varepsilon=\varepsilon_{0}+q E z(t) \tag{9.159}
\end{equation*}
$$

where (for the notation simplicity) I took $z(0)=0$. Requiring Eq. (159) to give the same $\varepsilon^{2}$ as Eq. (157), we get a quadratic equation for $z(t)$,

$$
\begin{equation*}
\varepsilon_{0}^{2}+c^{2}(q E t)^{2}=\left[\varepsilon_{0}+q E z(t)\right]^{2}, \tag{9.160}
\end{equation*}
$$

whose solution (with the sign before the square root corresponding to $E>0$, i.e. $z \geq 0$ ) is

$$
\begin{equation*}
z(t)=\frac{\varepsilon_{0}}{q E}\left\{\left[1+\left(\frac{c q E t}{\varepsilon_{0}}\right)^{2}\right]^{1 / 2}-1\right\} . \tag{9.161}
\end{equation*}
$$

Now let us find particle's trajectory. Selecting axis $x$ so that the initial velocity vector (and hence the velocity vector at any further instant) is within the $[x, z]$ plane, i.e. $y(t) \equiv 0$, we may use Eqs. (155) to calculate trajectory's slope, at its arbitrary point, as

$$
\begin{equation*}
\frac{d z}{d x}=\frac{d z / d t}{d x / d t}=\frac{M u_{z}}{M u_{x}}=\frac{p_{z}}{p_{x}}=\frac{q E t}{p_{0}} . \tag{9.162}
\end{equation*}
$$

Now let us use Eq. (160) to express the numerator of this fraction, $q E t$, as a function of $z$ :

$$
\begin{equation*}
q E t=\frac{1}{c}\left[\left(\varepsilon_{0}+q E z\right)^{2}-\varepsilon_{0}^{2}\right]^{1 / 2} . \tag{9.163}
\end{equation*}
$$

Plugging this expression into Eq. (161), we get

$$
\begin{equation*}
\frac{d z}{d x}=\frac{1}{c p_{0}}\left[\left(\varepsilon_{0}+q E z\right)^{2}-\varepsilon_{0}^{2}\right]^{1 / 2} \tag{9.164}
\end{equation*}
$$

This differential equation may be readily integrated, separating variables $z$ and $x$, and using the following substitution: $\xi \equiv \cosh ^{-1}\left(q E z / \varepsilon_{0}+1\right)$. Selecting the origin of axis $x$ at the initial point, so that $x(0)=0$, we finally get the trajectory:

$$
\begin{equation*}
z=\frac{\varepsilon_{0}}{q E}\left(\cosh \frac{q E x}{c p_{0}}-1\right) \tag{9.165}
\end{equation*}
$$

At the initial part of the trajectory, where $q E x \ll c p_{0}(0)$, this expression may be approximated by the first nonvanishing term of the Taylor series, giving a parabola:

$$
\begin{equation*}
z=\frac{\varepsilon_{0} q E}{2}\left(\frac{x}{c p_{0}}\right)^{2}, \tag{9.166}
\end{equation*}
$$

so that if the initial velocity of the particle is much less than $c$ (i.e. $p_{0} \approx m u_{0}, \varepsilon_{0} \approx m c^{2}$ ), we get the familiar non-relativistic formula:

$$
\begin{equation*}
z=\frac{q E}{2 m u_{0}^{2}} x^{2}=\frac{a}{2} t^{2}, \quad a=\frac{F}{m}=\frac{q E}{m} . \tag{9.167}
\end{equation*}
$$

This solution may be readily generalized to the case of an arbitrary direction of particle's initial velocity; this generalization is left for reader's exercise.
(iii) Crossed uniform magnetic and electric fields $(\mathbf{E} \perp \mathbf{B})$. In the view of how bulky the solution of the previous problem (i.e. the particular case of the current problem for $\mathbf{B}=0$ ) was, one might think that this problem should be forbiddingly complex for an analytical solution. Counter-intuitively, it is not the case, due to the help from the field transform relations (135). Let us consider two possible cases.

Case I: $E / c<B$. Let us consider an inertial frame moving (relatively the "lab" reference frame 0 in which fields $\mathbf{E}$ and $\mathbf{B}$ are defined) with velocity

$$
\begin{equation*}
\mathbf{v}=\frac{\mathbf{E} \times \mathbf{B}}{B^{2}} \tag{9.168}
\end{equation*}
$$

whose magnitude $v=c \times(E / c) / B<c$. Selecting the coordinate axes as shown in Fig. 12, so that

$$
\begin{equation*}
E_{x}=0, \quad E_{y}=E, \quad E_{z}=0 ; \quad B_{x}=0, \quad B_{y}=0, \quad B_{z}=0, \tag{9.169}
\end{equation*}
$$

we see that the Cartesian components of this velocity are $v_{x}=v, v_{y}=v_{z}=0$.


Fig. 9.12. Particle's trajectory in crossed electric and magnetic fields (at $E / \mathrm{c}<B$ ).

Since this choice of coordinates complies with that used to derive Eqs. (134), we can readily use that simple form of the Lorentz transform to calculate field components in the moving reference frame:

$$
\begin{gather*}
E_{x}^{\prime}=0, \quad E_{y}^{\prime}=\gamma(E-v B)=\gamma\left(E-\frac{E}{B} B\right)=0, \quad E_{z}^{\prime}=0,  \tag{9.170}\\
B_{x}^{\prime}=0, \quad B_{y}^{\prime}=0, \quad B_{z}^{\prime}=\gamma\left(B-\frac{v E}{c^{2}}\right)=\gamma B\left(1-\frac{v E}{B c^{2}}\right)=\gamma B\left(1-\frac{v^{2}}{c^{2}}\right)=\frac{B}{\gamma} \leq B, \tag{9.171}
\end{gather*}
$$

where the Lorentz parameter $\gamma \equiv\left(1-v^{2} / c^{2}\right)^{-1 / 2}$ corresponds to velocity (168) rather than that of the particle.

Thus in this special reference frame the particle only sees a (re-normalized) uniform magnetic field $B^{\prime} \leq B$, parallel to the initial field, i.e. perpendicular to velocity (168). Using the result of the above example (i), we see that in this frame the particle will move along either a circle or a spiral winding about the direction of the magnetic field, with angular speed (151),

$$
\begin{equation*}
\omega_{c}^{\prime}=\frac{q B^{\prime}}{\varepsilon^{\prime} / c^{2}}, \tag{9.172}
\end{equation*}
$$

and radius (148):

$$
\begin{equation*}
R^{\prime}=\frac{p_{\perp}^{\prime}}{q B^{\prime}} . \tag{9.173}
\end{equation*}
$$

Hence in the lab frame, the particle will perform such orbital motion plus a "drift" with constant velocity $\mathbf{v}$ (Fig. 12). As the result, the lab-frame trajectory of the particle (or rater its projection onto the plane perpendicular to the magnetic field) is a trochoid-like curve ${ }^{53}$ that, depending on the initial velocity, may be either prolate (self-crossing), as in Fig. 12, or curtate (stretched so much that it is not selfcrossing).

[^408]Such looped motion of electrons (in practice, with $v \ll c$ ) is used, in particular, in magnetrons generators of microwave radiation. In these devices (Fig. 13a), the magnetic field, usually created by specially-shaped permanent magnets, is nearly uniform (in the region of electron motion) and directed along magnetron's axis, while the electric field of magnitude $E \ll c B$, created by the dc voltage applied between the anode and cathode, is virtually radial. As a result, the above simple theory is only approximately valid, and electron trajectories are close to epicycloids rather than trochoids. The applied electric field is adjusted so that these trajectories pass close to the gap openings to cylindrical microwave cavities drilled in magnetron's bulk anode (Fig. 13b). The fundamental mode of each cavity is quasi-lumped, with cylindrical walls working mostly as lumped inductances, and gaps as lumped capacitances, with the microwave electric field concentrated in the gap openings. This is why the mode is strongly coupled to the passing electrons, and their interaction creates large positive feedback (equivalent to negative damping) that results in intensive microwave self-oscillations at cavities' eigenfrequency. ${ }^{54}$ The oscillation energy, of course, is taken from the dc-field-accelerated electrons; due to the energy loss each electron gradually moves closer to the anode and finally lands on its surface. The wide use of such generators (in particular, in microwave ovens, which operate in a narrow frequency band around 2.45 GHz , allocated for these devices to avoid their interference with wireless communication systems) is due to their simplicity and high (up to 65\%) efficiency.

(b)

Fig. 9.13. Magnetron. (Adapted from http://microwavetubes.iwarp.com.)

Case II: $E / c>B$. In this case, the speed given by Eq. (168) would be above the speed of light, so let us introduce a reference frame moving with a different velocity,

$$
\begin{equation*}
\mathbf{v}=\frac{\mathbf{E} \times \mathbf{B}}{(E / c)^{2}} \tag{9.174}
\end{equation*}
$$

whose direction is the same as before (Fig. 12), and magnitude $v=c \times B /(E / c)$ is again below $c$. A calculation absolutely similar to the one performed above for Case I, yields

$$
\begin{equation*}
E_{x}^{\prime}=0, \quad E_{y}^{\prime}=\gamma(E-v B)=\gamma E\left(1-\frac{v B}{E}\right)=\gamma E\left(1-\frac{v^{2}}{c^{2}}\right)=\frac{E}{\gamma} \leq E, \quad E_{z}^{\prime}=0, \tag{9.175}
\end{equation*}
$$

[^409]\[

$$
\begin{equation*}
B_{x}^{\prime}=0, \quad B_{y}^{\prime}=0, \quad B_{z}^{\prime}=\gamma\left(B-\frac{v E}{c^{2}}\right)=\gamma\left(B-\frac{E B}{E}\right)=0 . \tag{9.176}
\end{equation*}
$$

\]

so that in the moving frame the particle sees only an electric field $E^{\prime} \leq E$. According to the solution of our previous problem (ii), the trajectory of the particle in the moving frame is hyperbolic, so that in the lab frame it has an "open", hyperbolic character as well.

To conclude this section, let me note that if the electric and magnetic fields are non-uniform, the particle motion is much more complex, and in most cases the integration of equations (144), (148) may be carried out only numerically. However, if the field nonuniformity is small, (approximate) analytical methods may be very effective. For example, if the magnetic field has a small transverse gradient $\nabla B$ in a direction perpendicular to the vector $\mathbf{B}$ itself, such that

$$
\begin{equation*}
\eta \equiv \frac{|\nabla B|}{B} \ll \frac{1}{R}, \tag{9.177}
\end{equation*}
$$

where $R$ is the cyclotron radius (153), then it is straightforward to use Eq. (150) to show ${ }^{55}$ that the cyclotron orbit drifts perpendicular to both $\mathbf{B}$ and $\nabla B$, with speed

$$
\begin{equation*}
v_{d} \approx \frac{\eta}{\omega_{c}}\left(\frac{1}{2} u_{\perp}^{2}+u_{\|}^{2}\right) \ll u . \tag{9.178}
\end{equation*}
$$

The physics of this drift is rather simple: according to Eq. (153), the instant curvature of the cyclotron orbit is proportional to the local value of the field. Hence if the field is nonuniform, the trajectory bends more on its parts passing through stronger field, thus acquiring a shape close to a curate trochoid.

For engineering and experimental practice, effects of longitudinal gradients of magnetic field on charged particle motion are much more important, but let me postpone their discussion until we have got a little bit more analytical tools in the next section.

### 9.7. Analytical mechanics of charged particles

Equation (145) gives a full description of relativistic particle dynamics in electric and magnetic fields, just as the $2^{\text {nd }}$ Newton law (1) does it in the non-relativistic limit. However, we know that in the latter case, the Lagrange formalism of analytical mechanics allows an easier solution of many problems. ${ }^{56}$ We can fully expect that to be true in relativistic mechanics as well, so let us expand the analysis of Sec. 3 to particles in the field.

Let recall that for a free particle, our main result was Eq. (68), which may be rewritten as

$$
\begin{equation*}
\gamma \mathcal{L}=-m c^{2}, \tag{9.179}
\end{equation*}
$$

showing that this product is Lorentz-invariant. How can the electromagnetic field affect this relation? In electrostatics, we could write

$$
\begin{equation*}
\mathcal{L}=T-U=T-q \phi . \tag{9.180}
\end{equation*}
$$

[^410]However, in relativity the scalar potential $\phi$ is just one component of the potential 4-vector (116). The only way to get a Lorentz-invariant contribution to $\gamma \mathcal{L}$ from the full 4 -vector, that would be also proportional to the Lorentz force, i.e. to the first power of particle's velocity (to account for the magnetic component of the Lorentz force), is evidently

$$
\begin{equation*}
\gamma \mathcal{L}=-m c^{2}+\text { const } \times u^{\alpha} A_{\alpha} \tag{9.181}
\end{equation*}
$$

where $u^{\alpha}$ is the 4 -velocity (63). In order to comply with Eq. (180) in electrostatics, the constant factor should be equal to ( $-q c$ ), so that Eq. (182) becomes

$$
\begin{equation*}
\gamma \mathcal{L}=-m c^{2}-q u^{\alpha} A_{\alpha}, \tag{9.182}
\end{equation*}
$$

and, finally,

$$
\begin{equation*}
\mathcal{L}=-\frac{m c^{2}}{\gamma}-q \phi+q \mathbf{u} \cdot \mathbf{A} \tag{9.183}
\end{equation*}
$$

i.e., in the Cartesian form,

$$
\begin{equation*}
\mathcal{L}=-m c^{2}\left(1-\frac{u_{x}^{2}+u_{y}^{2}+u_{z}^{2}}{c^{2}}\right)^{1 / 2}-q \phi+q\left(u_{x} A_{x}+u_{y} A_{y}+u_{z} A_{z}\right) \tag{9.184}
\end{equation*}
$$

Let us see whether this relation (that admittedly was obtained above by an educated guess rather than by a strict derivation) passes a natural sanity check. For the case of unconstrained motion of a particle, we can select its three Cartesian coordinates $r_{j}(j=1,2,3)$ as the generalized coordinates, and linear velocity components $u_{j}$ as the corresponding generalized velocities. In this case, the Lagrange equations of motion are ${ }^{57}$

$$
\begin{equation*}
\frac{d}{d t} \frac{\partial \mathcal{L}}{\partial u_{j}}-\frac{\partial \mathcal{L}}{\partial r_{j}}=0 \tag{9.185}
\end{equation*}
$$

For example, for $r_{1}=x$, Eq. (184) yields

$$
\begin{equation*}
\frac{\partial \mathcal{L}}{\partial u_{x}}=\frac{m u_{x}}{\left(1-u^{2} / c^{2}\right)^{1 / 2}}+q A_{x}=p_{x}+q A_{x}, \quad \frac{\partial \mathcal{L}}{\partial x}=-q \frac{\partial \phi}{\partial x}+q \mathbf{u} \cdot \frac{\partial \mathbf{A}}{\partial x} \tag{9.186}
\end{equation*}
$$

so that Eq. (185) takes the form

$$
\begin{equation*}
\frac{d p_{x}}{d t}=-q \frac{\partial \phi}{\partial x}+q \mathbf{u} \cdot \frac{\partial \mathbf{A}}{\partial x}-q \frac{d A_{x}}{d t} . \tag{9.187}
\end{equation*}
$$

In equations of motion, field values have to be taken at the instant position of the particle, so that the last (full) derivative has components due to both the actual field change (at a fixed point of space) and the particle's motion. Such addition is described by the so-called convective derivative ${ }^{58}$

$$
\begin{equation*}
\frac{d}{d t}=\frac{\partial}{\partial t}+\mathbf{u} \cdot \nabla \tag{9.188}
\end{equation*}
$$

Convective derivative

[^411]Spelling out both scalar products, we may group the terms remaining after cancellations as follows:

$$
\begin{equation*}
\frac{d p_{x}}{d t}=q\left[\left(-\frac{\partial \phi}{\partial x}-\frac{\partial A_{x}}{\partial t}\right)+u_{y}\left(\frac{\partial A_{y}}{\partial x}-\frac{\partial A_{x}}{\partial y}\right)-u_{z}\left(\frac{\partial A_{x}}{\partial z}-\frac{\partial A_{z}}{\partial x}\right)\right] . \tag{9.189}
\end{equation*}
$$

But taking into account relations (121) between the electric and magnetic fields and potentials, this expression is nothing more than

$$
\begin{equation*}
\frac{d p_{x}}{d t}=q\left(E_{x}+u_{y} B_{z}-u_{z} B_{y}\right)=q(\mathbf{E}+\mathbf{u} \times \mathbf{B})_{x}, \tag{9.190}
\end{equation*}
$$

i.e. the $x$-component of Eq. (144). Since other Cartesian coordinates participate in Eq. (184) in a similar way, it is evident that the Lagrangian equations of motion along other coordinates yield other components of the same vector equation of motion.

So, Eq. (183) does indeed give the correct Lagrangian function, and we can use it for the further analysis, in particular to discuss the first of Eqs. (186). This relation shows that in the electromagnetic field, the generalized momentum corresponding to particle's coordinate $x$ is not $p_{x}=m \gamma u_{x}$, but ${ }^{59}$

$$
\begin{equation*}
P_{x} \equiv \frac{\partial \mathscr{L}}{\partial u_{x}}=p_{x}+q A_{x} . \tag{9.191}
\end{equation*}
$$

Thus, as was already mentioned in brief in Sec. 6.3, particle's motion in a field may be is described by two momentum vectors: the kinetic momentum p, defined by Eq. (70), and the canonical (or "conjugate") momentum ${ }^{60}$

$$
\begin{equation*}
\mathbf{P}=\mathbf{p}+q \mathbf{A} \tag{9.192}
\end{equation*}
$$

In order to facilitate the discussion of this notion, let us generalize expression (72) for the Hamiltonian function $\not \subset$ of a free particle to the case of a particle in the field:

$$
\begin{equation*}
\mathcal{H}=\mathbf{P} \cdot \mathbf{u}-\mathcal{L}=(\mathbf{p}+q \mathbf{A}) \cdot \mathbf{u}-\left(-\frac{m c^{2}}{\gamma}+q \mathbf{u} \cdot \mathbf{A}-q \phi\right)=\mathbf{p} \cdot \mathbf{u}+\frac{m c^{2}}{\gamma}+q \phi . \tag{9.193}
\end{equation*}
$$

Merging the first two terms exactly as it was done in Eq. (72), we get an extremely simple result,

$$
\begin{equation*}
\nexists=\gamma m c^{2}+q \phi, \tag{9.194}
\end{equation*}
$$

that may leave us wondering: where is the vector-potential $\mathbf{A}$ here - and the field effects is has to describe? The resolution of this puzzle is easy: for a practical use (e.g., for the alternative derivation of the equations of motion), $\nexists$ has to be presented as a function of particle's generalized coordinates (in the case of unconstrained motion, these may be the Cartesian components of vector $\mathbf{r}$ that serves as an argument for potentials $\mathbf{A}$ and $\phi$ ), and the generalized momenta, i.e. the Cartesian components of vector $\mathbf{P}$ (plus, generally, time). Hence, velocity $u$ and factor $\gamma$ should be eliminated from Eq. (194). This may be done using relation (192), $\gamma m \mathbf{u}=\mathbf{P}-q \mathbf{A}$. For such elimination, it is sufficient to notice that according

[^412]to Eq. (193), difference ( $\not \boldsymbol{\nless}-q \phi$ ) is equal to the right-hand part of Eq. (72), so that the generalization of Eq. (78) is ${ }^{61}$
\[

$$
\begin{equation*}
(\not Z-q \phi)^{2}=\left(m c^{2}\right)^{2}+c^{2}(\mathbf{P}-q \mathbf{A})^{2} . \tag{9.195}
\end{equation*}
$$

\]

Particle's Hamiltonian

It is straightforward to verify that the Hamilton equations of motion for three Cartesian coordinates of the particle, obtained in the regular way ${ }^{62}$ from this $\mathcal{H}$, may be merged into the same vector equation (144). In the non-relativistic limit, the Taylor expansion of Eq. (195) to the first term in $p^{2}$ yields the following generalization of Eq. (74):

$$
\begin{equation*}
\nexists-m c^{2} \approx \frac{p^{2}}{2 m}+U=\frac{1}{2 m}(\mathbf{P}-q \mathbf{A})^{2}+U, \quad U=q \phi . \tag{9.196}
\end{equation*}
$$

This expression for $\mathcal{H}$, and Eq. (183) for $\mathcal{L}$, give a clear view of the electromagnetic field effect account in analytical mechanics. The electric part of the total Lorentz force $q(\mathbf{E}+\mathbf{u} \times \mathbf{B})$ can perform work on the particle, i.e. change its kinetic energy - see Eq. (148) and its discussion. As a result, the scalar potential $\phi$, whose gradient gives a contribution into $\mathbf{E}$, may be directly associated with potential energy $U=q \phi$. On the contrary, the magnetic component $q \mathbf{u} \times \mathbf{B}$ of the Lorentz force is always perpendicular to particle's velocity $\mathbf{u}$, and cannot work on it, and as a result cannot be described by a contribution to $U$. However, if A did not participate in functions $\mathcal{L}$ and/or $\not \subset$ at all, analytical mechanics would be unable to describe effects of magnetic field $\mathbf{B}=\nabla \times \mathbf{A}$ on particle's motion. Relations (183) and (197) show the wonderful way in which physics (or Mother Nature herself?) solves this problem: the vector-potential gives such contributions to both $\mathcal{L}$ and $\not \not \notin$ (if the latter is considered, as it should be, a function of $\mathbf{P}$ rather than $\mathbf{p}$ ) that cannot be uniquely attributed to either kinetic or potential energy, but ensure the correct equation of motion (144) in both the Lagrange and Hamilton formalisms.

I believe I still owe the reader a clear discussion of the physical sense of the canonical momentum $\mathbf{P}$. For that, let us consider a particle moving near a region of localized magnetic field $\mathbf{B}(\mathbf{r}, t)$, but not entering this region. If there is no electrostatic field (no other electric charges nearby), we can select such a local gauge that $\phi(\mathbf{r}, t)=0$ and $\mathbf{A}=\mathbf{A}(t)$, so that Eq. (144) is reduced to

$$
\begin{equation*}
\frac{d \mathbf{p}}{d t}=q \mathbf{E}=-q \frac{d \mathbf{A}}{d t}, \tag{9.197}
\end{equation*}
$$

immediately giving

$$
\begin{equation*}
\frac{d \mathbf{P}}{d t}=0 \tag{9.198}
\end{equation*}
$$

Hence, even if the magnetic field is changed in time, so that the induced electric field accelerates the particle, its conjugate momentum does not change. Hence $\mathbf{P}$ is a variable more stable to magnetic field changes than its kinetic counterpart $\mathbf{p}$. This conclusion may be criticized because it relies on a specific gauge, and generally $\mathbf{P} \equiv \mathbf{p}+q \mathbf{A}$ is not gauge-invariant, because vector-potential $\mathbf{A}$ isn't. ${ }^{63}$ However, as
${ }^{61}$ This relation may be also obtained from the expression for the Lorentz-invariant norm, $p^{\alpha} p_{\alpha}=(m c)^{2}$, of the 4momentum (75), $p^{\alpha}=\{\varepsilon / c, \mathbf{p}\}=\{(\nexists-q \phi) / c, \mathbf{P}-q \mathbf{A}\}$.
${ }^{62}$ See, e.g., CM Sec. 10.1.
${ }^{63}$ The kinetic momentum $\mathbf{p}=M \mathbf{u}$ is just the usual mu product modified for relativistic effects, so that this variable is evidently gauge- (though not Lorentz-) invariant.
was already discussed in Sec. 5.3, integral $\int \mathbf{A} \cdot d \mathbf{r}$ over a closed contour does not depend on the chosen gauge and equals to the magnetic flux $\Phi$ through the area limited by the contour - see Eq. (5.65). Integrating Eq. (197) over a closed trajectory of a particle (Fig. 14), and over the time of one orbit, we get

$$
\begin{equation*}
\Delta \oint_{C} \mathbf{p} \cdot d \mathbf{r}=-q \Delta \Phi, \quad \text { so that } \Delta \oint_{C} \mathbf{P} \cdot d \mathbf{r}=0, \tag{9.199}
\end{equation*}
$$

where $\Delta \Phi$ is the change of flux during that time. This gauge-invariant result confirms the above conclusion about the stability of the canonical momentum to magnetic field variations.


Fig. 9.14. Particle's motion around a localized magnetic flux.

Generally, Eq. (199) is invalid if a particle moves inside a magnetic field and/or changes its trajectory at the field variation. However, if the field is almost uniform, i.e. its gradient small in the sense of Eq. (177), this result is (approximately) applicable. Indeed, analytical mechanics ${ }^{64}$ tells us that for any canonical coordinate-momentum pair $\left\{q_{j}, p_{j}\right\}$, the corresponding action variable,

$$
\begin{equation*}
J_{j} \equiv \frac{1}{2 \pi} \oint p_{j} d q_{j} \tag{9.200}
\end{equation*}
$$

is asymptotically constant at slow variations of motion conditions. According to Eq. (191), for a particle in magnetic field, the generalized momentum corresponding to Cartesian coordinate $r_{j}$ is $P_{j}$ rather than $p_{j}$. Thus forming the net action variable $J \equiv J_{x}+J_{y}+J_{z}$, we may write

$$
\begin{equation*}
2 \pi J=\oint \mathbf{P} \cdot d \mathbf{r}=\oint \mathbf{p} \cdot d \mathbf{r}+q \Phi=\text { const } . \tag{9.201}
\end{equation*}
$$

Let us apply this relation to the motion of a non-relativistic particle in an almost uniform magnetic field, with a small longitudinal velocity, $\cdot u_{\|} / u_{\perp} \rightarrow 0$ (Fig. 15).


Fig. 9.15. Particle in a magnetic field with a small longitudinal gradient $\nabla B \|$ B .

In this case, $\Phi$ in Eq. (201) is the flux encircled by a cyclotron orbit, equal to $\left(-\pi R^{2} B\right)$, where $R$ is its radius given by Eq. (153), and the negative sign accounts for the fact that the "correct" direction of

[^413]the normal vector $\mathbf{n}$ in the definition of flux, $\Phi=\int \mathbf{B} \cdot \mathbf{n} d^{2} r$, is antiparallel to vector $\mathbf{B}$. At $u \ll c$, the kinetic momentum is just $p_{\perp}=m u_{\perp}$, while Eq. (153) yields
\[

$$
\begin{equation*}
m u_{\perp}=q B R . \tag{9.202}
\end{equation*}
$$

\]

Plugging these relations into Eq. (201), we get

$$
\begin{equation*}
2 \pi J=m u_{\perp} 2 \pi R-q \pi R^{2} B=m \frac{q R B}{m} 2 \pi R-q \pi R^{2} B=(2-1) q \pi R^{2} B=-q \Phi . \tag{9.203}
\end{equation*}
$$

This means that even if the circular orbit slowly moves in the magnetic field, the flux encircled by the cyclotron orbit should remain constant. One manifestation of this effect is the result already mentioned in the end of Sec. 6: if a small gradient of the magnetic field is perpendicular to the field itself, particle orbit's drift is perpendicular to $\nabla B$, so that $\Phi$ stays constant. Now let us analyze the case of a small longitudinal gradient, $\nabla B \| \mathbf{B}$ (Fig. 15). If the small initial longitudinal velocity $u \|$ is directed toward the higher field region, in order to keep $\Phi$ constant, the cyclotron orbit has to gradually shrink. Rewriting Eq. (202) as

$$
\begin{equation*}
m u_{\perp}=q \frac{\pi R^{2} B}{\pi R}=q \frac{|\Phi|}{\pi R} \tag{9.204}
\end{equation*}
$$

we see that this reduction of $R$ (at constant $\Phi$ ) should increase the orbiting speed $u_{\perp}$. But since the magnetic field cannot do work on the particle, its kinetic energy,

$$
\begin{equation*}
\varepsilon=\frac{m}{2}\left(u_{\|}^{2}+u_{\perp}^{2}\right) \tag{9.205}
\end{equation*}
$$

should stay constant, so that the longitudinal velocity $u_{\|}$has to decrease. Hence eventually orbit's drift has to stop, and then the orbit has to start moving back toward the region of lower fields, being essentially repulsed from the high-field region. This effect is very important, in particular, for plasma confinement: two coaxial magnetic coils, inducing magnetic fields of the same direction (Fig. 16), naturally form a "magnetic bottle" that traps charged particles injected, with sufficiently low longitudinal velocities, into the region between the coils. Such bottles are the core components of the (generally, very complex) systems used for plasma confinement, in particular in the context of the longterm efforts to achieve controllable nuclear fusion. ${ }^{65}$


Fig. 9.16. Magnetic bottle (VERY schematically).

Returning to the constancy of magnetic flux encircled by free particles, it reminds us of the Meissner-Ochsenfeld effect discussed in Sec. 6.3, and gives a motivation for a brief revisit of the electrodynamics of superconductivity. As was emphasized in that section, superconductivity is a

[^414]substantially quantum phenomenon; nevertheless the notion of the conjugate momentum $\mathbf{P}$ helps to understand its description. Indeed, the general rule of quantization of physical systems ${ }^{66}$ is that each canonical pair $\left\{q_{j}, p_{j}\right\}$ of a generalized coordinate and the corresponding momentum is described by quantum-mechanical operators that obey the following commutation relation
\[

$$
\begin{equation*}
\left[\hat{q}_{j}, \hat{p}_{j^{\prime}}\right]=i \hbar \delta_{j j^{\prime}} . \tag{9.206}
\end{equation*}
$$

\]

According to Eq. (191), for Cartesian coordinates $r_{j}$ of a particle in electromagnetic field, the corresponding generalized momenta are $P_{j}$, so that their operators should obey the following commutation relations:

$$
\begin{equation*}
\left[\hat{r}_{j}, \hat{P}_{j^{\prime}}\right]=i \hbar \delta_{j j^{\prime}} . \tag{9.207}
\end{equation*}
$$

In the coordinate representation of quantum mechanics, canonical momentum operators are described by Cartesian components of the vector operator -i $\hbar \nabla$. As a result, ignoring the rest energy $m c^{2}$ (which gives an inconsequential phase factor $\exp \left\{-i m c^{2} t / \hbar\right\}$ in the wave function), we can use Eq. (196) to rewrite the non-relativistic Schrödinger equation,

$$
\begin{equation*}
i \hbar \frac{\partial \psi}{\partial t}=\hat{\nexists} \psi \psi \tag{9.208}
\end{equation*}
$$

as follows:

$$
\begin{equation*}
i \hbar \frac{\partial \psi}{\partial t}=\left(\frac{\hat{p}^{2}}{2 m}+U\right) \psi=\left[\frac{1}{2 m}(-i \hbar \nabla-q \mathbf{A})^{2}+q \phi\right] \psi . \tag{9.209}
\end{equation*}
$$

Thus, I believe I have finally delivered on my promise to justify the replacement (6.44) which had been used in Chapter 6 to discuss electrodynamics of superconductors, including the MeissnerOchsenfeld effect. ${ }^{67}$

### 9.8. Analytical mechanics of electromagnetic field

We have just seen that analytical mechanics of a particle in an electromagnetic field may be used to get some important results. The same is true for the analytical mechanics of the field alone, and the field-particle system as a whole, which will be discussed in this section. For such a space-distributed system as the field, governed by local dynamics laws (Maxwell equations), we need to apply analytical mechanics to the local densities $\ell$ and $h$ of the Lagrangian and Hamiltonian functions, defined by relations

$$
\begin{equation*}
\mathcal{L}=\int \ell d^{3} r, \quad \nexists=\int h d^{3} r . \tag{9.210}
\end{equation*}
$$

Let us start, as usual, from the Lagrange formalism. Some clue on the possible structure of the Lagrangian density $\ell$ may be obtained from that of the description of the particle-field interaction in this

[^415]formalism, which was discussed in the last section. For the case of a single particle, the interaction is described by the last two terms of Eq. (183):
\[

$$
\begin{equation*}
\mathcal{L}_{\mathrm{int}}=-q \phi-q \mathbf{u} \cdot \mathbf{A} . \tag{9.211}
\end{equation*}
$$

\]

It is obvious that if charge $q$ is continuously distributed over some volume, we may present $\mathcal{L}$ as a volume integral of Lagrangian density

$$
\begin{equation*}
\ell_{\text {int }}=-\rho \phi+\mathbf{j} \cdot \mathbf{A}=-j_{\alpha} A^{\alpha} . \tag{9.212}
\end{equation*}
$$

## Interaction Lagrangian density

Notice that the density (in contrast to $\mathcal{L}_{\text {int }}$ itself) is Lorentz-invariant. (This is due to the contraction of the longitudinal coordinate, and hence volume, at the Lorentz transform.) Hence we may expect the density of field's Lagrangian to be Lorentz-invariant as well. Moreover, in the view of the simple, local structure of the Maxwell equations (containing only first spatial and temporal derivatives of the fields), $\ell$ should be a simple function of potential's 4 -vector and its 4 -derivative:

$$
\begin{equation*}
\ell=\ell\left(A^{\alpha}, \partial_{\alpha} A^{\beta}\right) . \tag{9.213}
\end{equation*}
$$

Also, the density should be selected in such a way that the 4-vector analog of the Lagrangian equations of motion,

$$
\begin{equation*}
\partial_{\alpha} \frac{\partial \ell}{\partial\left(\partial_{\alpha} A^{\beta}\right)}-\frac{\partial \ell}{\partial A^{\beta}}=0, \tag{9.214}
\end{equation*}
$$

gave us correct inhomogeneous Maxwell equations (127). ${ }^{68,69}$ It is clear that the field part $\ell_{\text {field }}$ of the total Lagrangian density $\ell$ should be a scalar, and a quadratic form of the field strength, i.e. of $F^{\alpha \beta}$, so that the natural choice is

$$
\begin{equation*}
\ell_{\text {field }}=\text { const } \times F_{\alpha \beta} F^{\alpha \beta} . \tag{9.215}
\end{equation*}
$$

with implied summation over both indices. Indeed, adding to this expression the interaction Lagrangian (212),

$$
\begin{equation*}
\ell=\ell_{\text {field }}+\ell_{\text {int }}=\operatorname{const} \times F_{\alpha \beta} F^{\alpha \beta}-j_{\alpha} A^{\alpha}, \tag{9.216}
\end{equation*}
$$

and performing differentiation, we may check that Eq. (214) indeed yields Eqs. (127), provided that the constant factor equals $\left(-1 / 4 \mu_{0}\right) \cdot{ }^{70}$ With that, the field Lagrangian

$$
\begin{equation*}
\ell_{\text {field }}=-\frac{1}{4 \mu_{0}} F_{\alpha \beta} F^{\alpha \beta}=\frac{1}{2 \mu_{0}}\left(\frac{E^{2}}{c^{2}}-B^{2}\right)=\frac{\varepsilon_{0}}{2} E^{2}-\frac{B^{2}}{2 \mu_{0}}=u_{e}-u_{m} \tag{9.217}
\end{equation*}
$$

Field's
Lagrangian density
where $u_{e}$ is the local density of the electric field energy density (1.67), and $u_{m}$ is the magnetic field energy density (5.57).

[^416]Let me hope the reader agrees that Eq. (217) is a wonderful result, because the Lagrangian function has the structure absolutely similar to the well-known expression $\mathcal{L}=T-U$ of the classical mechanics. So, for the field alone, the "potential" and "kinetic" energies are separable again. ${ }^{71}$

As a sanity check, let us explore whether we can calculate a 4 -vector analog of the Hamiltonian function $\mathcal{H}$. In the generic analytical mechanics,

$$
\begin{equation*}
\mathcal{H}=\sum_{j} \frac{\partial \mathscr{L}}{\partial \dot{q}_{j}} \dot{q}_{j}-\mathscr{L} \tag{9.218}
\end{equation*}
$$

However, just as for the Lagrangian function, for a field we should find the spatial density $h$ of the Hamiltonian, defined by the second of Eqs. (210), for which a natural 4-form of Eq. (218) is

$$
\begin{equation*}
h^{\alpha \beta}=\frac{\partial \ell}{\partial\left(\partial_{\alpha} A^{\gamma}\right)} \partial^{\beta} A^{\gamma}-g^{\alpha \beta} \ell . \tag{9.219}
\end{equation*}
$$

Calculated for the field alone, i.e. using Eq. (217) for $\ell$, this definition yields

$$
\begin{equation*}
h_{\text {field }}^{\alpha \beta}=\theta^{\alpha \beta}-\tau_{D}^{\alpha \beta}, \tag{9.220}
\end{equation*}
$$

where tensor

Symmetric energymomentum tensor

$$
\begin{equation*}
\theta^{\alpha \beta} \equiv \frac{1}{\mu_{0}}\left(g^{\alpha \gamma} F_{\gamma \delta} F^{\delta \beta}+\frac{1}{4} g^{\alpha \beta} F_{\gamma \delta} F^{\gamma \delta}\right), \tag{9.221}
\end{equation*}
$$

is gauge-invariant, while the remaining term,

$$
\begin{equation*}
\tau_{D}^{\alpha \beta} \equiv \frac{1}{\mu_{0}} g^{\alpha \gamma} F_{\gamma \delta} \partial^{\delta} A^{\beta} \tag{9.222}
\end{equation*}
$$

is not, so that it cannot correspond to any measurable variables. Fortunately, it is straightforward to verify that tensor $\tau_{D}$ may be presented in the form

$$
\begin{equation*}
\tau_{D}^{\alpha \beta}=\frac{1}{\mu_{0}} \partial_{\gamma}\left(F^{\gamma \alpha} A^{\beta}\right), \tag{9.223}
\end{equation*}
$$

and as a result obeys the following relations:

$$
\begin{equation*}
\partial_{\alpha} \tau_{D}^{\alpha \beta}=0, \quad \int \tau_{D}^{0 \beta} d^{3} r=0 \tag{9.224}
\end{equation*}
$$

so it does not interfere with the conservation properties of the gauge-invariant, symmetric energymomentum tensor (also called the symmetric stress tensor) $\theta^{\alpha \beta}$, to be discussed below.

Using Eqs. (125), components of the latter tensor may be expressed via the electric and magnetic fields. For $\alpha=\beta=0$,

$$
\begin{equation*}
\theta^{00}=h_{\text {field }}=\frac{\varepsilon_{0}}{2} E^{2}+\frac{B^{2}}{2 \mu_{0}}=u_{e}+u_{m}=u \tag{9.225}
\end{equation*}
$$

[^417]i.e. the expression for the total energy density $u$ - see Eq. (6.104b). The other 3 components of the same row/column turn out to be just the Cartesian components of the Poynting vector, divided by $c$ :
\[

$$
\begin{equation*}
\theta^{j 0}=\frac{1}{\mu_{0}}\left(\frac{\mathbf{E}}{c} \times \mathbf{B}\right)_{j}=\left(\frac{\mathbf{E}}{c} \times \mathbf{H}\right)_{j}=\frac{S_{j}}{c}, \quad \text { for } j=1,2,3 \tag{9.226}
\end{equation*}
$$

\]

The remaining 9 components $\theta_{j j^{\prime}}$ of the tensor, with $j^{\prime}=1,2,3$, are usually presented as

$$
\begin{equation*}
\theta^{j j^{\prime}}=-\tau_{j j^{\prime}}^{(M)} \tag{9.227}
\end{equation*}
$$

where $\tau^{(M)}$ is the so-called Maxwell stress tensor:

$$
\begin{equation*}
\tau_{j j^{\prime}}^{(M)}=\varepsilon_{0}\left(E_{j} E_{j^{\prime}}-\frac{\delta_{i j j^{\prime}}}{2} E^{2}\right)+\frac{1}{\mu_{0}}\left(B_{j} B_{j^{\prime}}-\frac{\delta_{i j^{\prime}}}{2} B^{2}\right), \tag{9.228}
\end{equation*}
$$

so that the whole symmetric energy-momentum tensor may be conveniently presented in the following symbolic way:

$$
\theta^{\alpha \beta}=\left(\begin{array}{c:cc}
u & \leftarrow & \mathbf{S} / c  \tag{9.229}\\
\hdashline \uparrow & & \rightarrow \\
\mathbf{S} & -\tau_{j j^{\prime}}^{(M)} \\
\hdashline c &
\end{array}\right) .
$$

The physical meaning of this tensor may be revealed in the following way. Considering Eq. (221) just as the definition of tensor $\theta^{\alpha \beta},{ }^{72}$ and using the 4 -vector form of Maxwell equations, given by Eqs. (127) and (129), it is straightforward to verify an extremely simple result for the 4-derivative of the symmetric tensor:

$$
\begin{equation*}
\partial_{\alpha} \theta^{\alpha \beta}=-F^{\beta \gamma} j_{\gamma} . \tag{9.230}
\end{equation*}
$$

Maxwell
stress
tensor

This expression is valid in the presence of the electromagnetic field sources, e.g., for any system of charged particles and the field they have created. Of these 4 equations (for 4 values of index $\beta$ ), the temporal one (with $\beta=0$ ) may be simply expressed via the energy density (225) and Poynting vector (226):

$$
\begin{equation*}
\frac{\partial u}{\partial t}+\nabla \cdot \mathbf{S}=-\mathbf{j} \cdot \mathbf{E} \tag{9.231}
\end{equation*}
$$

while 3 spatial equations (with $\beta=j=1,2,3$ ) may be presented in the form

$$
\begin{equation*}
\frac{\partial}{\partial t} \frac{S_{j}}{c^{2}}-\sum_{j^{\prime}=1}^{3} \frac{\partial}{\partial r_{j^{\prime}}} \tau_{j j^{\prime}}^{(M)}=-(\rho \mathbf{E}+\mathbf{j} \times \mathbf{B})_{j} \tag{9.232}
\end{equation*}
$$

Integrated over a volume $V$ limited by surface $S$, with the account of the divergence theorem, Eq. (231) returns us to the Poynting theorem (6.103):

[^418]\[

$$
\begin{equation*}
\int_{V}\left(\frac{\partial u}{\partial t}+\mathbf{j} \cdot \mathbf{E}\right) d^{3} r+\oint_{S} S_{n} d^{2} r=0 \tag{9.233}
\end{equation*}
$$

\]

while Eq. (232) yields: ${ }^{73}$

$$
\begin{equation*}
\int_{V}\left[\frac{\partial}{\partial t} \frac{\mathbf{S}}{c^{2}}+\mathbf{f}\right]_{j} d^{3} r=\sum_{j^{\prime}=1}^{3} \oint_{S} \tau_{j j^{\prime}}^{(M)} d A_{j^{\prime}}, \quad \text { with } \mathbf{f} \equiv \rho \mathbf{E}+\mathbf{j} \times \mathbf{B} \tag{9.234}
\end{equation*}
$$

where $d A_{j}=n_{j} d A=n_{j} d^{2} r$ is the $j^{\text {th }} \quad$ component of the elementary area vector $d \mathbf{A}=\mathbf{n} d A=\mathbf{n} d^{2} \mathbf{r}$ that is normal to volume's surface, and directed out of the volume - see Fig. 17.

Since, according to Eq. (5.10), vector $\mathbf{f}$ is nothing else than the density of volume-distributed forces applied from the field to the particles, we can use the $2^{\text {nd }}$ Newton law, in its relativistic form (144), to rewrite Eq. (234), for a stationary volume $V$, as

dynamics

$$
\begin{equation*}
\frac{d}{d t}\left[\int_{V} \frac{\mathbf{S}}{c^{2}} d^{3} r+\mathbf{p}_{\text {part }}\right]=\mathbf{F} \tag{9.235}
\end{equation*}
$$

where $\mathbf{p}_{\text {part }}$ is the total mechanical (relativistic) momentum of all particles in volume $V$, and vector $\mathbf{F}$ is defined by its Cartesian components:


Fig. 9.17. Force $d \mathbf{F}$ exerted on a boundary element $d \mathbf{A}$ of volume $V$ occupied by the field.

Force via the Maxwell tensor

Electromagnetic field's momentum um

discussion. As has been emphasized at this discussion, vector $\mathbf{S}=\mathbf{E} \times \mathbf{H}$ in this case does not correspond to any measurable energy flow. However, the corresponding momentum (237) of the field is not only real, but may be measured by the recoil impulse ${ }^{74}$ it gives to the field sources (say, to a magnetic coil inducing field $\mathbf{H}$ and to the capacitor plates creating field $\mathbf{E}$ ).

Now let us turn to our second result, Eq. (236). It tells us that the $3 \times 3$-element Maxwell stress tensor complies with the general definition of the stress tensor ${ }^{75}$ characterizing force $\mathbf{F}$ exerted by external forces on the boundary of a volume, in this case occupied by the electromagnetic field (Fig. 17). ${ }^{76}$ Let us use this important result to analyze two simple examples for static fields.
(i) Electrostatic field's effect on a perfect conductor. Since Eq. (235) has been derived for a free space region, we have to select volume $V$ outside the conductor, but we may align one of its faces with conductor's surface (Fig. 18).


Fig. 9.18. Electrostatic field near conductor's surface.

From Chapter 2, we know that the electrostatic field has to be perpendicular to the conductor's surface. Selecting axis $z$ in this direction, we have $E_{x}=E_{y}=0, E_{z}= \pm E$, so that only diagonal components of the tensor (228) are not equal to zero:

$$
\begin{equation*}
\tau_{x x}^{(M)}=\tau_{y y}^{(M)}=-\frac{\varepsilon_{0}}{2} E^{2}, \quad \tau_{z z}^{(M)}=\frac{\varepsilon_{0}}{2} E^{2}, \tag{9.238}
\end{equation*}
$$

Since the elementary surface area vector has just one nonvanishing component, $d A_{z}$, according to Eq. (236), only the last component (that is positive regardless of the sign of $E$ ) gives a contribution to the surface force $\mathbf{F}$. We see that the force exerted by the conductor (and eventually by external forces that hold the conductor in its equilibrium position) on the field is normal to the conductor and directed out of the field volume: $d F_{z} \geq 0$. Hence, by the $3^{\text {rd }}$ Newton law, the force exerted by the field on conductor's surface is directed toward the field-filled space:

$$
\begin{equation*}
d F_{\text {surface }}=-d F_{z}=-\frac{\varepsilon_{0}}{2} E^{2} d A \tag{9.239}
\end{equation*}
$$

[^419]This important result could be obtained by simpler means as well. For example, one could argue, quite convincingly, that the local relation between the force and field should not depend on the global

[^420]configuration creating the field, and consider a planar capacitor (Fig. 2.2) with surfaces of both plates charged by equal and opposite charges of density $\sigma= \pm \varepsilon_{0} E$. According to the Coulomb law, the charges should attract each other, pulling each plate toward the field region, so that Maxwell-tensor result gives the correct direction of the force. The force's magnitude (240) can be verified either by the direct integration of the Coulomb law, or by the following simple reasoning. In the plane capacitor, field $E_{z}=$ $\sigma / \varepsilon_{0}$ is equally contributed by two surface charges; hence the field created by the negative charge of the counterpart plate (not shown in Fig. 18) is $E_{-}=\sigma / 2 \varepsilon_{0}$, and the force it exerts of the elementary surface charge $d Q=\sigma d A$ of the positively charged plate is $d F=E_{-} d Q=\sigma^{2} d A / 2 \varepsilon_{0}=\varepsilon_{0} E^{2} d A / 2$, in accordance with Eq. (239). ${ }^{77}$

Quantitatively, even for such high electric field as $E=3 \mathrm{MV} / \mathrm{m}$ (close to the electric breakdown in air), the "negative pressure" ( $d F / d A$ ) given by Eq. (240) is of the order of $500 \mathrm{~Pa}\left(\mathrm{~N} / \mathrm{m}^{2}\right)$, i.e. below one thousandth of the ambient atmospheric pressure ( $1 \mathrm{bar} \approx 10^{5} \mathrm{~Pa}$ ). Still, these forces may be substantial in some cases, especially in good dielectrics (such as high-quality $\mathrm{SiO}_{2}$, grown at high temperature, which is broadly used in integrated circuits) that can withstand fields up to $\sim 10^{9} \mathrm{~V} / \mathrm{m}$.
(ii) Static magnetic field's effect on its source ${ }^{78}$ - say, solenoid's wall or superconductor's surface (Fig. 19).


Fig. 9.19. Static magnetic field near a current-carrying surface.

With the choice of coordinates shown in Fig. 19, we have $B_{x}= \pm B, B_{y}=B_{z}=0$, so that the Maxwell stress tensor (228) is diagonal again:

$$
\begin{equation*}
\tau_{x x}^{(M)}=\frac{1}{2 \mu_{0}} B^{2}, \quad \tau_{y y}^{(M)}=\tau_{z z}^{(M)}=-\frac{1}{2 \mu_{0}} B^{2} . \tag{9.240}
\end{equation*}
$$

However, but since for this geometry only $d A_{z}$ differs from 0 in Eq. (236), the sign of the resulting force is opposite to that in electrostatics: $d F_{z} \leq 0$, and the force exerted by the magnetic field upon the conductor's surface,

$$
\begin{equation*}
d F_{\text {surface }}=-d F_{z}=\frac{1}{2 \mu_{0}} B^{2} d A \tag{9.241}
\end{equation*}
$$

[^421]corresponds to a positive pressure. For good laboratory magnets ( $B \sim 10 \mathrm{~T}$ ), this pressure is of the order of $4 \times 10^{7} \mathrm{~Pa} \approx 400$ bars, i.e. is very substantial, so the magnets require solid mechanical design.

The direction of force (241) could be also readily predicted elementary magnetostatics arguments. Indeed, we can imagine the magnetic field volume limited by another, parallel wall with the opposite direction of surface current. According to the starting point of magnetostatics, Eq. (5.1), such surface currents of opposite directions have to repulse each other - doing that via the magnetic field.

Another explanation of the fundamental sign difference between the electric and magnetic field pressures may be provided on the electric circuit language. As we know from Chapter 2, the potential energy of the electric field stored in a capacitor may be presented in two equivalent forms,

$$
\begin{equation*}
U_{e}=\frac{C V^{2}}{2}=\frac{Q^{2}}{2 C} . \tag{9.242}
\end{equation*}
$$

Similarly, the magnetic field energy of in an inductive coil is

$$
\begin{equation*}
U_{m}=\frac{L I^{2}}{2}=\frac{\Phi^{2}}{2 L} \tag{9.243}
\end{equation*}
$$

If we do not want to consider the work of external sources on a virtual change of the system dimensions, we should use the latter forms of these relations, i.e. consider a galvanically detached capacitor ( $Q=$ const) and an externally-shorted inductance ( $\Phi=$ const). ${ }^{99}$ Now if we let the electric field forces (239) drag capacitor's plates in the direction they "want", i.e. toward each other, this would lead to a reduction of the capacitor thickness, and hence to an increase of capacitance $C$, and hence to a decrease of $U_{e}$. Similarly, for a solenoid, allowing pressure (242) to move its walls would lead to an increase of the solenoid volume, and hence of its inductance $L$, so that the potential energy $U_{m}$ would be also reduced as it should be. It is remarkable (actually, beautiful) how do the local field formulas (239) and (241) "know" about these global circumstances.

Finally, let us see whether the major results (237) and (241), obtained in this section, match each other. For that, let us return to the normal incidence of a plane, monochromatic wave from free space on the plane surface of a perfect conductor (see Fig. 7.8 and its discussion), and use those results to calculate the time average of pressure $d F_{\text {surface }} / d A$ imposed by the wave on the surface. At elastic reflection from conductor's surface, electromagnetic field's momentum retains its amplitude but changes its sign, so that the momentum transferred to a unit area of the surface (i.e. average pressure) is

$$
\begin{equation*}
\frac{\overline{d F_{\text {surface }}}}{d A}=2 c g_{\text {incident }}=2 c \frac{\overline{S_{\text {incident }}}}{c^{2}}=2 c \frac{1}{c^{2}} \frac{E_{\omega} H_{\omega}^{*}}{2}=\frac{E_{\omega} H_{\omega}^{*}}{c}, \tag{9.244}
\end{equation*}
$$

where $E_{\omega}$ and $H_{\omega}$ are complex amplitudes of the incident wave. Using relation (7.7) between these amplitudes (for $\varepsilon=\varepsilon_{0}$ and $\mu=\mu_{0}$ giving $E_{\omega}=c B_{\omega}$ ), we get

$$
\begin{equation*}
\frac{\overline{d F_{\text {surface }}}}{d A}=\frac{1}{c} c B_{\omega} \frac{B_{\omega}^{*}}{\mu_{0}}=\frac{\left|B_{\omega}\right|^{2}}{\mu_{0}} . \tag{9.245}
\end{equation*}
$$

[^422]On the other hand, as was discussed in Sec. 7.4, at the surface of the perfect mirror the electric field vanishes while the magnetic field doubles, so that we can use Eq. (241) with $B \rightarrow B(t)=2 \operatorname{Re}\left[B_{\omega} \mathrm{e}\{-\right.$ $i \omega t\}]$. Averaging the pressure over time, we get

$$
\begin{equation*}
\frac{\overline{d F_{\text {surface }}}}{d A}=\frac{1}{2 \mu_{0}} \overline{\left(2 \operatorname{Re}\left[B_{\omega} e^{-i \omega t}\right]\right)^{2}}=\frac{\left|B_{\omega}\right|^{2}}{\mu_{0}}, \tag{9.246}
\end{equation*}
$$

i.e. the same result as Eq. (245).

For the physics intuition development, it is useful to estimate the electromagnetic radiation pressure's magnitude. Even for a relatively high wave intensity $S_{n}$ of $1 \mathrm{~kW} / \mathrm{m}^{2}$ (close to that of the direct sunlight at Earth's orbit), the pressure $2 \mathrm{cg}_{n}=2 S_{n} / \mathrm{c}$ is somewhat below $10^{-5} \mathrm{~Pa} \sim 10^{-10}$ bar. Still, this extremely small effect was experimentally observed (by P. Lebedev) as early as in 1899, giving one more confirmation of the Maxwell's theory.

### 9.9. Exercise problems

9.1. Use the non-relativistic Doppler effect picture to derive Eq. (4).
9.2. Show that two successive Lorentz space/time transforms in the same direction, with velocities $u$ ' and $v$, are equivalent to a single transform with velocity $u$ given by Eq. (25).
9.3. $N+1$ reference frames, numbered by index $n$ (taking values $0,1, \ldots, N$ ), move in the same direction as a particle. Express the particle's velocity in frame $n=0$ via its velocity $u_{N}$ in frame number $N$ and the set of velocities $v_{n}$ of frame number $n$ relative to the frame number $(n-1)$.
9.4. A spaceship, moving with constant velocity $v$ directly from the Earth, sends back brief flashes of light with period $\Delta t_{s}$ - as measured by spaceship's clock. Calculate the period with which Earth's observers receive the signals - as measured by Earth's clock.
9.5. From the point of view of reference frame $0^{\prime}$, a straight rod, parallel to axis $x^{\prime}$, is moving, without rotation, with constant velocity $\mathbf{u}^{\prime}$ directed along axis $y^{\prime}$. The reference frame $0^{\prime}$ is itself moving relative to another ("lab") reference frame 0 , with similarly oriented axes, with a constant velocity $v$ along axis $x$, also without rotation - see Fig. on the right. Calculate:
(i) the direction of rod's velocity, and
(ii) the orientation of the rod on the $[x, y]$ plane,
as observed from the lab reference frame. Is the velocity perpendicular to the rod?
9.6. A relativistic particle moving with velocity $u$ decays into two particles with zero rest mass.
(i) Calculate the smallest possible angle between the decay product velocities (in the lab frame).
(ii) What is the largest possible energy of one product particle?
9.7. Starting from the rest at $t=0$, a spaceship moves with a constant acceleration, as measured in its instantaneous rest frame. Find its displacement $x(t)$ from the starting point, as measured from the lab frame, and interpret the result.
9.8. Calculate the first relativistic correction to the frequency of a harmonic oscillator as a function of its amplitude.
9.9. A particle with rest mass $m$ decays into two particles, with rest masses $m_{1}$ and $m_{2}$. Calculate the total energy of the first decay product, in the rest frame of the decayed particle.
9.10. A relativistic particle, propagating with velocity $\mathbf{v}$ outside of external fields, decays into two photons. ${ }^{80}$ Calculate the angular dependence of the probability of photon detection.
9.11. Photon with wavelength $\lambda$ is scattered by an electron, initially at rest. Considering the photon as an ultrarelativistic particle (with the rest mass $m=0$ ), find wavelength $\lambda$ ' of the scattered photon as a function of the scattering angle $\alpha$-see Fig. on the right. ${ }^{81}$

9.12. Calculate the threshold energy of a $\gamma$-photon for the reaction

$$
\gamma+\mathrm{p} \rightarrow \mathrm{p}+\pi^{0}
$$

if the proton was initially at rest.
Hint: For protons $m_{p} c^{2} \approx 938 \mathrm{MeV}$, while for neutral pions $m_{\pi} c^{2} \approx 135 \mathrm{MeV}$.
9.13. A relativistic particle with energy $\varepsilon$ and rest mass $m$ collides with a similar particle, initially at rest in the laboratory frame. Find:
(i) the final velocity of the center of mass of the system, in the lab frame,
(ii) the total energy of the system, in the center-of-mass frame, and
(iii) the final velocities of both particles (in the lab frame), if they move along the same direction.
9.14. A "primed" reference frame moves with the reduced velocity $\boldsymbol{\beta} \equiv \mathbf{v} / c=\mathbf{n}_{\chi} \beta$ relative to the "lab" frame. Use Eq. (109) to spell out components $T^{, 00}$ and $T^{, 0 j}$ (with $j=1,2,3$ ) of an arbitrary contravariant 4-tensor $T^{\gamma \delta}$.
9.15. Static fields $\mathbf{E}$ and $\mathbf{B}$ are uniform but arbitrary (both in magnitude and in direction). What should be the velocity of an inertial reference frame to have the vectors $\mathbf{E}$ ' and $\mathbf{B}$ ', observed from that frame, parallel? Is this solution unique?
9.16. Two charged particles, moving with the same constant velocity $\mathbf{u}$, are offset by distance $\mathbf{R}=\{a, b\}$ (see Fig. on the right), as measured in the lab frame. Calculate the forces between the particles - also in the lab frame.


[^423]9.17. Each of two very thin, long, parallel beams of electrons of the same velocity $\mathbf{u}$ carries electric charge of density $\lambda$ per unit length (as measured in the coordinate frame moving with electrons).
(i) Calculate the distribution of the electric and magnetic fields in the system (outside the beams), as measured in the lab frame.
(ii) Calculate the interaction force between the beams (per particle) and the resulting acceleration, both in the lab frame and in the system moving with the electrons. Compare the results and give a brief discussion of the comparison.
9.18. Spell out the Lorentz transform of the scalar potential and the vector potential components, and use the result to calculate the potentials of a point charge $q$, moving with a constant velocity $\mathbf{u}$, as measured in the lab reference frame.
9.19. Calculate the scalar and vector potentials created by a time-independent electric dipole $\mathbf{p}$, as measured in a reference frame which moves relatively to the dipole with a constant velocity $\mathbf{v}$, with the shortest distance ("impact parameter") equal to $b$.
9.20. Calculate the scalar and vector potentials created by a time-independent magnetic dipole $\mathbf{m}$, as measured in a reference frame which moves relatively to the dipole with a constant velocity $v \ll$ $c$, with the shortest distance ("impact parameter") equal to $b$.
9.21. Assuming that the magnetic monopole does exist and has magnetic charge $g$, calculate the change $\Delta \Phi$ of magnetic flux in a superconductor ring due to the passage of single monopole through it. Evaluate $\Delta \Phi$ for the monopole charge conjectured by Dirac, $g=n g_{0} \equiv n(2 \pi \hbar / e)$, where $n$ is an integer; compare the result with the magnetic flux quantum $\Phi_{0}$ (6.55) and discuss their relation.
9.22.* Calculate the trajectory of a relativistic particle in a uniform electrostatic field $\mathbf{E}$ for the case of arbitrary direction of its initial velocity $\mathbf{u}(0)$, using two different approaches - one of them different from the approach used in Sec. 6 for the case $\mathbf{u}(0) \perp \mathbf{E}$.
9.23. A charged relativistic particle with velocity $u$ performs planar cyclotron rotation in a uniform external magnetic field $B$. How much would the velocity and orbit radius change at a slow change of the field to a new magnitude $B^{\prime \prime}$ ?
9.24.* Analyze the motion of a relativistic particle in uniform, mutually perpendicular fields $\mathbf{E}$ and $\mathbf{B}$, for the particular case when $E$ is exactly equal to $c B$.
9.25.* Find the law of motion of a relativistic particle in uniform, parallel, static fields $\mathbf{E}$ and $\mathbf{B}$.
9.26. Neglecting relativistic effects, calculate the smallest voltage $V$ that has to be applied between the anode and cathode of a magnetron (see Fig. 13 and its discussion) to enable electrons to reach the anode in the absence of electron-electron interactions and collisions with the residual gas molecules. You may model the cathode and anode as two coaxial round cylinders, of radii $R_{1}$ and $R_{2}$, respectively, assume that the magnetic field $\mathbf{B}$, directed along their common axis, is uniform, and neglect the initial velocity of the electrons emitted by the cathode. (After the solution, estimate the validity of the last assumption for reasonable values of parameters.)
9.27. A charged, relativistic particle has been injected into a uniform electric field that oscillates in time with frequency $\omega$. Calculate the time dependence of the particle's velocity, as observed from a lab frame.
9.28. Analyze motion of a non-relativistic particle in a region where the electric and magnetic fields are both constant and uniform, but not necessarily parallel or perpendicular to each other.
9.29. A static distribution of electric charge in otherwise free space has created a timeindependent distribution $\mathbf{E}(\mathbf{r})$ of the electric field. Use two different approaches to express the energy density $u$ ' and the Poynting vector $\mathbf{S}^{\prime}$, as observed in a reference frame moving with constant velocity $\mathbf{v}$, via the components of vector $\mathbf{E}$. In particular, is $\mathbf{S}^{\prime}$ equal to ( $-\mathrm{v} \mathbf{u}^{\prime}$ )?
9.30. A plane wave, of frequency $\omega$ and intensity $S$, is normally incident on a perfect mirror, moving with velocity $v$ in the same direction as the wave.
(i) Calculate the reflected wave's frequency, as observed in the lab reference frame, and
(ii) use the Lorentz transform of the fields to calculate the reflected wave's intensity

- both as observed from the lab reference frame.
9.31. Carry out the second task of the previous problem by using the relations between wave's energy, power, and momentum.

Hint: As a byproduct, this approach should also give you the pressure exerted by the wave on the moving mirror.
9.32. Consider the simple model of plane capacitor charging by a lumped current source, shown in Fig. on the right, and prove that the momentum given by the constant, uniform external magnetic field $\mathbf{B}$ to the current-carrying conductor is equal and opposite to the momentum of the electromagnetic field that current $I(t)$ builds up in the capacitor. (You may let the capacitor be planar and very broad, and neglect the fringe field effects.)

9.33. Consider an electromagnetic plane wave packet propagating in free space, with the electric field represented as the Fourier integral

$$
\mathbf{E}(\mathbf{r}, t)=\operatorname{Re} \int_{-\infty}^{+\infty} \mathbf{E}_{k} e^{i \psi_{k}} d k, \quad \text { with } \psi_{k} \equiv k z-\omega_{k} t, \quad \text { and } \omega_{k} \equiv c|k| .
$$

Express the full linear momentum (per unit area of wave's front) of the packet via the complex amplitudes $\mathbf{E}_{k}$. Does the momentum depend on time? (In contrast with Problem 7.7, in this case the wave packet is not necessarily narrow.)
9.34. Calculate the pressure exerted on well-conducting walls of a waveguide with rectangular $(a \times b)$ cross-section by a wave propagating along it in the fundamental $\left(H_{10}\right)$ mode. Give an interpretation of the result.

## Chapter 10. Radiation by Relativistic Charges

In this chapter, we return to the electromagnetic wave radiation by moving charges, because the review of the special relativity background in the previous chapter enables an analysis of the radiation effects for arbitrary speed of the charged particle. After an analysis of such important particular cases as synchrotron radiation and "Bremsstrahlung" (brake radiation), we will discuss the apparently unrelated effect of Coulomb losses, which nevertheless will lead us to such important phenomena as the Cherenkov radiation and transitional radiation. In the end of the chapter, I will briefly review the effects of back action of the emitted radiation on the emitting particle, whose analysis reveals some limitations of classical electrodynamics.

### 10.1. Liénard-Wiechert potentials

A convenient starting point for the discussion of radiation by relativistic moving charges is provided by Eqs. (8.17) for retarded potentials. In free space these formulas are reduced to

$$
\begin{equation*}
\phi(\mathbf{r}, t)=\frac{1}{4 \pi \varepsilon_{0}} \int \frac{\rho\left(\mathbf{r}^{\prime}, t-R / c\right)}{R} d^{3} r^{\prime}, \quad \mathbf{A}(\mathbf{r}, t)=\frac{\mu_{0}}{4 \pi} \int \frac{\mathbf{j}\left(\mathbf{r}^{\prime}, t-R / c\right)}{R} d^{3} r^{\prime} . \tag{10.1}
\end{equation*}
$$

Here $R$ is the magnitude of the vector,

$$
\begin{equation*}
\mathbf{R}=\mathbf{r}-\mathbf{r}^{\prime}, \tag{10.2}
\end{equation*}
$$

that connects the source point $\mathbf{r}$ ' to the observation point $\mathbf{r}$. As a reminder, Eqs. (1) were derived from the Maxwell equations without any restrictions, and are very convenient for situations with continuous distribution of charge and current. On the other hand, for point charges, with delta-functional $\rho$ and $\mathbf{j}$, it is more convenient to recast these relations into a simpler form that would not require the integration over the $\mathbf{r}$ 'space.

This reduction, however, requires care. Indeed, for a single point charge $q$ moving with velocity $\mathbf{u}$, such integration of Eqs. (1), if carried out naïvely, would yield the following apparent result:

$$
\begin{equation*}
\phi(\mathbf{r}, t)=\frac{1}{4 \pi \varepsilon_{0}} \frac{q}{R_{r}}, \quad \text { i.e. } \frac{\phi(\mathbf{r}, t)}{c}=\frac{\mu_{0}}{4 \pi} \frac{q c}{R_{r}} ; \quad \mathbf{A}(\mathbf{r}, t)=\frac{\mu_{0}}{4 \pi} \frac{q \mathbf{u}_{r}}{R_{r}}, \quad[\mathrm{WRONG}!] \tag{10.3}
\end{equation*}
$$

where index $r$ marks the variables to be calculated at time $t-R_{r} / c$. This is a good example how the science of relativity (even the special one :-) cannot be taken too lightly. Indeed, 4-vectors (9.84)-(9.85), formed from potentials (3), would not obey the Lorentz transform rule (9.91), because distance $R_{r}$ also depends on the reference frame it is measured in.

In order to correct the error, we need, first of all, to specify what exactly is $R_{r}$ for a point charge. Evidently, in this case, only one space-time point $\left\{\mathbf{r}^{\prime}, t^{\prime}\right\}$ may contribute to integrals (1) for any observation point $\{\mathbf{r}, \mathrm{t}\}$. The point should be found from the retardation condition $t^{\prime}=t-R_{r} / c$, i.e.

$$
\begin{equation*}
c\left(t-t^{\prime}\right)=\left|\mathbf{r}(t)-\mathbf{r}^{\prime}\left(t^{\prime}\right)\right| . \tag{10.4}
\end{equation*}
$$

Figure 1 depicts the graphical solution of this self-consistency equation as the point of intersection of the light cone of the observation point (see Fig. 9.9 and its discussion) and the trajectory of the charged
particle. ${ }^{1}$ As in Eq. (3), I will use index $r$ to mark all variables corresponding to the retarded point $\{\mathbf{r}$,, $\left.t^{\prime}\right\}$ that satisfies Eq. (4); for example, $t^{\prime} \equiv t_{r}, c\left(t-t_{r}\right) \equiv R_{r}$ (see Fig. 1), $\mathbf{u}\left\{\mathbf{r}^{\prime}, t_{r}\right) \equiv \mathbf{u}_{r}$, etc, as measured in the "lab" reference frame - generally, any inertial frame that moves with the same velocity as the observation point at the moment $t$ we are considering.


Fig. 10.1. Graphical solution of Eq. (4).

Now let us write Eqs. (1) for a point charge in another inertial reference frame 0 ', whose velocity (as measured in the lab frame) coincides, at moment $t_{r}$, with the same velocity ( $\mathbf{u}_{r}$ ) of the point charge. In that frame the charge rests, so that

$$
\begin{equation*}
\phi^{\prime}=\frac{q}{4 \pi \varepsilon_{0} R^{\prime}}, \quad \mathbf{A}^{\prime}=0 \tag{10.5}
\end{equation*}
$$

but let us remember that this $R$ ' may not be equal to $R$, because the latter distance is measured in the "lab" reference frame. Let us use the identity $1 / \varepsilon_{0} \equiv \mu_{0} c^{2}$ to rewrite Eq. (5) in the form of components of a 4-vector similar in structure to Eq. (3):

$$
\begin{equation*}
\frac{\phi^{\prime}}{c}=\frac{\mu_{0}}{4 \pi} q \frac{c}{R^{\prime}}, \quad \mathbf{A}^{\prime}=0 \tag{10.6}
\end{equation*}
$$

Now it is easy to guess the correct answer for the whole 4-potential:

$$
\begin{equation*}
A^{\alpha}=\frac{\mu_{0}}{4 \pi} q \frac{c u^{\alpha}}{u_{\beta} R^{\beta}} \tag{10.7}
\end{equation*}
$$

where (just as a reminder), $A^{\alpha} \equiv\{\phi / c, \mathbf{A}\}, u^{\alpha} \equiv \gamma\{c, \mathbf{u}\}$, and $R^{\alpha}$ is a 4-vector of the event distance, formed similarly to that of a single event - cf. Eq. (9.48):

$$
\begin{equation*}
R^{\alpha} \equiv\left\{c\left(t-t^{\prime}\right), \mathbf{R}\right\} \equiv\left\{c\left(t-t^{\prime}\right), \mathbf{r}-\mathbf{r}^{\prime}\right\} \tag{10.8}
\end{equation*}
$$

Indeed, we need the 4 -vector $A^{\alpha}$ that would:
(i) obey the Lorentz transform,
(ii) have its spatial components $A_{j}$ scaling as $u_{j}$, and
(iii) be reduced to the correct result (5) in the reference frame moving with the charge.

[^424]Formula (7) evidently satisfies all these requirements, because the scalar product in its denominator is just

$$
\begin{equation*}
u_{\beta} R^{\beta}=\gamma\{c,-\mathbf{u}\} \cdot\left\{c\left(t-t^{\prime}\right), \mathbf{R}\right\}=\gamma\left[c^{2}\left(t-t^{\prime}\right)-\mathbf{u} \cdot \mathbf{R}\right]=\gamma c(R-\boldsymbol{\beta} \cdot \mathbf{R})=\gamma c R(1-\boldsymbol{\beta} \cdot \mathbf{n}), \tag{10.9}
\end{equation*}
$$

where $\mathbf{n} \equiv \mathbf{R} / R$ is a unit vector in the observer's direction, $\boldsymbol{\beta} \equiv \mathbf{u} / c$ is the normalized velocity of the particle, and $\gamma \equiv 1 /\left(1-u^{2} / c^{2}\right)^{1 / 2} .^{2}$ In the reference frame of the charge (in which $\beta=0$ and $\gamma=1$ ), expression (9) is reduced to $c R$, so that Eq. (7) is correctly reduced to Eq. (6). Now let us spell out components of Eq. (7) in the lab frame (in which $t^{\prime}=t_{r}$ and $R=R_{r}$ ):

LiénardWiechert potentials

$$
\begin{gather*}
\phi(\mathbf{r}, t)=\frac{1}{4 \pi \varepsilon_{0}} \frac{q}{(R-\boldsymbol{\beta} \cdot \mathbf{R})_{r}}=\frac{1}{4 \pi \varepsilon_{0}} q\left[\frac{1}{R(1-\boldsymbol{\beta} \cdot \mathbf{n})}\right]_{r},  \tag{10.10a}\\
\mathbf{A}(\mathbf{r}, t)=\frac{\mu_{0}}{4 \pi} q\left(\frac{\mathbf{u}}{R-\boldsymbol{\beta} \cdot \mathbf{R}}\right)_{r}=\frac{\mu_{0}}{4 \pi} q c\left[\frac{\boldsymbol{\beta}}{R(1-\boldsymbol{\beta} \cdot \mathbf{n})}\right] r=\phi(\mathbf{r}, t) \frac{\mathbf{u}_{r}}{c^{2}} . \tag{10.10b}
\end{gather*}
$$

These formulas are called the Liénard-Wiechert potentials. ${ }^{3}$ In the non-relativistic limit, they coincide with the naïve guess (3), but in the general case include the additional factor (1- $\boldsymbol{\beta} \cdot \mathbf{n}$ ) in the denominator, which describes the apparent increase of the effective charge density of the source due to the apparent change of distance $R$, at $\beta \sim 1$. In order to understand its origin, let us consider a simple 1D model of the radiation: a uniformly charged rod, of length $l$, moving directly toward an observer located at point $\mathbf{r}$, with a constant speed $u$ (Fig. 2). As a result of this motion, the observer may measure the field (1) induced by the rod, within a certain time interval $\left[t_{\text {start }}, t_{\text {stop }}\right]$.


Fig. 10.2. Geometric effect behind factor (1- $\boldsymbol{\beta} \cdot \mathbf{n}$ ) in the Liénard-Wiechert potentials.

That trailing end of this field pulse, observed at $t=t_{\text {stop }}$, is emitted by the far (in Fig. 2, leftmost) end of the rod at moment $t$ 'stop. Due to the limited speed of the rod, $u<c$, the moment $t^{\prime}$ stop comes earlier than the moment $t_{\text {start, }}^{\prime}$, at which the front end of the rod emits the field that starts the observed pulse. During the positive time interval ( $t^{\prime}$ start $-t^{\prime}$ stop $)$, the rod passes an additional distance $u\left(t^{\prime}\right.$ start $\left.-t_{\text {stop }}^{\prime}\right)-$ see the bottom panel of Fig. 2. Using the evident relations shown on each of the two panels of Fig. 2 to express $r$, and requiring them to give the same result, we get the following relation

$$
\begin{equation*}
c\left(t_{\text {stop }}-t_{\text {stop }}^{\prime}\right)=u\left(t_{\text {start }}^{\prime}-t_{\text {stop }}^{\prime}\right)+l+c\left(t_{\text {start }}-t_{\text {start }}^{\prime}\right) \tag{10.11}
\end{equation*}
$$

[^425]Using it to express the difference $\Delta t^{\prime}(u) \equiv t_{\text {start }}^{\prime}-t_{\text {start }}>0$ in the limit when $t_{\text {stop }} \rightarrow t_{\text {start, }}$, i.e. when the observed radiation pulse is short, we get

$$
\begin{equation*}
\Delta t^{\prime}(u)=\frac{l}{c-u}=\frac{l / c}{1-\beta} \equiv \frac{\Delta t(0)}{1-\beta}, \quad \text { where } \Delta t^{\prime}(0) \equiv \frac{l}{c}, \tag{10.12}
\end{equation*}
$$

is a factor of $1 /(1-\beta)$ smaller than what is would be at negligible source speed. Hence the time interval between the retarded moments $t_{r}$ for two ends of the rod is compressed as $u$ is increased. Since the total charge of the rod does not depend on $u$, its linear charge density is increased, and the field in the observation point is increased accordingly. Somewhat counter-intuitively, Eq. (12) shows that this field re-normalization is independent of the source size $l$, and hence takes place even in the limit $l \rightarrow 0$, e.g., for a point source. ${ }^{4}$

So, the 4 -vector formalism has provided a big help for the calculation of field potentials. Now, the electric and magnetic field corresponding to the potentials may be found by the plugging Eqs. (10) into the general formulas (6.106). This operation should be also performed very carefully, because Eqs. (6.106) require the differentiation over the coordinates $\{\mathbf{r}, t\}$ of the observation point, while we want the fields to be expressed via particle's velocity $\mathbf{u}_{\mathrm{r}} \equiv\left(d \mathbf{r}^{\prime} / d t^{\prime}\right)_{r}$ that participates in Eqs. (10). In order to find the relation between derivatives over $t$ and $t^{\prime}$, let us differentiate Eq. (4), rewritten as

$$
\begin{equation*}
R_{r}=c\left(t-t_{r}\right) \tag{10.13}
\end{equation*}
$$

over $t$ and $t_{r}$. In order to calculate derivative $\partial R_{r} / \partial t_{r}$, let us first differentiate identity $R^{2}=\mathbf{R} \cdot \mathbf{R}$ :

$$
\begin{equation*}
2 R_{r} \frac{\partial R_{r}}{\partial t_{r}}=2 \mathbf{R}_{r} \cdot \frac{\partial \mathbf{R}_{r}}{\partial t_{r}} \tag{10.14}
\end{equation*}
$$

Since $\partial \mathbf{R}_{r} / \partial t_{r}=\partial\left(\mathbf{r}-\mathbf{r}^{\prime}\right) / \partial t_{r}=-\partial \mathbf{r}^{\prime} / \partial t_{r}=-\mathbf{u}$, Eq. (14) yields

$$
\begin{equation*}
\frac{\partial R_{r}}{\partial t_{r}}=\frac{\mathbf{R}_{r}}{R_{r}} \cdot \frac{\partial \mathbf{R}_{r}}{\partial t_{r}}=-(\mathbf{n} \cdot \mathbf{u})_{r} . \tag{10.15}
\end{equation*}
$$

Now let us differentiate the same function $R_{r}$ over $t$, keeping $\mathbf{r}$ fixed. On one hand, Eq. (13) yields

$$
\begin{equation*}
\frac{\partial R_{r}}{\partial t}=c-c \frac{\partial t_{r}}{\partial t} . \tag{10.16}
\end{equation*}
$$

On the other hand, according to Eq. (4), if $\mathbf{r}$ is fixed, $t^{\prime}$ is a function of $t$ alone, so that, using Eq. (15), we may write

$$
\begin{equation*}
\frac{\partial R}{\partial t}=\frac{\partial R_{r}}{\partial t_{r}} \frac{\partial t_{r}}{\partial t}=-(\mathbf{n} \cdot \mathbf{u})_{r} \frac{\partial t_{r}}{\partial t} . \tag{10.17}
\end{equation*}
$$

Requiring Eqs. (16) and (17) to give the same result, we get the same factor that participates in the Liénard-Wiechert potentials (10) and Eq. (12):

[^426]\[

$$
\begin{equation*}
\frac{\partial t_{r}}{\partial t}=\frac{c}{c-(\mathbf{n} \cdot \mathbf{u})_{r}}=\left(\frac{1}{1-\boldsymbol{\beta} \cdot \mathbf{n})_{r}}\right)_{r} \tag{10.18}
\end{equation*}
$$

\]

This relation may be readily interpreted - at least semi-quantitatively. At fixed $\mathbf{r}$, variation $\partial t$ of the observation time corresponds to a small vertical shift of the light cone in Fig. 2, while $\partial t_{r}$ is the corresponding shift of the retarded time $t_{r}$, i.e. of the point where the world line $\mathbf{r}^{\prime}\left(t^{\prime}\right)$ crosses the light cone at the observation point $\mathbf{r}(t)$. It is evident from that figure that if the particle does not move (i.e. its world trajectory in a vertical straight line), then $\partial t_{r}=\partial t$. On the other hand, if the particles moves fast (with speed $u \approx \mathrm{c}$ ) toward the observation point, its world line crosses the light cone at a small ("grazing") angle, so that $\partial t_{r} \gg \partial t$, in accordance with Eq. (18).

Since the retarded time $t_{r}$, as the solution of Eq. (3), depends not only on the observation time $t$, but also the observation point $\mathbf{r}$, so we also need to calculate its spatial derivative - the gradient in $\mathbf{r}$ space. A calculation, absolutely similar to that carried above, yields

$$
\begin{equation*}
\nabla t_{r}=-\left[\frac{\mathbf{n}}{c(1-\boldsymbol{\beta} \cdot \mathbf{n})}\right]_{r} . \tag{10.19}
\end{equation*}
$$

Using Eqs. (6.106), (18) and (19), the calculation of fields from Eqs. (10) is straightforward but tedious, and is left for reader's exercise. For the electric field, the result is:

Electric magnetic fields of relativistic particle

$$
\begin{equation*}
\mathbf{E}=\frac{q}{4 \pi \varepsilon_{0}}\left[\frac{\mathbf{n}-\boldsymbol{\beta}}{\gamma^{2}(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3} R^{2}}+\frac{\mathbf{n} \times\{(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3} c R}\right]_{r} . \tag{10.20a}
\end{equation*}
$$

The only good news about this uncomfortably bulky result is that a similar differentiation gives essentially the same formula for the magnetic field, which may be expressed via Eq. (20a): ${ }^{5}$

$$
\begin{equation*}
\mathbf{B}=\mathbf{n}_{r} \times \frac{\mathbf{E}}{c}, \quad \text { i.e. } \mathbf{H}=\frac{1}{Z_{0}} \mathbf{n}_{r} \times \mathbf{E} . \tag{10.20b}
\end{equation*}
$$

Thus the magnetic and electric fields are always perpendicular to each other, and related just as in a plane wave - cf. Eq. (7.6), ${ }^{6}$ with the only difference that now vector $\mathbf{n}_{r}$ may be a function of time.

As a sanity check, let us use Eq. (20a) as an alternative way to find the electric field of a charge moving without acceleration, i.e. uniformly, along a straight line - see Fig. 9.11 (reproduced in Fig. 3) and its discussion in Sec. 5. (This example will also exhibit the challenges of practical application of the Liénard-Wiechert formulas.) In this case vector $\beta$ does not change in time, so that the second term in Eq. (20a) vanishes, and all we need to do is to spell out the Cartesian components of the first term. Let us select the coordinate axes and time origin in the same way as shown in Fig. 3, and make a clear distinction between the actual position, $\mathbf{r}^{\prime}(t)=\{u t, 0,0\}$ of the charged particle at the instant $t$ we are
${ }^{5}$ An alternative way to derive Eqs. (20) is to plug the 4 -vector of potentials, given by Eq. (7), into Eq. (9.124) to calculate the field strength tensor. This calculation yields

$$
F^{\alpha \beta}=\frac{\mu_{0} q}{4 \pi} \frac{1}{u_{\gamma} R^{\gamma}} \frac{d}{d \tau}\left[\frac{R^{\alpha} u^{\beta}-R^{\beta} u^{\alpha}}{u_{\delta} R^{\delta}}\right] .
$$

Now the elements of this tensor may be identified with fields components in accordance with Eq. (9.125).
${ }^{6}$ Superficially, Eq. (20b) contradicts the electrostatics where B should vanish while E stays finite. However, note that according to the Coulomb law for a point charge, in this case $\mathbf{E}=E \mathbf{n}=E \mathbf{n}_{r}$, so that $\mathbf{B} \propto \mathbf{n}_{r} \times \mathbf{E} \propto \mathbf{n}_{r} \times \mathbf{n}_{r}=0$.
considering, and its retarded position $\mathbf{r}$ ' $\left(t_{r}\right)$, where $t_{r}$ is the solution of Eq. (4), i.e. the moment when the particle's field, moving with the speed of light, reaches the observation point $\mathbf{r}$. In these coordinates

$$
\begin{equation*}
\boldsymbol{\beta}=\{\beta, 0,0\}, \quad \mathbf{r}=\{0,0, b\}, \quad \mathbf{r}^{\prime}\left(t_{r}\right)=\left\{u t_{r}, 0,0\right\}, \quad \mathbf{n}_{r}=\{\cos \theta, 0, \sin \theta\} \tag{10.21}
\end{equation*}
$$

with $\cos \theta=-u t^{\prime} / R_{r}$, so that $\left[(\mathbf{n}-\boldsymbol{\beta})_{x}\right]_{r}=-u t^{\prime} / R_{r}-\beta$, and for the longitudinal component of the electric field, Eq. (20a) yields

$$
\begin{equation*}
E_{x}=\frac{q}{4 \pi \varepsilon_{0}}\left[\frac{-u t_{r} / R-\beta}{\gamma^{2}(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3} R^{2}}\right]_{r}=\frac{q}{4 \pi \varepsilon_{0}}\left[\frac{-u t_{r}-\beta R}{\gamma^{2}(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3} R^{3}}\right]_{r} . \tag{10.22}
\end{equation*}
$$



Fig. 10.3. Geometry of the linearly moving charge problem.

But according to Eq. (13), product $\beta R_{r}$ may be presented as $\beta c\left(t-t_{r}\right)=u\left(t-t_{r}\right)$. Plugging this expression into Eq. (22), we may eliminate the explicit dependence of $E_{x}$ on time $t^{\prime}$ :

$$
\begin{equation*}
E_{x}=\frac{q}{4 \pi \varepsilon_{0}} \frac{-u t}{\gamma^{2}[(1-\boldsymbol{\beta} \cdot \mathbf{n}) R]_{r}^{3}} . \tag{10.23}
\end{equation*}
$$

The nonvanishing transverse component of the field also has a similar form:

$$
\begin{equation*}
E_{y}=\frac{q}{4 \pi \varepsilon_{0}}\left[\frac{\sin \theta}{\gamma^{2}(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3} R^{2}}\right]_{r}=\frac{q}{4 \pi \varepsilon_{0}} \frac{b}{\gamma^{2}[(1-\boldsymbol{\beta} \cdot \mathbf{n}) R]_{r}^{3}}, \tag{10.24}
\end{equation*}
$$

while $E_{z}=0$. Hence, the only combination of $t_{r}$ and $R_{r}$ we still need to calculate is $[(1-\boldsymbol{\beta} \cdot \mathbf{n}) R]_{r}$. From Fig. 3, $\boldsymbol{\beta} \cdot \mathbf{n}_{r}=\beta \cos \theta=-\beta u t^{\prime} / R_{r}$, so that $(1-\beta \cdot \mathbf{n}) R_{r}=R_{r}+\beta u t_{r}=c\left(t-t_{r}\right)+c \beta^{2} t_{r}=c t-c t_{r} / \gamma^{2}$. What remains is to find time $t_{r}$ from the self-consistency equation (13) that in our case (Fig. 3) takes the form

$$
\begin{equation*}
R_{r}^{2} \equiv c^{2}\left(t-t_{r}\right)^{2}=b^{2}+\left(u t_{r}\right)^{2} . \tag{10.25}
\end{equation*}
$$

After solving this quadratic equation (with the appropriate negative sign before the square root, in order to get $t_{r}<t$ ),

$$
\begin{equation*}
t_{r}=\gamma^{2} t-\left[\left(\gamma^{2} t\right)^{2}-\gamma^{2}\left(t^{2}-b^{2} / c^{2}\right)\right]^{1 / 2}=\gamma^{2} t-\frac{\gamma}{c}\left(u^{2} \gamma^{2} t^{2}+b^{2}\right)^{1 / 2} \tag{10.26}
\end{equation*}
$$

we obtain a simple result:

$$
\begin{equation*}
[(1-\boldsymbol{\beta} \cdot \mathbf{n}) R]_{\mathrm{r}}=\frac{c}{\gamma^{2}}\left(u^{2} \gamma^{2} t^{2}+b^{2}\right)^{1 / 2} \tag{10.27}
\end{equation*}
$$

so that the electric field components are

$$
\begin{equation*}
E_{x}=-\frac{q}{4 \pi \varepsilon_{0}} \frac{\gamma u t}{\left(b^{2}+\gamma^{2} u^{2} t^{2}\right)^{3 / 2}}, \quad E_{y}=\frac{q}{4 \pi \varepsilon_{0}} \frac{\gamma b}{\left(b^{2}+\gamma^{2} u^{2} t^{2}\right)^{3 / 2}}, \quad E_{z}=0 . \tag{10.28}
\end{equation*}
$$

These are exactly Eqs. (9.139), ${ }^{7}$ which had been obtained in Sec. 9.5 by simpler means, without the necessity to solve the self-consistency equation for $t_{r}$. However, that alternative approach was essentially based on the inertial motion of the particle, and cannot be used in problems in which particle moves with acceleration. In those problems, the second term in Eq. (20a), describing wave radiation, is essential and most important.

### 10.2. Radiation power

Let us calculate the angular distribution of particle's radiation. For that, we need to return to use Eqs. (20) to find the Poynting vector $\mathbf{S}=\mathbf{E} \times \mathbf{H}$, and in particular its component $S_{n}=\mathbf{S} \cdot \mathbf{n}_{r}$, at large distances $R$ from the particle. Following tradition, let us express the result as the radiated energy per unit solid angle per unit time interval $d t_{r}$ of the radiation (rather than its measurement), using Eq. (18):

$$
\begin{equation*}
\frac{d \mathcal{P}}{d \Omega} \equiv-\frac{d \varepsilon}{d \Omega d t_{r}}=\left[R^{2} S_{n} \frac{\partial t}{\partial t_{r}}\right]_{r}=\left[R^{2}(\mathbf{E} \times \mathbf{H}) \cdot \mathbf{n}(1-\boldsymbol{\beta} \cdot \mathbf{n})\right]_{r} . \tag{10.29}
\end{equation*}
$$

At sufficiently large distances from the particle, i.e. in the limit $R \rightarrow \infty$, the contribution of the first (essentially, the Coulomb field) term in the square brackets of Eq. (20a) vanishes as $1 / R^{2}$, so that we get a key formula valid for an arbitrary law of particle motion: ${ }^{8}$

$$
\begin{equation*}
\frac{d \mathcal{P}}{d \Omega}=\frac{Z_{0} q^{2}}{(4 \pi)^{2}} \frac{|\mathbf{n} \times[(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}]|^{2}}{(1-\mathbf{n} \cdot \boldsymbol{\beta})^{5}} \tag{10.30}
\end{equation*}
$$

Now, let us apply this important result to some simple cases. First of all, Eq. (30) says that a charge moving with constant velocity $\beta$ does not radiate at all. This might be expected from our analysis of this case in Sec. 9.5, because in the reference frame moving with the charge it produces only the Coulomb electrostatic field, i.e. no radiation.

Next, let us consider a linear motion of a point charge with a nonvanishing acceleration evidently directed along the motion line. With the coordinate axes directed as shown in Fig. 4a, each of the vectors involved in Eq. (30) has at most two nonvanishing Cartesian components:

$$
\begin{equation*}
\mathbf{n}=\{\sin \theta, 0, \cos \theta\}, \quad \boldsymbol{\beta}=\{0,0, \beta\}, \quad \dot{\boldsymbol{\beta}}=\{0,0, \dot{\beta}\} . \tag{10.31}
\end{equation*}
$$

where $\theta$ is the angle between the directions of particle's motion and radiation propagation. Plugging these expressions into Eq. (30) and performing the vector multiplications, we get

$$
\begin{equation*}
\frac{d P}{d \Omega}=\frac{Z_{0} q^{2}}{(4 \pi)^{2}} \dot{\beta}^{2} \frac{\sin ^{2} \theta}{(1-\beta \cos \theta)^{5}} \tag{10.32}
\end{equation*}
$$

[^427]

Fig. 10.4. Radiation at linear acceleration: (a) geometry of the problem, and (b) the last fraction in Eq. (32) as a function of angle $\theta$.

Figure 4 b shows the angular distribution of this radiation, for three values of particle's speed. If it is relatively low ( $\beta \ll 1$ ), the denominator in Eq. (32) is close to 1 for all observation angles $\theta$, so that the angular distribution of the radiation power is close to $\sin ^{2} \theta$ - just as it follows from the general nonrelativistic formula (8.26). However, as the velocity is increased, the denominator is less than 1 for $\theta<$ $\pi / 2$, i.e. for the forward-looking directions, and is larger than 1 for back directions. As a result, the radiation toward particle's velocity is increased (somewhat counter-intuitively, regardless of the acceleration sign!), while that in the back direction is suppressed. For ultra-relativistic particles ( $\beta \rightarrow 1$ ), this trend is enormously exacerbated, and radiation to very small forward angles dominates. In order to describe this main part of the distribution, we may expand the trigonometric functions of $\theta$, participating in Eq. (32), into the Taylor series in small $\theta$, and keep only their leading terms: $\sin \theta \approx \theta, \cos \theta \approx 1-\theta$ ${ }^{2} / 2$, so that $(1-\beta \cos \theta) \approx\left(1+\gamma^{2} \theta^{2}\right) / 2 \gamma^{2}$. The resulting expression,

$$
\begin{equation*}
\frac{d P}{d \Omega} \approx \frac{2 Z_{0} q^{2}}{\pi^{2}} \dot{\beta}^{2} \gamma^{8} \frac{(\gamma \theta)^{2}}{\left(1+\gamma^{2} \theta^{2}\right)^{5}}, \text { for } \gamma \gg 1 \tag{10.33}
\end{equation*}
$$

describes a narrow distribution of radiation, with a maximum at angle

$$
\begin{equation*}
\theta_{0}=\frac{1}{2 \gamma} \ll 1 \tag{10.34}
\end{equation*}
$$

Note that due to the axial symmetry of the result, and the fact that according to Eq. (33), $d \mathcal{P} / d \Omega=0$ in the exact direction of particle's propagation $(\theta=0)$, Eq. (40) describes a narrow circular "hollow cone" of radiation. Another important aspect of this result is how fast does the maximum radiation brightness grows with the Lorentz factor $\gamma$, i.e. with particle's energy $\varepsilon=\gamma m c^{2}$.

Still, the total radiated power $P$ (into all observation angles) at linear acceleration is not too high for any practicable values of parameters. In order to show this, it is convenient to calculate $P$ for an arbitrary motion of the particle first. It is possible to do this by a straightforward integration of Eq. (30) over the full solid angle, but let me demonstrate how $\mathcal{P}$ may be found (or rather guessed) from the general relativistic arguments. In Sec. 8.2, we have derived Eq. (8.27) for the electric dipole radiation for non-relativistic particle motion. That result is valid, in particular, for one charged particle whose electric dipole moment's derivative over time may be expressed as $d(q \mathbf{r}) / d t=(q / m) \mathbf{p}$, where $\mathbf{p}$ is
particle's mechanical momentum (not its electric dipole moment). As the result, the Larmor formula (8.27) in free space, i.e. with $v=c$, reduces to

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0}}{6 \pi c^{2}}\left(\frac{q}{m} \frac{d p}{d t}\right)^{2}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d \mathbf{p}}{d t} \cdot \frac{d \mathbf{p}}{d t}\right) \tag{10.35}
\end{equation*}
$$

This is evidently not a Lorentz-invariant result, but it gives a clear hint how such an invariant, that is reduced to Eq. (35) in the non-relativistic limit, may be formed:

$$
\begin{equation*}
\mathcal{P}=-\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d p_{\alpha}}{d \tau} \cdot \frac{d p^{\alpha}}{d \tau}\right)=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left[\left(\frac{d \mathbf{p}}{d \tau}\right)^{2}-\frac{1}{c^{2}}\left(\frac{d \varepsilon}{d \tau}\right)^{2}\right] . \tag{10.36}
\end{equation*}
$$

Plugging in the relativistic expressions, $\mathbf{p}=\gamma m c \boldsymbol{\beta}, \varepsilon=\gamma m c^{2}$, and $d \tau=d t / \gamma$, the last formula may be recast into the Liénard extension of the Larmor formula: ${ }^{9}$

Total
radiation power via $\beta$

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi} \gamma^{6}\left[(\dot{\boldsymbol{\beta}})^{2}-(\boldsymbol{\beta} \times \dot{\boldsymbol{\beta}})^{2}\right] \equiv \frac{Z_{0} q^{2}}{6 \pi} \gamma^{4}\left[(\dot{\boldsymbol{\beta}})^{2}+\gamma^{2}(\boldsymbol{\beta} \cdot \dot{\boldsymbol{\beta}})^{2}\right], \tag{10.37}
\end{equation*}
$$

which may be also obtained by a direct integration of Eq. (30) over the full solid angle, thus confirming our guess. However, for some applications, it is beneficial to express $P$ the via the time evolution of particle's momentum alone. For that, we may differentiate the fundamental relativistic relation (9.78), $\varepsilon^{2}=\left(m c^{2}\right)^{2}+(p c)^{2}$, over the proper time $\tau$ to get

$$
\begin{equation*}
2 \varepsilon \frac{d \varepsilon}{d \tau}=2 c^{2} p \frac{d p}{d \tau}, \text { i.e. } \frac{d \varepsilon}{d \tau}=\frac{c^{2} p}{\varepsilon} \frac{d p}{d \tau}=u \frac{d p}{d \tau} \tag{10.38}
\end{equation*}
$$

where, at the last transition, the magnitude of the relativistic vector relation mentioned in Chapter 9, $c^{2} \mathbf{p} / \mathcal{E}=\mathbf{u}$, has been used. Plugging this relation into Eq. (36), we may rewrite it as

Total radiation power via $\mathbf{p}$

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left[\left(\frac{d \mathbf{p}}{d \tau}\right)^{2}-\beta^{2}\left(\frac{d p}{d \tau}\right)^{2}\right] \tag{10.39}
\end{equation*}
$$

Note the difference between the squared derivatives in this expression: in the first of them we have to differentiate the momentum vector $\mathbf{p}$, and only then form a scalar by squaring the resulting vector derivative, while in the second case, only the magnitude of the vector is differentiated. For example, for a circular motion with constant speed (to be analyzed in detail in the next section), the second term is zero, while the first one is not.

However, if we return to the simplest case of linear acceleration (Fig. 4), then $(d \mathbf{p} / d \tau)^{2}=$ $(d p / d \tau)^{2}$, and Eq. (39) is reduced to

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d p}{d \tau}\right)^{2}\left(1-\beta^{2}\right)=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d p}{d \tau}\right)^{2} \frac{1}{\gamma^{2}}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d p}{d t^{\prime}}\right)^{2}, \tag{10.40}
\end{equation*}
$$

[^428](where $t^{\prime} \equiv t_{r}$ is the time of emitting radiation as measured as in the lab frame), i.e. formally coincides with non-relativistic Eq. (35). In order to get a better feeling of the magnitude of this radiation, we may use the fact that $d p / d t=d \varepsilon / d z^{\prime}$. This allows us to rewrite Eq. (40) in the following form:
\[

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d \varepsilon}{d z}\right)^{2}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}} \frac{d \varepsilon}{d z^{\prime}} \frac{d \varepsilon}{d t^{\prime}} \frac{d t^{\prime}}{d z^{\prime}}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2} u} \frac{d \varepsilon}{d z^{\prime}} \frac{d \varepsilon}{d t^{\prime}} . \tag{10.41}
\end{equation*}
$$

\]

For the most important case of ultra-relativistic motion $(u \rightarrow c)$, this result may be presented as

$$
\begin{equation*}
\frac{P}{d \varepsilon / d t^{\prime}} \approx \frac{2}{3} \frac{d\left(\varepsilon / m c^{2}\right)}{d\left(z^{\prime} / r_{\mathrm{c}}\right)} \tag{10.42}
\end{equation*}
$$

where $r_{c}$ is the classical radius of the particle, given by Eq. (8.41). This formula shows that the radiated power, i.e. the change of particle's energy due to radiation, is much smaller than that due to the accelerating field, unless energy as large as $m c^{2}$ is gained on the classical radius of the particle. For example, for an electron, such acceleration would require the accelerating electric field of the order of $(0.5 \mathrm{MV}) /\left(3 \times 10^{-15} \mathrm{~m}\right) \sim 10^{14} \mathrm{MV} / \mathrm{m}$, while practicable accelerating fields are below $10^{3} \mathrm{MV} / \mathrm{m}$, limited by the electric breakdown effects. Such smallness of radiative losses of energy is actually a large advantage of linear electron accelerators - such as the famous 2-mile-long SLAC ${ }^{10}$ that can accelerate electrons or positrons to energies up to 50 GeV , i.e. to $\gamma \approx 10^{5}$.

### 10.3. Synchrotron radiation

Now let me show that in circular accelerators, the radiation is much larger. Consider a charged particle being accelerated in the direction perpendicular to its velocity $\mathbf{u}$ (for example by a the magnetic component of the Lorentz force), so that its speed $u$, and hence the magnitude $p$ of its momentum, do not change. In this case, the second term in Eq. (39) vanishes, and it yields

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d \mathbf{p}}{d \tau}\right)^{2}=\frac{Z_{0} q^{2}}{6 \pi m^{2} c^{2}}\left(\frac{d \mathbf{p}}{d t^{\prime}}\right)^{2} \gamma^{2} . \tag{10.43}
\end{equation*}
$$

Comparing this expression with Eq. (40), we see that for the same acceleration magnitude, the electromagnetic radiation is a factor of $\gamma^{2}$ larger. For modern accelerators, with $\gamma \sim 10^{4}-10^{5}$, such a factor creates an enormous difference. For example, if a particle is on a cyclotron orbit in a constant magnetic field (as was analyzed in Sec. 9.6), both $\mathbf{u}$ and $\mathbf{p}=\gamma m \mathbf{u}$ obey Eq. (9.150), so that

$$
\begin{equation*}
\left|\frac{d \boldsymbol{p}}{d t^{\prime}}\right|=\omega_{c} p=\frac{u}{R} p=\beta^{2} \gamma \frac{m c^{2}}{R} \tag{10.44}
\end{equation*}
$$

(where $R$ is orbit's radius), so that for the power of this synchrotron radiation, Eq. (43) yields

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi} \beta^{4} \gamma^{4} \frac{c^{2}}{R^{2}} \tag{10.45}
\end{equation*}
$$

According to Eq. (9.153), at fixed magnetic field (in particle accelerators, limited to a few Tesla produced by the beam-bending magnets), the synchrotron orbit radius $R$ scales as $\gamma$, so that according to

[^429]Eq. (45), $\mathcal{P}_{\text {scales as }} \gamma^{2}$, i.e. grows fast with particle's energy $\varepsilon \propto \gamma$. For example, for typical parameters of the first electron cyclotrons (such as the General Electric machine in which the synchrotron radiation was first noticed in 1947), $R \sim 1 \mathrm{~m}, \varepsilon \sim 0.3 \mathrm{GeV}$ ( $\gamma \sim 600$ ), Eq. (45) gives a very modest electron energy loss per one revolution: $P \Delta t^{\prime} \approx 2 \pi P R / c \sim 1 \mathrm{keV}$. However, already by the mid-1970s, electron accelerators, with $R \sim 100 \mathrm{~m}$, have reached energies $\mathcal{E} \sim 10 \mathrm{GeV}$, and the energy loss per revolution has grown to $\sim 10 \mathrm{MeV}$, becoming the major energy loss mechanism. ${ }^{11}$ However, what is bad for particle accelerators and storage rings is good for the so-called synchrotron light sources - the electron accelerators designed specially for the generation of intensive synchrotron radiation - with the spectrum extending well beyond the visible light range. Let us now analyze the angular and spectral distributions of such radiation.

To calculate the angular distribution, let us select the coordinate axes as shown in Fig. 5, with the origin at the current location of the orbiting particle, axis $z$ along its instant velocity (i.e. vector $\beta$ ), and axis $x$ toward the orbit center.


Fig. 10.5. Geometry of the synchrotron radiation problem.

In the general case, the unit vector $\mathbf{n}$ toward the radiation observer is not within any of the coordinate planes, and hence should be described by two angles - the polar angle $\theta$ and the azimuthal angle $\varphi$ between the $x$ axis and projection 0 P of vector $\mathbf{n}$ on plane $[x, y]$. Since the length of segment 0 P is $\sin \theta$, the Cartesian coordinates of the relevant vectors are as follows:

$$
\begin{equation*}
\mathbf{n}=\{\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta\}, \quad \boldsymbol{\beta}=\{0,0, \beta\}, \quad \dot{\boldsymbol{\beta}}=\{\dot{\beta}, 0,0\} . \tag{10.46}
\end{equation*}
$$

Plugging these coordinates into the general Eq. (30), we get

Synchrotron radiation's angular distribution

$$
\begin{equation*}
\frac{d \mathcal{P}}{d \Omega}=\frac{2 Z_{0} q^{2}}{\pi^{2}}|\dot{\boldsymbol{\beta}}|^{2} \gamma^{6} f(\theta, \varphi), \text { with } f(\theta, \varphi) \equiv \frac{1}{8 \gamma^{6}(1-\beta \cos \theta)^{3}}\left[1-\frac{\sin ^{2} \theta \cos ^{2} \varphi}{\gamma^{2}(1-\beta \cos \theta)^{2}}\right], \tag{10.47}
\end{equation*}
$$

According to this result, just as at the linear acceleration, in the ultra-relativistic limit, most radiation goes to a narrow cone (of width $\Delta \theta \sim \gamma^{-1} \ll 1$ ) around vector $\beta$, i.e. around the instant direction of particle's propagation. For such small angles, and $\gamma \gg 1$, the second of Eqs. (47) is reduced to

[^430]\[

$$
\begin{equation*}
f(\theta, \varphi) \approx \frac{1}{\left(1+\gamma^{2} \theta^{2}\right)^{3}}\left[1-\frac{4 \gamma^{2} \theta^{2} \cos ^{2} \varphi}{\left(1+\gamma^{2} \theta^{2}\right)^{2}}\right] . \tag{10.48}
\end{equation*}
$$

\]

Left panel of Fig. 6 shows the angular distribution $f(\theta, \varphi)$ color-coded, on the plane perpendicular to particle's instant velocity (in Fig. 5, plane $[x, y]$ ), while its right panel shows the intensity as a function of $\theta$ in two perpendicular directions: within the particle rotation plane (along axis $x$ ) and perpendicular to this plane (along axis $y$ ). The result shows, first of all, that, in contrast to the case of linear acceleration, the narrow radiation cone is now not hollow: the intensity maximum is reached exactly at $\theta=0$, i.e. in particle's motion direction. Second, the radiation cone is not axiallysymmetric: the intensity drops faster within the particle rotation plane (and even has nodes at $\theta= \pm 1 / \gamma$ ).


Fig. 10.6. Angular distribution of the synchrotron radiation at $\gamma \gg 1$.

Let us consider the time/frequency structure of the synchrotron radiation, now from the point of view of the observer rather than the particle itself. (In the latter picture, due to the axial symmetry of the problem, the total radiation power $\mathcal{P}$ is evidently constant.) Its semi-quantitative picture may be obtained from the angular distribution we have just analyzed. Indeed, if an ultra-relativistic particle's radiation is observed from a point in (or close to) the rotation plane, ${ }^{12}$ the observer is being "struck" by the narrow radiation cone once each rotation period, each "strike" giving a pulse of a short duration $\Delta t$ $\ll \omega_{c}-$ see Fig. 7.

[^431]

Fig. 10.7. (a) Synchrotron radiation cones at $\gamma \gg 1$, and (b) the in-plane component of their electric field, observed in the rotation plane, as a function of observation time $t$-schematically.

The evaluation of the time duration $\Delta t$ of each pulse requires some care: its estimate $\Delta t^{\prime} \sim 1 / \gamma \omega_{c}$ is correct for the duration of the time of particle's motion while its cone is aimed at the observer. However, due to the time compression effect, discussed in detail in Sec. 1 and described by Eqs. (12) and (18), the pulse duration as seen by observer is a factor of $1 /(1-\beta)$ shorter, so that

$$
\begin{equation*}
\Delta t=(1-\beta) \Delta t^{\prime} \sim \frac{1-\beta}{\gamma \omega_{c}} \sim \frac{1}{\gamma^{3} \omega_{c}} . \tag{10.49}
\end{equation*}
$$

From the Fourier theorem, we can expect that the frequency spectrum of the radiation consists of numerous $\left(N \sim \gamma^{3} \gg 1\right.$ ) harmonics of the rotation frequency $\omega_{\mathrm{c}}$, with comparable amplitudes. However, if the orbital frequency fluctuates even slightly $\left(\delta \omega_{c} / \omega_{c}>1 / N \sim 1 / \gamma^{3}\right)$, as it happens in most practical systems, the radiation pulses are not coherent, so that the average radiation power spectrum may be calculated as that of one pulse, multiplied by number of pulses per second. In this case, the spectrum is continuous, extending from low frequencies all the way to approximately

$$
\begin{equation*}
\omega_{\max } \sim 1 / \Delta t \sim \gamma^{3} \omega_{c} . \tag{10.50}
\end{equation*}
$$

In order to verify this estimate, let us calculate the spectrum of radiation, due to a single pulse. For that, we should first make the general notion of spectrum quantitative. Let us present an arbitrary electric field (say that of the synchrotron radiation we are studying now), considered as a function of the observation time $t$ (at fixed $\mathbf{r}$ ), as a Fourier integral: ${ }^{13}$

$$
\begin{equation*}
\mathbf{E}(t)=\int_{-\infty}^{+\infty} \mathbf{E}_{\omega} e^{-i \omega t} d t \tag{10.51}
\end{equation*}
$$

This expression may be plugged into the following formula for the total energy of the radiation pulse (i.e. of particle energy's loss) per unit solid angle: ${ }^{14}$

[^432]\[

$$
\begin{equation*}
-\frac{d \varepsilon}{d \Omega} \equiv \int_{-\infty}^{+\infty} S_{n}(t) R^{2} d t=\frac{R^{2}}{Z_{0}} \int_{-\infty}^{+\infty}|\mathbf{E}(t)|^{2} d t \tag{10.52}
\end{equation*}
$$

\]

This substitution, plus a natural change of integration order, yield

$$
\begin{equation*}
\frac{d \varepsilon}{d \Omega}=\frac{R^{2}}{Z_{0}} \int_{-\omega}^{+\omega} d \omega \int_{-\omega}^{+\omega} d \omega^{\prime} \mathbf{E}_{\omega} \cdot \mathbf{E}_{\omega^{\prime}} \int_{-\infty}^{+\infty} d t e^{-i\left(\omega+\omega^{\prime}\right) t} \tag{10.53}
\end{equation*}
$$

But the inner integral (over $t$ ) is just $2 \pi \delta\left(\omega+\omega^{\prime}\right) .{ }^{15}$ This delta-function kills one of the frequency integrals (say, one over $\omega^{\prime}$ ), and Eq. (53) gives a result which may be recast as

$$
\begin{equation*}
-\frac{d \varepsilon}{d \Omega}=\int_{0}^{+\infty} I(\omega) d \omega, \quad \text { with } I(\omega) \equiv \frac{4 \pi R^{2}}{Z_{0}} \mathbf{E}_{\omega} \cdot \mathbf{E}_{-\omega}=4 \pi Z_{0} \varepsilon_{0}^{2}(c R)^{2} \mathbf{E}_{\omega} \mathbf{E}_{\omega}^{*} \tag{10.54}
\end{equation*}
$$

where the evident frequency symmetry of the scalar product $\mathbf{E}_{\omega} \cdot \mathbf{E}_{-\omega}$ has been utilized to fold the integral of $I(\omega)$ to positive frequencies only. The first of Eqs. (51) and the first of Eqs. (54) make the physical sense of function $I(\omega)$ clear: this is the so-called spectral density of the electromagnetic radiation (per unit solid angle, per unit pulse). ${ }^{16}$

In order to calculate the spectral density, we need to express function $\mathbf{E}_{\omega}$ via $\mathbf{E}(t)$ using the Fourier transform reciprocal to Eq. (51):

$$
\begin{equation*}
\mathbf{E}_{\omega}=\frac{1}{2 \pi} \int_{-\infty}^{+\omega} \mathbf{E}(t) e^{i \omega t} d t \tag{10.55}
\end{equation*}
$$

In the particular case of radiation by a single point charge, we should use the second term of Eq. (20a):

$$
\begin{equation*}
\mathbf{E}_{\omega}=\frac{1}{2 \pi} \frac{q}{4 \pi \varepsilon_{0}} \frac{1}{c R} \int_{-\infty}^{+\infty} \frac{\mathbf{n} \times\{(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{3}} e^{i \omega t} d t \tag{10.56}
\end{equation*}
$$

Since vectors $\mathbf{n}$ and $\beta$ are natural functions of the radiation (retarded) time $t^{\prime}$, let us use Eqs. (18) to change integration in Eq. (52) from the observation time $t$ to time $t^{\prime}$ :

$$
\begin{equation*}
\mathbf{E}_{\omega}=\frac{q}{4 \pi \varepsilon_{0}} \frac{1}{2 \pi} \frac{1}{c R} \int_{-\infty}^{+\infty} \frac{\mathbf{n} \times\{(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{2}} \exp \left\{i \omega\left(t^{\prime}+\frac{R_{r}}{c}\right)\right\} d t^{\prime} \tag{10.57}
\end{equation*}
$$

The strong inequality $R_{r} \gg r$ ' that is implied from the beginning of this section allows us to consider the unit vector $\mathbf{n}$ as constant and, moreover, to use approximation (8.19) to reduce Eq. (57) to

$$
\begin{equation*}
\mathbf{E}_{\omega}=\frac{1}{2 \pi} \frac{q}{4 \pi \varepsilon_{0}} \frac{1}{c R} \exp \left\{\frac{i \omega r}{c}\right\} \int_{-\infty}^{+\infty} \frac{\mathbf{n} \times\{(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{2}} \exp \left\{i \omega\left(t^{\prime}-\frac{\mathbf{n} \cdot \mathbf{r}^{\prime}}{c}\right)\right\} d t^{\prime} \tag{10.58}
\end{equation*}
$$

Plugging this expression into Eq. (54), we get ${ }^{17}$

[^433]\[

$$
\begin{equation*}
I(\omega)=\frac{Z_{0} q^{2}}{16 \pi^{3}}\left|\int_{-\infty}^{+\infty} \frac{\mathbf{n} \times\{(\mathbf{n}-\boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{2}} \exp \left\{i \omega\left(t^{\prime}-\frac{\mathbf{n} \cdot \mathbf{r}^{\prime}}{c}\right)\right\} d t^{\prime}\right|^{2} . \tag{10.59}
\end{equation*}
$$

\]

Let me remind the reader that $\beta$ inside this integral is supposed to be taken at the retarded point $\left\{\mathbf{r}^{\prime}, t^{\prime}\right\}$, so that Eq. (59) is fully sufficient for finding the spectral density from the law $\mathbf{r}^{\prime}\left(t^{\prime}\right)$ of particle's motion. However, this result may be further simplified by noticing that the fraction before the exponent may be presented as a full derivative over $t^{\prime}$,

$$
\begin{equation*}
\frac{\mathbf{n} \times\left\{(\mathbf{n}-\boldsymbol{\beta}) \times d \boldsymbol{\beta} / d t^{\prime}\right\}}{(1-\boldsymbol{\beta} \cdot \mathbf{n})^{2}}=\frac{d}{d t^{\prime}}\left[\frac{\mathbf{n} \times(\mathbf{n} \times \boldsymbol{\beta})}{1-\boldsymbol{\beta} \cdot \mathbf{n}}\right], \tag{10.60}
\end{equation*}
$$

and working out the resulting integral by parts. At this operation, the time differentiation of the parentheses in the exponent, $d\left(t^{\prime}-\mathbf{n} \cdot \mathbf{r}^{\prime} / c\right) / d t^{\prime}=1-\mathbf{n} \cdot \mathbf{u} / c=1-\boldsymbol{\beta} \cdot \mathbf{n}$, leads to the cancellation of denominator's remains and hence to a surprisingly simple result: ${ }^{18}$

$$
\begin{equation*}
I(\omega)=\frac{Z_{0} q^{2} \omega^{2}}{16 \pi^{3}} \int_{-\infty}^{+\infty} \mathbf{n} \times\left.(\mathbf{n} \times \boldsymbol{\beta}) \exp \left\{i \omega\left(t^{\prime}-\frac{\mathbf{n} \cdot \mathbf{r}^{\prime}}{c}\right)\right\} d t^{\prime}\right|^{2} \tag{10.61}
\end{equation*}
$$

Returning to the particular case of synchrotron radiation, it is beneficial to choose the origin of time $t^{\prime}$ so that at $t^{\prime}=0$, angle $\theta$ takes its smallest value $\theta_{0}$, i.e., in terms of Fig. 5, vector $\mathbf{n}$ is within plane $[y, z]$. Fixing this direction of axes in time, we can redraw that figure as shown in Fig. 8. In these coordinates,

$$
\begin{equation*}
\mathbf{n}=\left\{0, \sin \theta_{0}, \cos \theta_{0}\right\}, \quad \mathbf{r}^{\prime}=\{R(1-\cos \alpha), 0, R \sin \alpha\}, \quad \boldsymbol{\beta} \equiv\{\beta \sin \alpha, 0, \beta \cos \alpha\} \tag{10.62}
\end{equation*}
$$

where $\alpha \equiv \omega_{c} t^{\prime}$, and an easy multiplication yields

$$
\begin{align*}
& \mathbf{n} \times(\mathbf{n} \times \boldsymbol{\beta})=\beta\left\{\sin \alpha, \sin \theta_{0} \cos \theta_{0} \cos \alpha,-\sin ^{2} \theta_{0} \sin \alpha\right\},  \tag{10.63}\\
& \quad \exp \left\{i \omega\left(t^{\prime}-\frac{\mathbf{n} \cdot \mathbf{r}^{\prime}}{c}\right)\right\}=\exp \left\{i \omega\left(t^{\prime}-\frac{R}{c} \cos \theta_{0} \sin \alpha\right)\right\} . \tag{10.64}
\end{align*}
$$



Fig. 10.8. Deriving the spectral density of synchrotron radiation. Vector $\mathbf{n}$ is fixed in plane $[y, z]$, while vectors $\mathbf{r}^{\prime}\left(t^{\prime}\right)$ and $\beta\left(t^{\prime}\right)$ rotate in plane $[x, y]$ with angular velocity $\omega_{c}$.

[^434]As we already know, in the (most interesting) ultra-relativistic limit $\gamma \gg 1$, most radiation is confined to short pulses, so that only small angles $\alpha \sim \omega_{\mathrm{c}} \Delta t^{\prime} \sim \gamma^{-1}$ may contribute to the integral in Eq. (61). Moreover, since most radiation goes to small angles $\theta \sim \gamma^{-1}$, it makes sense to consider only small angles $\theta_{0} \sim \gamma^{-1} \ll 1$. Expanding both trigonometric functions of these small angles, participating in parentheses of Eq. (64), into Taylor series, and keeping only terms up to $O\left(\gamma^{-3}\right)$, we can present them as

$$
\begin{equation*}
\left(t^{\prime}-\frac{R}{c} \cos \theta_{0} \sin \alpha\right)=\left(t^{\prime}-\frac{R}{c} \omega_{c} t^{\prime}+\frac{R}{c} \frac{\theta_{0}^{2}}{2} \omega_{c} t^{\prime}+\frac{R}{c} \frac{\omega_{c}^{3} t^{\prime 3}}{6}\right) . \tag{10.65}
\end{equation*}
$$

Since $(R / c) \omega_{c}=u / c=\beta \approx 1$, in two last terms we may approximate this parameter by 1 . However, it is crucial to distinguish the difference of two first terms, proportional to $(1-\beta) t^{\prime}$, from zero, and as we have done before we may approximate it with $t^{\prime} / 2 \gamma^{2}$. In Eq. (63), which does not have such critical differences, we may be more bold, taking ${ }^{19}$

$$
\begin{equation*}
\mathbf{n} \times(\mathbf{n} \times \boldsymbol{\beta}) \approx\left\{\alpha, \theta_{0}, 0\right\}=\left\{\omega_{c} t^{\prime}, \theta_{0}, 0\right\} . . \tag{10.66}
\end{equation*}
$$

As a result, Eq. (61) is reduced to

$$
\begin{equation*}
I(\omega)=\frac{Z_{0} q^{2}}{16 \pi^{3}}\left|a_{x} \mathbf{n}_{x}+a_{y} \mathbf{n}_{y}\right|^{2}=\frac{Z_{0} q^{2}}{16 \pi^{3}}\left(\left|a_{x}\right|^{2}+\left|a_{y}\right|^{2}\right), \tag{10.67}
\end{equation*}
$$

where $a_{x}$ and $a_{y}$ are the dimensionless factors,

$$
\begin{align*}
& a_{x} \equiv \omega \int_{-\infty}^{+\infty} \omega_{c} t^{\prime} \exp \left\{\frac{i \omega}{2}\left(\left(\theta_{0}^{2}+\gamma^{-2}\right) t^{\prime}+\frac{\omega_{c}^{2}}{3} t^{\prime 3}\right)\right\} d t^{\prime},  \tag{10.68}\\
& a_{y} \equiv \omega \int_{-\infty}^{+\infty} \theta_{0} \exp \left\{\frac{i \omega}{2}\left(\left(\theta_{0}^{2}+\gamma^{-2}\right) t^{\prime}+\frac{\omega_{c}^{2}}{3} t^{\prime 3}\right)\right\} d t^{\prime}
\end{align*}
$$

which describe the frequency spectra of two components of the synchrotron radiation, with mutually perpendicular directions of polarization. Defining a dimensionless parameter

$$
\begin{equation*}
v \equiv \frac{\omega}{3 \omega_{c}}\left(\theta_{0}^{2}+\gamma^{-2}\right)^{3 / 2} \tag{10.69}
\end{equation*}
$$

proportional to the observation frequency, and changing the integration variable to $\xi \equiv \omega_{c} t^{\prime} /\left(\theta_{0}{ }^{2}+\gamma^{-2}\right)^{1 / 2}$, integrals (68) may be reduced to the modified Bessel functions of the second kind:

$$
\begin{align*}
& a_{x}=\frac{\omega}{\omega_{c}}\left(\theta_{0}^{2}+\gamma^{-2}\right) \int_{-\infty}^{+\infty} \xi \exp \left\{\frac{3}{2} i v\left(\xi+\frac{\xi^{3}}{3}\right)\right\} d \xi=\frac{2 \sqrt{3} i}{\left(\theta_{0}^{2}+\gamma^{-2}\right)^{1 / 2}} v K_{2 / 3}(v),  \tag{10.70}\\
& a_{y}=\frac{\omega}{\omega_{c}} \theta_{0}\left(\theta_{0}^{2}+\gamma^{-2}\right)^{1 / 2} \int_{-\infty}^{+\infty} \exp \left\{\frac{3}{2} i v\left(\xi+\frac{\xi^{3}}{3}\right)\right\} d \xi=\frac{2 \sqrt{3} \theta_{0}}{\theta_{0}^{2}+\gamma^{-2}} v K_{1 / 3}(v)
\end{align*}
$$

[^435]Figure 9a shows the dependence of amplitudes $a_{x}$ and $a_{y}$ of the normalized observation frequency $v$. It is clear that the in-plane component, proportional to $a_{x}$, is larger. (The off-plane component disappears altogether at $\theta_{0}=0$, i.e. at observation within the particle rotation plane $[x, y]$, due to the evident mirror symmetry of the problem about the plane.) It is also clear that the spectrum changes rather slowly (note the log-log scale of the plot!) until the normalized frequency, defined by Eq. (69), reaches $\sim 1$. For most important observation angles $\theta_{0} \sim \gamma$ this means that our estimate (50) is indeed correct, though theoretically the frequency spectrum extends to infinity. ${ }^{20}$


Fig. 10.9. Synchrotron radiation frequency spectra of: (a) two polarization amplitudes and (b) the total (polarization- and angle-averaged) radiation.

Naturally, a similar frequency behavior is valid for the spectral density integrated over the full solid angle. Without performing the integration, ${ }^{21}$ let me give the result (also valid for $\gamma \gg 1$ only) for reader's reference:

$$
\begin{equation*}
\oint_{4 \pi} I(\omega) d \Omega=\frac{\sqrt{3}}{4 \pi} q^{2} \gamma \zeta \int_{\zeta}^{\infty} K_{5 / 3}(\xi) d \xi, \quad \zeta \equiv \frac{2}{3} \frac{\omega}{\omega_{c} \gamma^{3}} . \tag{10.71}
\end{equation*}
$$

Figure 8 b shows the dependence of this integral on the normalized frequency $\zeta$. (This plot is sometimes called the "universal flux curve".) In accordance with estimate (50), it reaches maximum at

$$
\begin{equation*}
\zeta_{\max } \approx 0.3, \text { i.e. } \omega_{\max } \approx \frac{\omega_{c}}{2} \gamma^{3} . \tag{10.72}
\end{equation*}
$$

For the new National Synchrotron Light Source (NSLS-II), that is under construction in the Brookhaven National Laboratory very close to our campus, with the ring circumference of 792 m , the electron revolution period $T$ will be $2.64 \mu \mathrm{~s}$. Calculating $\omega_{c}$ as $2 \pi / T \approx 2.4 \times 10^{6} \mathrm{~s}^{-1}$, for the planned $\gamma \approx$

[^436]$6 \times 10^{3}(\varepsilon \approx 3 \mathrm{GeV}),{ }^{22}$ we get $\omega_{\max } \sim 3 \times 10^{17} \mathrm{~s}^{-1}$, corresponding to photon energy $\hbar \omega_{\max } \sim 200 \mathrm{eV}$, corresponding to soft X-rays. In the light of this estimate, the reader may be surprised by Fig. 10 that shows the projected spectra of radiation which this facility is designed to produce, with maximum photon energies up to a few keV.


Fig. 10.10. Design brightness of various synchrotron radiation sources of the NSLS-II facility. For bend magnets and wigglers, the "brightness" may be obtained by multiplication of the spectral density $I(\omega)$ from one electron pulse, calculated above, by the number of electrons passing the source per second. (Note the non-SI units, commonly used in the synchrotron radiation community.) However, for undulators, there is an additional factor due to the partial coherence of radiation - see below. (Data from document NSLS-II Source Properties and Floor Layout, available online at http://www.nsls.bnl.gov/.)

The reason of this discrepancy is that in NLLS-II, and in all modern synchrotron light sources, most radiation is produced not by the circular orbit itself, but rather using special devices inserted into the electron beam path. These devices include bend magnets with magnetic field stronger than the average

[^437]field on the orbit (which, according to Eq. (9.112), produce higher effective value of $\omega_{c}$ and hence of $\omega_{\max }$ ), and wigglers and undulators: strings of several strong magnets with alternating field direction (Fig. 11), that induce periodic bending of electron trajectory, with radiation emitted at each bend.


Fig. 10.11. The generic magnetic structure common for wigglers, undulators and freeelectron lasers. (Adapted from http://wwwxfel.spring8.or.jp/cband/e/Undulator.htm.)

The difference between wigglers and undulators is more quantitative than qualitative: the former devices have a larger spatial period $\lambda$ (distance between the adjacent magnets of the same polarity, see Fig. 11), giving enough space for the electron beam to bend by an angle larger than $\gamma^{-1}$, i.e. larger than the radiation cone angle. As a result, the pulses radiated at each period arrive to an in-plane observer as a periodic sequence of individual pulses (Fig. 12a). The shape of each pulse, and hence its frequency spectrum, are similar to those discussed above, ${ }^{23}$ but with much higher local values of $\omega_{c}$ and $\omega_{\max }$ - see Fig. 9. Another difference is a much higher frequency of the peaks. Indeed, the fundamental Eq. (18) allows us to calculate the time distance between them, for the observer, as

$$
\begin{equation*}
\Delta t \approx \frac{\partial t}{\partial t^{\prime}} \Delta t^{\prime} \approx(1-\beta) \frac{\lambda}{u} \approx \frac{1}{2 \gamma^{2}} \frac{\lambda}{c} \ll \frac{\lambda}{c}, \tag{10.73}
\end{equation*}
$$

where the first two relations are valid at $\lambda \ll R$ (the relation typically satisfied very well, see Fig. 10), and the last two relations also require the ultra-relativistic limit. As a result, the radiation intensity, that is proportional to the number of poles, is much higher than that from the bend magnets - in the NLSL-II case, more than by 2 orders of magnitude, clearly visible in Fig. 10.

(b)

Fig. 10.12. Radiation (with in-plane polarization) from (a) a wiggler and (b) an undulator - schematically.

[^438]The situation in different in undulators - similar structures with smaller spatial period $\lambda$, in which electron's velocity vector oscillates with angular amplitude smaller that $\gamma^{-1}$. As a result, the radiation pulses overlap (Fig. 12b) and the radiation waveform is closer to sinusoidal one. As a result, the radiation spectrum narrows to the central frequency ${ }^{24}$

$$
\begin{equation*}
\omega_{0}=\frac{2 \pi}{\Delta t} \approx 2 \gamma^{2} \frac{2 \pi c}{\lambda} . \tag{10.74}
\end{equation*}
$$

For example, for the LSNL-II undulators with $\lambda=20 \mathrm{~mm}$, this formula predicts the radiation peak at phonon energy $\hbar \omega_{0} \approx 4 \mathrm{keV}$, in a reasonable agreement with results of quantitative calculations, shown in Fig. 10. ${ }^{25}$ Due to the spectrum narrowing, the intensity of undulators radiation is higher that that of wigglers using the same electron beam.

This spectrum-narrowing trend is brought to its logical conclusion in the so-called free-electron lasers ${ }^{26}$ whose basic structure is the same as that of wigglers and undulators (Fig. 11), but the radiation at each beam bend is so intense and narrow-focused that it affects the electron motion downstream the radiation cone. As a result, the radiation of all bends becomes synchronized, so its spectrum is a narrow line at frequency (74), with electromagnetic wave amplitude proportional to the number $N$ of electrons in the structure, and hence its power proportional to $N^{2}$ (rather than to $N$ as in wigglers and undulators).

Finally, note that wigglers, undulators, and free-electron lasers may be also used at the end of a linear electron accelerator (such as SLAC) that, as was noted above, may provide extremely high values of $\gamma$, and hence radiation frequencies, due to the absence of the radiation energy losses at the electron acceleration stage.

### 10.4. Bremsstrahlung and Coulomb losses

Surprisingly, a very similar mechanism of radiation by charged particles works at much lower spatial scale, namely at their scattering by charged particles of the propagation medium, the so-called bremsstrahlung - German for "brake radiation". This effect responsible, in particular, for the continuous part of the frequency spectrum of the radiation produced by standard vacuum X-ray tubes, its incidence on a solid "anticathode". 27

The bremsstrahlung in condensed matter is generally a rather complicated phenomenon, because of simultaneous involvement of many particles, and some quantum electrodynamic effect involvement.

[^439]This is why I will give only a very brief glimpse at the theoretical description of this effect, for the simplest case when scattering of incoming, relatively light charged particles (such as electrons, protons, $\alpha$-particles, etc.) is produced by atomic nuclei that remain virtually immobile during the scattering event (Fig. 13a). This is a reasonable approximation if the energy of incoming particles is not too low, otherwise most scattering is produced by atomic electrons whose dynamics is substantially quantum see below.

(b)


Fig. 10.13. Basic geometry of the bremsstrahlung and Coulomb loss problems in (a) direct and (b) reciprocal space.

To calculate the frequency spectrum of radiation emitted during a single scattering event, it is convenient to use a byproduct of the last section's analysis, namely Eq. (59) with replacement (60):28

$$
\begin{equation*}
I(\omega)=\left.\frac{1}{4 \pi^{2} c} \frac{q^{2}}{4 \pi \varepsilon_{0}} \int_{-\infty}^{+\infty} \frac{d}{d t^{\prime}}\left[\frac{\mathbf{n} \times(\mathbf{n} \times \boldsymbol{\beta})}{1-\boldsymbol{\beta} \cdot \mathbf{n}}\right] \exp \left\{i \omega\left(t^{\prime}-\frac{\mathbf{n} \cdot \mathbf{r}^{\prime}}{c}\right)\right\} d t^{\prime}\right|^{2} . \tag{10.75}
\end{equation*}
$$

The typical duration $\tau$ of a single scattering event, that is described by this formula, is of the order of $a_{0} / c \sim\left(10^{-10} \mathrm{~m}\right) /\left(3 \times 10^{8} \mathrm{~m} / \mathrm{s}\right) \sim 10^{-18} \mathrm{~s}$ in solids, and only an order of magnitude longer in gases at ambient conditions. This is why for most frequencies of interest, from zero all the way up to at least soft X-rays, ${ }^{29}$ we can use the so-called low-frequency approximation, taking the exponent in Eq. (75) for 1 through the whole collision event, i.e. the integration interval. This approximation immediately yields

$$
\begin{equation*}
I(\omega)=\frac{1}{4 \pi^{2} c} \frac{q^{2}}{4 \pi \varepsilon_{0}}\left|\frac{\mathbf{n} \times\left(\mathbf{n} \times \boldsymbol{\beta}_{f i n}\right)}{1-\boldsymbol{\beta}_{\text {fin }} \cdot \mathbf{n}}-\frac{\mathbf{n} \times\left(\mathbf{n} \times \boldsymbol{\beta}_{i n i}\right)}{1-\boldsymbol{\beta}_{i n i} \cdot \mathbf{n}}\right|^{2} . \tag{10.76}
\end{equation*}
$$

In the non-relativistic limit $\left(\beta_{\text {ini }}, \beta_{\text {fin }} \ll 1\right)$, this formula in reduced to ${ }^{30}$

$$
\begin{equation*}
I(\omega)=\frac{1}{4 \pi c} \frac{q^{2}}{4 \pi^{2} \varepsilon_{0}} \frac{q^{2}}{m^{2} c^{3}} \sin ^{2} \theta \tag{10.77}
\end{equation*}
$$

where $g$ is the momentum transferred from the scattering center to the scattered charge (Fig. 13b):31

[^440]\[

$$
\begin{equation*}
\boldsymbol{q} \equiv \mathbf{p}_{f i n}-\mathbf{p}_{i n i}=m \Delta \mathbf{u}=m c \Delta \boldsymbol{\beta}=m c\left(\boldsymbol{\beta}_{f i n}-\boldsymbol{\beta}_{i n i}\right) \tag{10.78}
\end{equation*}
$$

\]

and $\theta$ is the angle between vector $g$ and the direction $\mathbf{n}$ toward the observer.
The most important feature of result (77) is the frequency-independent ("white") spectrum of the radiation, very typical for any rapid leaps, which may be approximated as theta-functions of time. (Note, however, that this is only valid for a fixed value of $g$, so that the statistics of this parameter, to be discussed in a minute, "colors" the radiation.) Note also the angular distribution of the radiation, forming the usual "doughnut" shape about the momentum transfer vector $\mathbf{g}$. In particular, this means that in typical cases when $q \sim p$, the bremsstrahlung produces a significant radiation flow in the direction back to the particle source - the fact significant for the operation of X-ray tubes.

Now integrating over all wave propagation angles, just as we did for the instant radiation power in Sec. 8.2, we get the spectral density of the full energy loss,

$$
\begin{equation*}
-\frac{d \varepsilon}{d \omega}=\oint_{4 \pi} I(\omega) d \Omega=\frac{2}{3 \pi c} \frac{q^{2}}{4 \pi^{2} \varepsilon_{0}} \frac{q^{2}}{m^{2} c^{3}} . \tag{10.79}
\end{equation*}
$$

The main new feature of bremsstrahlung (as of most scattering problems ${ }^{32}$ ), is the necessity to take into account the randomness of the impact parameter $b$ (Fig. 13a). For elastic ( $\beta_{\text {ini }}=\beta_{f i n} \equiv \beta$ ) Coulomb collisions we can use the so-called Rutherford formula for the differential cross-section of scattering ${ }^{33}$

$$
\begin{equation*}
\frac{d \sigma}{d \Omega^{\prime}}=\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0}}\right)^{2}\left(\frac{1}{2 p c \beta}\right)^{2} \frac{1}{\sin ^{4}\left(\theta^{\prime} / 2\right)} \tag{10.80}
\end{equation*}
$$

Here $d \sigma=2 \pi b d b$ is the elementary area of the sample cross-section (as visible from the direction of incident particles) corresponding to particle scattering into an elementary body angle ${ }^{34}$

$$
\begin{equation*}
d \Omega^{\prime}=2 \pi \sin \theta^{\prime} d \theta^{\prime} \tag{10.81}
\end{equation*}
$$

Differentiating the geometric relation that is evident from Fig. 13b,

$$
\begin{equation*}
q=2 p \sin \frac{\theta^{\prime}}{2} \tag{10.82}
\end{equation*}
$$

we may present Eq. (80) in a more convenient form

$$
\begin{equation*}
\frac{d \sigma}{d q}=8 \pi\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0}}\right)^{2} \frac{1}{u^{2} q^{3}} \tag{10.83}
\end{equation*}
$$

[^441]Now combining Eqs. (79) and (83), we get

$$
\begin{equation*}
-\frac{d \varepsilon}{d \omega} \frac{d \sigma}{d q}=\frac{16}{3} \frac{q^{2}}{4 \pi \varepsilon_{0}}\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0} m c^{2}}\right)^{2} \frac{1}{c \beta^{2}} \frac{1}{q} . \tag{10.84}
\end{equation*}
$$

This product is called the differential radiation cross-section. When averaged it over all values $g$ (which is equivalent to averaging over all values of the impact parameter), it gives a convenient measure of radiation intensity. Indeed, after the multiplication by the volume density $n$ of independent scattering centers, the integral gives particle's energy loss by unit bandwidth of radiation by unit path length $d^{2} \varepsilon / d \omega d x$. A technical problem here is that the integral of $1 / g$ formally diverges at both infinite and zero values of $\mathfrak{g}$. However, these divergences are very weak (logarithmic), and the integral converges due to virtually any reason unaccounted for by our simple analysis. The standard simple way to account for these effects is to write

$$
\begin{equation*}
-\frac{d^{2} \varepsilon}{d \omega d x} \approx \frac{16}{3} n \frac{q^{2}}{4 \pi \varepsilon_{0}}\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0} m c^{2}}\right)^{2} \frac{1}{c \beta^{2}} \ln \frac{q_{\max }}{g_{\min }}, \tag{10.85}
\end{equation*}
$$

and then plug, instead of $g_{\max }$ and $g_{\min }$, scales of the most important effects limiting the small momentum range. At classical analysis, according to Eq. (82), $g_{\max }=2 p$. To estimate $q_{\min }$, let us note that very small momentum transfer takes place when the impact parameter $b$ is very large and hence the effective scattering time $\tau \sim b / v$ is very long. Recalling the condition of the low-frequency approximation, we may associate $g_{\min }$ with $\tau \sim 1 / \omega$ and hence with $b \sim u \tau \sim v / \omega$. Since for the small scattering angles, $g$ may be estimated as the impulse $F \tau \sim\left(q q^{\prime} / 4 \pi \varepsilon_{0} b^{2}\right) \tau$ of the Coulomb force, so that $g_{\min } \sim\left(q q^{\prime} / 4 \pi \varepsilon_{0}\right) \omega / u^{2}$, and Eq. (85) becomes

$$
\begin{equation*}
-\frac{d^{2} \varepsilon}{d \omega d x} \approx \frac{16}{3} n \frac{q^{2}}{4 \pi \varepsilon_{0}}\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0} m c^{2}}\right)^{2} \frac{1}{c \beta^{2}} \ln \left(\frac{4 \pi \varepsilon_{0} 2 m u^{3}}{q q^{\prime} \omega}\right) . \tag{10.86}
\end{equation*}
$$

This is Bohr's formula for what is called the classical bremsstrahlung. We see that the low momentum cutoff indeed makes the spectrum colored, with more energy going to lower frequencies. There is even a formal divergence at $\omega \rightarrow 0$; however, this divergence is integrable, so it does not present a problem in finding the total energy radiative losses $(-d \mathcal{L} / d x)$ as an integral of Eq. (86) over all radiated frequencies $\omega$. A larger problem for this procedure is the upper integration limit, $\omega \rightarrow \infty$, at which the integral diverges. This means that our approximate description, which considers the collision as an elastic process, becomes wrong, and needs to be amended by taking into account the difference between the initial and final kinetic energies of the particle due to radiation of the energy quantum $\hbar \omega$ of the emitted photon:

$$
\begin{equation*}
\frac{p_{i n i}^{2}}{2 m}-\frac{p_{f i n}^{2}}{2 m}=\hbar \omega . \tag{10.87}
\end{equation*}
$$

As a result, taking into account that the minimum and maximum values of $\mathfrak{q}$ correspond to, respectively, the parallel and antiparallel alignments of vectors $\mathbf{p}_{i n i}$ and $\mathbf{p}_{f i n}$, we get

$$
\ln \frac{\boldsymbol{q}_{\max }}{\boldsymbol{q}_{\text {min }}}=\ln \frac{p_{i n i}+p_{\text {fin }}}{p_{\text {ini }}-p_{\text {fin }}}=\ln \frac{\left(p_{i n i}+p_{f i n}\right)^{2}}{p_{i n i}^{2}-p_{f i n}^{2}}=\ln \frac{\left[\varepsilon^{1 / 2}+(\varepsilon-\hbar \omega)^{1 / 2}\right]^{2}}{\hbar \omega} .
$$

Quantum bremsstrahlung

Plugged into Eq. (85), this expression yields the so-called Bethe-Heitler formula for quantum bremsstrahlung. ${ }^{35}$ Note that at this approach, $g_{\max }$ is close to that of the classical approximation, but $g_{\min }$ $\sim \hbar \omega / u$, so that

$$
\begin{equation*}
\frac{\left.\boldsymbol{q}_{\min }\right|_{\text {classical }}}{\left.\boldsymbol{q}_{\min }\right|_{\text {quantum }}} \sim \frac{\alpha z z^{\prime}}{\beta} \tag{10.89}
\end{equation*}
$$

where $z$ and $z$ ' are particles' charges in units of $e$, and $\alpha$ is the fine structure ("Sommerfeld") constant,

$$
\begin{equation*}
\left.\alpha \equiv \frac{e^{2}}{4 \pi \varepsilon_{0} \hbar c}\right|_{\mathrm{SI}}=\left.\frac{e^{2}}{\hbar c}\right|_{\text {Gaussian }} \approx \frac{1}{137} \ll 1, \tag{10.90}
\end{equation*}
$$

which is one of the basic notions of quantum mechanics. ${ }^{36}$ For most cases of practical interest, ratio (89) is smaller that 1 , and since we have to keep the highest value of $q_{\text {min }}$, the Bethe-Heitler formula should be used.

Now nothing prevents us from calculating the total radiative losses of energy per unit length:

$$
\begin{equation*}
-\frac{d \varepsilon}{d x}=\int_{0}^{\infty}\left(-\frac{d^{2} \varepsilon}{d \omega d z}\right) d \omega=\frac{16}{3} n \frac{q^{2}}{4 \pi \varepsilon_{0} c}\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0} m c^{2}}\right)^{2} \frac{1}{\beta^{2}} 2 \int_{0}^{\omega_{\max }} \ln \frac{\varepsilon^{1 / 2}-(\varepsilon-\hbar \omega)^{1 / 2}}{(\hbar \omega)^{1 / 2}} d \omega \tag{10.91}
\end{equation*}
$$

where $\hbar \omega_{\max }=\varepsilon$ is the maximum energy of the radiation quantum. By introducing the dimensionless integration variable $\xi \equiv \hbar \omega / \varepsilon=2 \hbar \omega /\left(m u^{2} / 2\right)$ this integral is reduced to the table one, ${ }^{37}$ and we get

$$
\begin{equation*}
-\frac{d \varepsilon}{d x}=\frac{16}{3} n \frac{q^{2}}{4 \pi \varepsilon_{0} c}\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0} m c^{2}}\right)^{2} \frac{1}{\beta^{2}} \frac{u^{2}}{\hbar}=\frac{16}{3} n\left(\frac{q^{\prime 2}}{4 \pi \varepsilon_{0} \hbar c}\right)\left(\frac{q^{2}}{4 \pi \varepsilon_{0}}\right)^{2} \frac{1}{m c^{2}} \tag{10.92}
\end{equation*}
$$

In my usual style, I would give you an estimate of the losses for a typical case; however, let me compare them to a parallel energy loss mechanism, the so-called Coulomb losses, due to the transfer of mechanical impulse from the scattered particle to the scattering center. (This energy eventually goes into an increase of the thermal energy of the scattering medium.) Using Eqs. (9.139) for the electric field of a linearly moving charge, we can readily find the momentum it transfers to charge $q^{\prime}: 3^{38}$

$$
\begin{equation*}
\Delta p^{\prime}=\left|\left(\Delta p^{\prime}\right)_{y}\right|=\left|\int_{-\infty}^{+\infty}\left(\dot{p}^{\prime}\right)_{y} d t\right|=\left|\int_{-\infty}^{+\infty} q^{\prime} E_{y} d t\right|=\frac{q q^{\prime}}{4 \pi \varepsilon_{0}} \int_{-\infty}^{+\infty} \frac{\gamma b}{\left(b^{2}+\gamma^{2} u^{2} t^{2}\right)^{3 / 2}} d t=\frac{q q^{\prime}}{4 \pi \varepsilon_{0}} \frac{2}{b u} . \tag{10.93}
\end{equation*}
$$

[^442]Hence, the kinetic energy acquired by the scattering center (equal to the loss of energy of the incident particle) is

$$
\begin{equation*}
-\Delta \varepsilon=\frac{\left(\Delta p^{\prime}\right)^{2}}{2 m^{\prime}}=\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0}}\right)^{2} \frac{2}{m^{\prime} u^{2} b^{2}} . \tag{10.94}
\end{equation*}
$$

Such energy losses have to be summed up over all collisions, with random values of the impact parameter $b$. At the scattering center density $n$, the number of collisions per small path length $d z$ per small range $d b$ is $d N=n 2 \pi b d b d x$, so that

$$
\begin{equation*}
-\frac{d \varepsilon}{d x}=\int(-\Delta \varepsilon) d N=n\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0}}\right)^{2} \frac{2}{m^{\prime} u^{2}} 2 \pi \int_{b_{\min }}^{b_{\max }} \frac{d b}{b}=4 \pi n\left(\frac{q q^{\prime}}{4 \pi \varepsilon_{0}}\right)^{2} \frac{\ln B}{m^{\prime} u^{2}}, \quad \text { where } B \equiv \frac{b_{\max }}{b_{\min }} . \tag{10.95}
\end{equation*}
$$

Here the logarithmic integral over $b$ was treated similarly to that over $g$ in the bremsstrahlung theory. This approach is adequate, because the ratio $b_{\text {max }} / b_{\text {min }}$ is much larger than 1 . Indeed, $b_{\text {min }}$ may be estimated from $\left(\Delta p^{\prime}\right)_{\max } \sim p=r m u$. For this value, Eq. (93) with $q^{\prime} \sim q$ gives $b_{\min } \sim r_{c}$ (see Eq. (8.41) and its discussion), which is, for elementary particles, of the order of $10^{-15} \mathrm{~m}$. On the other hand, for the most important case when charges $q$ ' belong to electrons (which, according to Eq. (94) are the most efficient Coulomb energy absorbers, due to their extremely low mass $m^{\prime}$ ), $b_{\text {max }}$ may be estimated from condition $\tau=b / \gamma u \sim 1 / \omega_{\max }$, where $\omega_{\max } \sim 10^{16} \mathrm{~s}^{-1}$ is the characteristic frequency of electron transitions in atoms. (Below this frequency, our classical analysis of scatterer's motion is invalid.) From here, we have the estimate $b_{\max } \sim \mu u / \omega_{\max }$, so that

$$
\begin{equation*}
B \equiv \frac{b_{\max }}{b_{\min }} \sim \frac{r u}{r_{c} \omega_{0}} \tag{10.96}
\end{equation*}
$$

for $\gamma \sim 1$ and $u \sim c \approx 3 \times 10^{8} \mathrm{~m} / \mathrm{s}$ giving $b_{\max } \sim 3 \times 10^{-8} \mathrm{~m}$, and $B \sim 10^{9}$ (give or take a couple orders of magnitude - this does not change the estimate $\ln B \sim 20$ too much). ${ }^{39}$

Now we can compare the Coulomb losses (95) with those due to the bremsstrahlung, given by Eq. (92):

$$
\begin{equation*}
\frac{-\left.d \varepsilon\right|_{\text {radiation }}}{-\left.d \varepsilon\right|_{\text {Coulomb }}} \sim \alpha \mathcal{F}^{\prime} \frac{m^{\prime}}{m} \beta^{2} \frac{1}{\ln B} \tag{10.97}
\end{equation*}
$$

Since $\alpha \sim 10^{-2} \ll 1$, for non-relativistic particles $(\beta \ll 1)$ the Coulomb losses of energy are much higher, and only for ultra-relativistic particles, the relation may be opposite.

According to Eq. (95), for electron-electron scattering ( $q=q^{\prime}=-e, m^{\prime}=m_{e}$ ), ${ }^{40}$ at the value $n$ $6 \times 10^{26} \mathrm{~m}^{-3}$ typical for air at ambient conditions, the characteristic length of energy loss,

[^443]\[

$$
\begin{equation*}
l_{c} \equiv \frac{\varepsilon}{(-d \varepsilon / d x)} \tag{10.98}
\end{equation*}
$$

\]

for electrons with kinetic energy $\varepsilon=6 \mathrm{keV}$ is close to $2 \times 10^{-4} \mathrm{~m}=0.2 \mathrm{~mm}$. (This is why you need vacuum in CRT monitors and electron microscope columns!) Since $l_{c} \propto \varepsilon^{2}$, more energetic particles penetrate deeper, until the bremsstrahlung steps in at very high energies.

### 10.5. Density effects and the Cherenkov radiation

For condensed matter, the Coulomb loss estimate made in the last section is not quite suitable, because it is based on the upper cutoff $b_{\max } \sim \mu u / \omega_{\max }$. For the example given above, incoming electron velocity $u$ is close to $5 \times 10^{7} \mathrm{~m} / \mathrm{s}$, and for the typical value $\omega_{\max } \sim 10^{16} \mathrm{~s}-1\left(\hbar \omega_{\max } \sim 10 \mathrm{eV}\right)$, this cutoff $b_{\max } \sim 5 \times 10^{-9} \mathrm{~m}=5 \mathrm{~nm}$. Even for air at ambient conditions, this is larger than the average distance ( $\sim 2$ nm ) between the molecules, so that at the high end of the impact parameter range, at $b \sim b_{\text {max }}$, the Coulomb loss events in adjacent molecules are not quite independent, and the theory needs corrections. For condensed matter, with much higher particle density $n$, most collisions satisfy condition

$$
\begin{equation*}
n b^{3} \gg 1, \tag{10.99}
\end{equation*}
$$

and the treatment of Coulomb collisions as independent events is completely inadequate. However, condition (99) enables the opposite approach: treating the medium as a continuum. In the time domain formulation, used in the previous sections of this chapter, this would be a very complex problem, because it would require an explicit description of medium dynamics. Here the frequency-domain approach, based on the Fourier transform in both time and space, helps a lot, provided that functions $\varepsilon(\omega)$ and $\mu(\omega)$ are considered known - either calculated or taken from experiment. Let us have a good look at such approach, because it gives some interesting (and practically important) results.

In Chapter 6, we have used the macroscopic Maxwell equations to derive Eqs. (6.109), which describe the time evolution of potentials in a medium with frequency-independent $\varepsilon$ and $\mu$. Looking for all functions participating in Eqs. (6.109) in the form of plane-wave expansion ${ }^{41}$

$$
\begin{equation*}
f(\mathbf{r}, t)=\int d^{3} k \int d \omega f_{\mathbf{k}, \omega} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)} \tag{10.100}
\end{equation*}
$$

and requiring all coefficients at similar exponents to be balanced, we get their Fourier image: ${ }^{42}$

$$
\begin{equation*}
\left[k^{2}-\omega^{2} \varepsilon \mu\right] \phi_{\mathbf{k}, \omega}=\frac{\rho_{\mathbf{k}, \omega}}{\varepsilon}, \quad\left[k^{2}-\omega^{2} \varepsilon \mu\right] \mathbf{A}_{\mathbf{k}, \omega}=\mu \mathbf{j}_{\mathbf{k}, \omega} . \tag{10.101}
\end{equation*}
$$

[^444]As was discussed in Chapter 7, in such a Fourier form, the Maxwell theory remain valid even for the dispersive media, so that Eq. (101) is generalized as

$$
\begin{equation*}
\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right] \phi_{\mathbf{k}, \omega}=\frac{\rho_{\mathbf{k}, \omega}}{\varepsilon(\omega)}, \quad\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right] \mathbf{A}_{\mathbf{k}, \omega}=\mu(\omega) \mathbf{j}_{\mathbf{k}, \omega} \tag{10.102}
\end{equation*}
$$

The evident advantage of these equations is that their formal solution is trivial:
potentials in a linear medium

$$
\begin{equation*}
\phi_{\mathbf{k}, \omega}=\frac{\rho_{\mathbf{k}, \omega}}{\varepsilon(\omega)\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]}, \quad \mathbf{A}_{\mathbf{k}, \omega}=\frac{\mu(\omega) \mathbf{j}_{\mathbf{k}, \omega}}{\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]} \tag{10.103}
\end{equation*}
$$

so that the "only" remaining things to do is to calculate the Fourier transforms of functions $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$, describing stand-alone charges and currents, using the transform reciprocal to Eq. (100), with one factor $1 / 2 \pi$ per each scalar dimension,

$$
\begin{equation*}
f_{\mathbf{k}, \omega}=\frac{1}{(2 \pi)^{4}} \int d^{3} r \int d t f(\mathbf{r}, t) e^{-i(\mathbf{k} \cdot \mathbf{r}-\omega t)} \tag{10.104}
\end{equation*}
$$

and than carry out the integration (100).
For our current problem of a single charge $q$, uniformly moving in the medium with velocity $\mathbf{u}$,

$$
\begin{equation*}
\rho(\mathbf{r}, t)=q \delta(\mathbf{r}-\mathbf{u} t), \quad \mathbf{j}(\mathbf{r}, t)=q \mathbf{u} \delta(\mathbf{r}-\mathbf{u} t), \tag{10.105}
\end{equation*}
$$

the first task is easy:

$$
\begin{equation*}
\rho_{\mathbf{k}, \omega}=\frac{q}{(2 \pi)^{4}} \int d^{3} r \int d t q \delta(\mathbf{r}-\mathbf{u} t) e^{-i(\mathbf{k} \cdot \mathbf{r}-\omega t)}=\frac{q}{(2 \pi)^{4}} \int e^{i(\omega t-\mathbf{k} \cdot \mathbf{u} t)} d t=\frac{q}{(2 \pi)^{3}} \delta(\omega-\mathbf{k} \cdot \mathbf{u}) . \tag{10.106}
\end{equation*}
$$

Since expressions (105) for $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$ differ only by a constant factor $\mathbf{u}$, it is clear that the absolutely similar calculation for current would give

$$
\begin{equation*}
\mathbf{j}_{\mathbf{k}, \omega}=\frac{q \mathbf{u}}{(2 \pi)^{3}} \delta(\omega-\mathbf{k} \cdot \mathbf{u}) . \tag{10.107}
\end{equation*}
$$

Let us summarize what we have got by now, plugging Eqs. (106) and (107) into Eqs. (103):

$$
\begin{equation*}
\phi_{\mathbf{k}, \omega}=\frac{1}{(2 \pi)^{3}} \frac{q \delta(\omega-\mathbf{k} \cdot \mathbf{u})}{\varepsilon(\omega)\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]}, \quad \mathbf{A}_{\mathbf{k}, \omega}=\frac{1}{(2 \pi)^{3}} \frac{\mu(\omega) q \mathbf{u} \delta(\omega-\mathbf{k} \cdot \mathbf{u})}{\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]}=\varepsilon(\omega) \mu(\omega) \mathbf{u} \phi_{\mathbf{k}, \omega} . \tag{10.108}
\end{equation*}
$$

Now, at the last step of calculations, namely integration (100), we are starting to pay a heavy price for the easiness of the first steps. This is why let us think well what exactly do we need from it. First of all, for the calculation of power losses, the electric field is more convenient to use than the potentials, so let us calculate the Fourier images of $\mathbf{E}$ and B. Plugging expansion (100) into the fundamental relations (6.106), and again requiring the balance of exponent's coefficients, we get

$$
\begin{equation*}
\mathbf{E}_{\mathbf{k}, \omega}=-i \mathbf{k} \phi_{k, \omega}+i \omega \mathbf{A}_{\mathbf{k}, \omega}=i[\omega \varepsilon(\omega) \mu(\omega) \mathbf{u}-\mathbf{k}] \phi_{\mathbf{k}, \omega}, \quad \mathbf{B}_{\mathbf{k}, \omega}=i \mathbf{k} \times \mathbf{A}_{\mathbf{k}, \omega}=i \varepsilon(\omega) \mu(\omega) \mathbf{k} \times \mathbf{u} \phi_{\mathbf{k}, \omega}, \tag{10.109}
\end{equation*}
$$

so that Eqs. (100) and (108) yield

$$
\begin{equation*}
\mathbf{E}(\mathbf{r}, t)=\int d^{3} k \int d \omega \mathbf{E}_{\mathbf{k}, \omega} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)}=\frac{i q}{(2 \pi)^{3}} \int d^{3} k \int d \omega \frac{[\omega \varepsilon(\omega) \mu(\omega) \mathbf{u}-\mathbf{k}] \delta(\omega-\mathbf{k} \cdot \mathbf{u})}{\varepsilon(\omega)\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)} \tag{10.110}
\end{equation*}
$$

With the notation used in Eq. (51), this integral may be partitioned as

$$
\begin{equation*}
\mathbf{E}(\mathbf{r}, t)=\int \mathbf{E}_{\omega} e^{-i \omega t} d \omega, \quad \mathbf{E}_{\omega}=\int \mathbf{E}_{\mathbf{k}, \omega} e^{i \mathbf{k} \cdot \mathbf{r}} d^{3} k=\frac{i q}{(2 \pi)^{3}} \int \frac{[\omega \varepsilon(\omega) \mu(\omega) \mathbf{u}-\mathbf{k}] \delta(\omega-\mathbf{k} \cdot \mathbf{u})}{\varepsilon(\omega)\left[k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)\right]} e^{i \mathbf{k} \cdot \mathbf{r}} d^{3} k .( \tag{10.111}
\end{equation*}
$$

Let us calculate the Cartesian components of the partial Fourier image $\mathbf{E}_{\omega}$, at a point separated by distance $b$ from particle's trajectory. Selecting the coordinates and time origin as shown in Fig. 9.11a, we have $\mathbf{r}=\{0, b, 0\}$, so that only $E_{x}$ and $E_{y}$ are not vanishing. In particular, according to Eq. (111),

$$
\begin{equation*}
\left(E_{x}\right)_{\omega}=\frac{i q}{(2 \pi)^{3} \varepsilon(\omega)} \int d k_{x} \int d k_{y} \int d k_{z} \frac{\omega \varepsilon(\omega) \mu(\omega) u-k_{x}}{k^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)} \delta\left(\omega-k_{x} u\right) e^{i k_{y} b} \tag{10.112}
\end{equation*}
$$

The delta-function kills one integral (over $k_{x}$ ) of three, and we get:

$$
\begin{equation*}
\left(E_{x}\right)_{\omega}=\frac{i q}{(2 \pi)^{3} \varepsilon(\omega) u}\left[\omega \varepsilon(\omega) \mu(\omega) u-\frac{\omega}{u}\right] \int e^{i k_{y} b} d k_{y} \int \frac{d k_{z}}{\omega^{2} / u^{2}+k_{y}^{2}+k_{z}^{2}-\omega^{2} \varepsilon(\omega) \mu(\omega)} . \tag{10.113}
\end{equation*}
$$

The last integral (over $k_{y}$ ) may be readily reduced to the table integral $\int d \xi /\left(1+\xi^{2}\right)$, in infinite limits, equal to $\pi .{ }^{43}$ The result may be presented as

$$
\begin{equation*}
\left(E_{x}\right)_{\omega}=-\frac{i \pi q \kappa^{2}}{(2 \pi)^{3} \omega \varepsilon(\omega)} \int \frac{e^{i k_{y} b}}{\left(k_{y}^{2}+\kappa^{2}\right)^{1 / 2}} d k_{y} \tag{10.114}
\end{equation*}
$$

where parameter $\kappa$ (generally, a complex function of frequency) is defined as

$$
\begin{equation*}
\kappa^{2} \equiv \omega^{2}\left(\frac{1}{u^{2}}-\varepsilon(\omega) \mu(\omega)\right) . \tag{10.115}
\end{equation*}
$$

The last integral may be expressed via the modified Bessel function of the second kind:44

$$
\begin{equation*}
\left(E_{x}\right)_{\omega}=-\frac{i q u \kappa^{2}}{(2 \pi)^{2} \omega \varepsilon(\omega)} K_{0}(\kappa b) . \tag{10.116}
\end{equation*}
$$

A similar calculation yields

$$
\begin{equation*}
\left(E_{y}\right)_{\omega}=\frac{q \kappa}{(2 \pi)^{2} \varepsilon(\omega)} K_{1}(\kappa b) . \tag{10.117}
\end{equation*}
$$

Now, instead of rushing to make the final integration (111) over frequency to calculate $\mathbf{E}(t)$, let us realize that what we need for power losses is only the total energy loss through the whole time of particle passage. Energy loss per unit volume is

$$
\begin{equation*}
-\frac{d \varepsilon}{d V}=\int \mathbf{j} \cdot \mathbf{E} d t \tag{10.118}
\end{equation*}
$$

[^445]where $\mathbf{j}$ is the current of bound charges in the medium, and should not be confused with the free particle's current (105). This integral may be readily expressed via the partial Fourier image $\mathbf{E}_{\omega}$ and the similarly defined image $\mathbf{j}_{\omega}$, just as it was done at the derivation of Eq. (54):
\[

$$
\begin{equation*}
-\frac{d \varepsilon}{d V}=\int d t \int d \omega e^{-i \omega t} \int d \omega^{\prime} e^{-i \omega^{\prime} t} \mathbf{j}_{\omega} \cdot \mathbf{E}_{\omega^{\prime}}=2 \pi \int d \omega \int d \omega^{\prime} \mathbf{j}_{\omega} \cdot \mathbf{E}_{\omega^{\prime}} \delta\left(\omega+\omega^{\prime}\right)=2 \pi \int \mathbf{j}_{\omega} \cdot \mathbf{E}_{-\omega} d \omega \tag{10.119}
\end{equation*}
$$

\]

In our approach, the Ohmic conductance is incorporated into the complex permittivity $\varepsilon(\omega)$, so that, according to the discussion in the end of Sec. 7.2, current's Fourier image is

$$
\begin{equation*}
\mathbf{j}_{\omega}=\sigma_{\mathrm{ef}}(\omega) \mathbf{E}_{\omega}=-i \omega \varepsilon(\omega) \mathbf{E}_{\omega} . \tag{10.120}
\end{equation*}
$$

As a result, Eq. (119) yields

$$
\begin{equation*}
-\frac{d \varepsilon}{d V}=-2 \pi i \int \varepsilon(\omega) \mathbf{E}_{\omega} \cdot \mathbf{E}_{-\omega} \omega d \omega=4 \pi \operatorname{Im} \int_{0}^{\infty} \varepsilon(\omega)\left|E_{\omega}\right|^{2} \omega d \omega \tag{10.121}
\end{equation*}
$$

(The last transition is possible due to the property $\delta(-\omega)=\varepsilon^{*}(\omega)$, which was discussed in Sec. 7.2.)
Finally, just as in the last section, we have to calculate the energy loss rate averaged over random values of the impact parameter $b$ :

$$
\begin{equation*}
\left.-\frac{d \varepsilon}{d x}=\int\left(-\frac{d \varepsilon}{d V}\right) d^{2} b=2 \pi \int_{b_{\text {min }}}^{\infty}\left(-\frac{d \varepsilon}{d V}\right) b d b=8 \pi^{2} \int_{b_{\text {min }}}^{\infty} b d b \int_{0}^{\infty}\left(\left|E_{x}\right|_{\omega}^{2}+\left|E_{y}\right|_{\omega}^{2}\right) \operatorname{Im} \varepsilon(\omega)\right) \omega d \omega . \tag{10.122}
\end{equation*}
$$

Note that we are cutting the resulting integral over $b$ from below at some $b_{\text {min }}$ where our theory looses legitimacy. (On that limit, we are not doing much better than in the past section). Plugging in the calculated expressions (116) and (117) for field components, swapping the integrals, and using recurrence relations (2.142), which are valid for any Bessel functions, we finally get:

$$
\begin{equation*}
-\frac{d \varepsilon}{d x}=\frac{2}{\pi} q^{2} \operatorname{Im} \int_{0}^{\infty}\left(\kappa^{*} b_{\min }\right) K_{1}\left(\kappa^{*} b_{\min }\right) K_{0}\left(\kappa^{*} b_{\min }\right) \frac{d \omega}{\omega \varepsilon(\omega)} \tag{10.123}
\end{equation*}
$$

This general result is valid for an arbitrary linear medium, with arbitrary dispersion relations $\varepsilon(\omega)$ and $\mu(\omega)$. (The last function participates in Eq. (123) only via Eq. (115) which defines parameter $\kappa$.) To get more concrete results, some particular model of the medium should be used. Let us explore the Lorentz oscillator model, which was discussed in Sec. 7.2, in its form (7.33) suitable for transition to quantum-mechanical description of atoms:

$$
\begin{equation*}
\varepsilon(\omega)=\varepsilon_{0}+\frac{n q^{\prime 2}}{m} \sum_{j} \frac{f_{j}}{\left(\omega_{j}^{2}-\omega^{2}\right)-2 i \omega \delta_{j}}, \quad \sum_{j} f_{j}=1, \quad \mu(\omega)=\mu_{0} . \tag{10.124}
\end{equation*}
$$

If the damping of the effective atomic oscillators is low, $\delta_{j} \ll \omega_{j}$, and particle's speed $u$ is much lower than the typical wave's phase velocity $v$ (and hence $c!$ ), then for most frequencies Eq. (115) gives

$$
\begin{equation*}
\kappa^{2} \equiv \omega^{2}\left(\frac{1}{u^{2}}-\frac{1}{v^{2}(\omega)}\right) \approx \frac{\omega^{2}}{u^{2}} \tag{10.125}
\end{equation*}
$$

i.e. $\kappa=\kappa^{*} \approx \omega / u$ is real. In this case, Eq. (123) may be shown to give Eq. (95) with

$$
\begin{equation*}
b_{\max }=\frac{1.123 u}{\langle\omega\rangle} . \tag{10.126}
\end{equation*}
$$

Good news here is that both approaches (the microscopic analysis of Sec. 4 and the macroscopic analysis of this section) give essentially the same result. This fact may be also perceived as bad news: the treatment of the medium as a continuum does not give any new results here. The situation somewhat changes at relativistic velocities at which such treatment provides noticeable corrections (called density effects), in particular reducing the energy loss estimates.

Let me, however, skip these details and focus on a much more important effect described by our formulas. Consider the dependence of the electric field components on the impact parameter $b$, i.e. on the closest distance between particle's trajectory and the field observation point. If $\kappa^{2}>0$, then $\kappa$ is real, and we can use, in Eqs. (116)-(117), the asymptotic formula (2.158),

$$
\begin{equation*}
K_{n}(\xi) \rightarrow\left(\frac{\pi}{2 \xi}\right)^{1 / 2} e^{-\xi}, \text { at } \xi \rightarrow \infty \tag{10.127}
\end{equation*}
$$

to conclude that the complex amplitudes $E_{\omega}$ of both components $E_{x}$ and $E_{y}$ of the electric field decrease exponentially, starting from $b \sim u /\langle\omega\rangle$. However, let us consider what happens at frequencies where $\kappa^{2}<$ 0 , i.e.

$$
\begin{equation*}
\varepsilon(\omega) \mu(\omega) \equiv \frac{1}{v^{2}(\omega)}<\frac{1}{u^{2}}<\frac{1}{c^{2}}=\varepsilon_{0} \mu_{0} . \tag{10.128}
\end{equation*}
$$

(This condition means that particle's velocity is larger than the phase velocity of waves, at this particular frequency.) In these intervals, $\kappa$ is purely imaginary, ${ }^{45}$ functions $\exp \{\kappa b\}$ become just phase factors, and

$$
\begin{equation*}
\left|E_{x}(\omega)\right| \propto\left|E_{y}(\omega)\right| \propto \frac{1}{b^{1 / 2}} . \tag{10.129}
\end{equation*}
$$

This means that the Poynting vector drops as $1 / b$, so that its flux through a surface of a round cylinder of radius $b$, with the axis on the particle trajectory (i.e. power flow), does not depend on $b$. Hence, this is wave emission - the famous Cherenkov radiation. ${ }^{46}$

The direction of its propagation may be readily found taking into account that at large distances from particle's trajectory the emitted wave has to be locally planar, so that the Cherenkov angle $\theta$ may be found from the ratio of the field components (Fig. 14a):

$$
\begin{equation*}
\tan \theta=-\frac{E_{x}}{E_{y}} \tag{10.130}
\end{equation*}
$$

[^446]


Fig. 10.14. (a) Cherenkov radiation's propagation angle $\theta$, and (b) its interpretation.
This ratio may be calculated by plugging the asymptotic formula (127) into Eqs. (116) and (117) and calculating their ratio:

$$
\begin{equation*}
\tan \theta=-\frac{E_{x}}{E_{y}}=\frac{i \kappa u}{\omega}=\left[\varepsilon(\omega) \mu(\omega) u^{2}-1\right]^{1 / 2}=\left(\frac{u^{2}}{v^{2}(\omega)}-1\right)^{1 / 2}, \tag{10.131a}
\end{equation*}
$$

so that

Cherenkov angle

$$
\begin{equation*}
\cos \theta=\frac{v(\omega)}{u}<1 \tag{10.131b}
\end{equation*}
$$

Remarkably, this direction does not depend on the emission time $t$, so that radiation of frequency $\omega$, at each instant, forms a hollow cone led by the particle. This simple result allows an evident interpretation (Fig. 14b): the cone is just the set of all observation points that may be reached by "signals" propagating with speed $v(\omega)<u$ from all previous points of particle's trajectory.

This phenomenon is closely related to the so-called Mach cone in fluid dynamics, ${ }^{47}$ besides that in the Cherenkov radiation there is a separate cone for each frequency (of the range in which $v(\omega)<u$ ): the smaller is the $\delta(\omega) \mu(\omega)$ product, i.e. the larger is wave velocity $v(\omega)=1 /[\varepsilon(\omega) \mu(\omega)]^{1 / 2}$, and the broader is the cone, i.e. the earlier the corresponding "shock wave" arrives to an observer. Please note that the Cherenkov radiation is a unique radiative phenomenon: it takes place even if a particle moves without acceleration, and (in agreement with our analysis in Sec. 2), is impossible in free space where $v$ $=c$ is always larger than $u$.

The intensity of the Cherenkov radiation intensity may be also readily found by plugging the asymptotic expression (127), with imaginary $\kappa$, into Eq. (123). The result is

Cherenkov radiation intensity

$$
\begin{equation*}
-\frac{d \varepsilon}{d x} \approx\left(\frac{\mathfrak{Y}}{4 \pi}\right)^{2} \int_{v(\omega)<u} \omega\left(1-\frac{v^{2}(\omega)}{u^{2}}\right) d \omega . \tag{10.132}
\end{equation*}
$$

For non-relativistic particles $(u \ll c)$, the Cherenkov radiation condition $u>v(\omega)$ may be fulfilled only in relatively narrow frequency intervals where the product $\varepsilon(\omega) \mu(\omega)$ is very large (usually, due to optical resonance peaks of the electric permittivity - see Fig. 7.5 and its discussion). In this case the emitted light consists of a few nearly monochromatic components. On the contrary, if the condition $u>v(\omega)$, i.e. $u^{2} / \varepsilon(\omega) \mu(\omega)>1$ is fulfilled in a broad frequency range (as it is for ultra-relativistic particles in

[^447]condensed media), the radiated power is clearly dominated by higher frequency of the range - hence the famous bluish color of the Cherenkov radiation glow in water nuclear reactors- see Fig. 15.


Fig. 10.15. The Cherenkov radiation glow coming from the Advanced Test Reactor of the Idaho National Laboratory. Adapted from http://en.wikipedia.org/wiki/Cherenkov radiation.

The Cherenkov radiation is broadly used for the detection of radiation in high energy experiments for particle identification and speed measurement (since it is easy to pass particles through media of various density and hence of the dielectric constant) - for example, in the so-called Ring Imaging Cherenkov (RICH) detectors that have been designed for the DELPHI experiment ${ }^{48}$ at the Large Electron-Positron Collider (LEP) in CERN.

A little bit counter-intuitively, the formalism described in this section is also very useful for the description of an apparently rather different effect - the so-called transition radiation that takes place when a charged particle crosses a border between two media. ${ }^{49}$ The effect may be understood as result of the time dependence of the electric dipole formed by the moving charge and its mirror image in the counterpart medium - see Fig. 16. In the non-relativistic limit, the effect allows a straightforward description combining the electrostatics picture of Sec. 3.4 (see Fig. 3.9 and its discussion), and Eq. (8.27) - slightly corrected for polarization effects of the media. However, if particle's velocity $u$ is comparable with the phase velocity of waves in either medium, the adequate theory of the transition radiation becomes very close to that of the Cherenkov radiation.


Fig. 10.16. Physics of the transition radiation.

[^448]In comparison with the Cherenkov radiation, the transition radiation is rather weak, and its practical use (mostly for the measurement of the relativistic factor $\gamma$, to which the radiation intensity is proportional) requires multi-layered stacks. ${ }^{50}$ In these systems, the radiation emitted at sequential borders may be coherent, and the system's physics becomes close to that of the undulators discussed in Sec. 4.

### 10.6. Radiation's back-action

An attentive reader could notice that so far our treatment of charged particle dynamics has never been fully self-consistent. Indeed, in Sec. 9.6 we have analyzed particle's motion in various external fields, ignoring the fields radiated by particle itself, while in Sec. 8.2 and earlier in this chapter these fields have been calculated (admittedly, just for a few simple cases), but, again, their back-action on the emitting particle have been ignored. Only in few cases we have taken the back effects of the radiation implicitly, via the energy conservation. However, even in these cases, the near-field components of the fields (such as the first term in Eq. (20a), that affect the moving particle most, have been ignored.

At the same time, it is clear that generally the interaction of a point charge with its own field cannot be always ignored. As the simplest example, if an electron is made to fly through a resonant cavity, thus inducing oscillations in it, and then is forced to return to it before the oscillations have decayed, its motion will be certainly affected by the oscillating fields, just as if they had been induced by another source. There is no conceptual problem with applying the Maxwell theory to such "fieldparticle rendezvous" effects; moreover, it is the basis of the engineering design of such electron devices as klystrons, magnetrons, and undulators.

A problem arises only when no finite "rendezvous" point is enforced by boundary conditions, so that the most important self-field effects are at $R \equiv|\mathbf{r}-\mathbf{r}| \rightarrow 0$, the most evident example being the radiation of particle in free space, described earlier in this chapter. We already know that radiation takes away a part of charge's kinetic energy, i.e. has to cause its deceleration. One should wonder, however, whether such self-action effects might be described in a more direct, non-perturbative way.

As the first attempt, let us try a phenomenological approach based on the already derived formulas for radiation power $P$. For the sake of simplicity, let us consider a non-relativistic point charge $q$ in free space, so that $P$ is described by Eq. (8.27), with electric dipole moment's derivative over time equal to $q \mathbf{u}$ :

$$
\begin{equation*}
\mathcal{P}=\frac{Z_{0} q^{2}}{6 \pi c^{2}} \dot{u}^{2}=\frac{2}{3 c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \dot{u}^{2} . \tag{10.133}
\end{equation*}
$$

The most naïve approach would be to write the equation of particle's motion in the form

$$
\begin{equation*}
m \dot{\mathbf{u}}=\mathbf{F}_{e x t}+\mathbf{F}_{\text {self }}, \tag{10.134}
\end{equation*}
$$

[^449]and try to calculate the radiation back-action force by requiring its instant power, $-\mathbf{F}_{\text {self }} \mathbf{u}$, to be equal to P. However, with Eq. (133), this approach (say, for 1D motion) would give a very unnatural result,
\[

$$
\begin{equation*}
F_{\text {self }} \propto \frac{\dot{u}^{2}}{u} \tag{10.135}
\end{equation*}
$$

\]

that might diverge at some points of particle's trajectory. This failure is clearly due to the retardation effect: as the reader may recall, Eq. (133) results from the analysis of radiation fields at large distances from the particle, e.g., from the second term in Eq. (20a), i.e. when the non-radiative first term (which is much larger at small distances, $R \rightarrow 0$ ) is ignored.

Before exploring the effects of this term, let us, however, make one more try with Eq. (133), considering its average effect on some periodic motion of the particle. To calculate the average, let us write

$$
\begin{equation*}
\overline{\dot{u}^{2}} \equiv \frac{1}{T} \int_{0}^{T} \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} d t \tag{10.136}
\end{equation*}
$$

and integrate this identity, over the motion period, by parts:

$$
\begin{equation*}
\overline{\mathcal{P}}=\frac{2}{3 c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \overline{(\dot{\mathbf{u}})^{2}}=\frac{2}{3 c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \frac{1}{T}\left(\left.\dot{\mathbf{u}} \cdot \mathbf{u}\right|_{0} ^{T}-\int_{0}^{T} \ddot{\mathbf{u}} \cdot \mathbf{u} d t\right)=-\frac{1}{T} \int_{0}^{T} \frac{2}{3 c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \ddot{\mathbf{u}} \cdot \mathbf{u} d t . \tag{10.137}
\end{equation*}
$$

One the other hand, the back-action force would give

$$
\begin{equation*}
\overline{\mathcal{P}}=-\frac{1}{T} \int_{0}^{T} \mathbf{F}_{\text {self }} \cdot \mathbf{u} d t \tag{10.138}
\end{equation*}
$$

These two averages coincide if ${ }^{51}$

$$
\begin{equation*}
\mathbf{F}_{\text {self }}=\frac{2}{3 c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \ddot{\mathbf{u}} \tag{10.139}
\end{equation*}
$$

This is the so-called Abraham-Lorentz force for self-action. Before going after a more serious derivation of this formula, let us estimate its scale, presenting Eq. (139) as

$$
\begin{equation*}
\mathbf{F}_{\text {self }}=m \tau \ddot{\mathbf{u}}, \quad \text { with } \tau \equiv \frac{2}{3 m c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}} \tag{10.140}
\end{equation*}
$$

where constant $\tau$ evidently has the dimension of time. Recalling definition (8.41) of the classical radius $r_{c}$ of the particle, Eq. (140) for $\tau$ may be rewritten as

$$
\begin{equation*}
\tau=\frac{2}{3} \frac{r_{c}}{c} . \tag{10.141}
\end{equation*}
$$

[^450]- the so-called Abraham-Lorentz-Dirac force.

For the electron, $\tau$ is of the order of $10^{-23} \mathrm{~s}$. This means that in most cases the Abrahams-Lorentz force is either negligible or leads to the same results as the perturbative treatments of energy loss we have used earlier in this chapter.

However, Eq. (140) brings some unpleasant surprises. For example, let us consider a 1D oscillator of eigenfrequency $\omega_{0}$. For it, Eq. (134), with the back-action force given by Eq. (140), is

$$
\begin{equation*}
m \ddot{x}+m \omega_{0}^{2} x=m \tau \dddot{x} \tag{10.142}
\end{equation*}
$$

Looking for the solution to this linear differential equation in the usual exponential form, $x(t) \propto$ $\exp \{\lambda t\}$, we get the following characteristic equation,

$$
\begin{equation*}
\lambda^{2}+\omega_{0}^{2}=\tau \lambda^{3} . \tag{10.143}
\end{equation*}
$$

It may look like that for any "reasonable" value of $\omega_{0} \ll 1 / \tau \sim 10^{23} \mathrm{~s}^{-1}$, the right-hand side of this nonlinear algebraic equation may be treated as a perturbation. Indeed, looking for its solutions in the natural form $\lambda_{ \pm}= \pm i \omega_{0}+\lambda^{\prime}$, with $\left|\lambda^{\prime}\right| \ll \omega_{0}$, expanding both parts of Eq. (143) in the Taylor series in small parameter $\lambda^{\prime}$, and keeping only linear terms, we get

$$
\begin{equation*}
\lambda^{\prime} \approx-\frac{\omega_{0}^{2} \tau}{2} \tag{10.144}
\end{equation*}
$$

This means that the energy of free oscillations decreases in time as $\exp \left\{2 \lambda^{\prime} t\right\}=\exp \left\{-\omega_{0}{ }^{2} \tau t\right\}$; this is exactly the radiative damping analyzed earlier. However, Eq. (143) is deceiving; it has the third root corresponding to unphysical, exponentially growing (so-called run-away) solutions. It is easiest to see for a free particle, with $\omega_{0}=0$. Then Eq. (143) becomes very simple,

$$
\begin{equation*}
\lambda^{2}=\tau \lambda^{3} \tag{10.145}
\end{equation*}
$$

and it is easy to find all its 3 roots explicitly: $\lambda_{1}=\lambda_{2}=0$ and $\lambda_{3}=1 / \tau$. While the first 2 roots correspond the values $\lambda_{ \pm}$found earlier, the last one describes exponential (and extremely fast!) acceleration..

In order to remove this artifact, let us try to develop a self-consistent approach to back action, taking into account the near-field terms of particle fields. For that, we need somehow overcome the divergence of Eqs. (10) and (20) at $R \rightarrow 0$. The most reasonable way to do this is to spread particle charge over a ball of radius $a$, with a spherically-symmetric (but not necessarily constant) density $\rho(r)$, and in the end of calculations trace the limit $a \rightarrow 0 .{ }^{52}$ Again sticking to the non-relativistic case (so that the magnetic component of the Lorentz force is not important), we should calculate

$$
\begin{equation*}
\mathbf{F}_{r a d}=\int_{V} \rho(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) d^{3} r, \tag{10.146}
\end{equation*}
$$

where the electric field is that of the charge itself, with field of any elementary charge $d q=\rho(r) d^{3} r$, described by Eqs. (20a).

[^451]In order to make analytical calculations doable, we need to make assumption $a \ll r_{c}$, treat ratio $R / r_{c} \sim a / r_{c}$ as a small parameter, and expand the result in the Taylor series in small $R$. This procedure yields

$$
\begin{equation*}
\mathbf{F}_{\text {self }}=-\frac{2}{3} \frac{1}{4 \pi \varepsilon_{0}} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{c^{n+2} n!} \frac{d^{n+1} \mathbf{u}}{d t^{n+1}} \int_{V} d^{3} r \int_{V} d^{3} r^{\prime} \rho(r) R^{n-1} \rho\left(r^{\prime}\right) . \tag{10.147}
\end{equation*}
$$

Distance $R$ cancels only in the term with $n=1$,

$$
\begin{equation*}
\mathbf{F}_{1}=\frac{2}{3 c^{3}} \frac{\ddot{\mathbf{u}}}{4 \pi \varepsilon_{0}} \int_{V} d^{3} r \int_{V} d^{3} r^{\prime} \rho(r) \rho\left(r^{\prime}\right)=\frac{q^{2}}{6 \pi \varepsilon_{0} c^{3}} \ddot{\mathbf{u}}, \tag{10.148}
\end{equation*}
$$

showing that we have recovered (now in an apparently legitimate fashion) Eq. (139) for the AbrahamsLorentz force. One could argue that in the limit $a \rightarrow 0$ the terms higher in $R \sim a$ (with $n>1$ ) could be ignored. However, we have to notice that the main contribution to into series (147) is not described by Eq. (148) for $n=1$, but is given by the larger term with $n=0$ :

$$
\begin{equation*}
\mathbf{F}_{0}=-\frac{2}{3} \frac{1}{4 \pi \varepsilon_{0}} \frac{\dot{\mathbf{u}}}{c^{2}} \int_{V} d^{3} r \int_{V} d^{3} r^{\prime} \frac{\rho(r) \rho\left(r^{\prime}\right)}{R}=-\frac{4}{3} \frac{\dot{\mathbf{u}}}{c^{2}} \frac{1}{8 \pi \varepsilon_{0}} \int_{V} d^{3} r \int_{V} d^{3} r^{\prime} \frac{\rho(r) \rho\left(r^{\prime}\right)}{R}=-\frac{4}{3 c^{2}} \dot{\mathbf{u}} U, \tag{10.149}
\end{equation*}
$$

This term may be interpreted as the inertial "force" $-m_{\mathrm{e} f} \mathbf{a}^{53}$ with the effective electromagnetic mass

$$
\begin{equation*}
m_{\mathrm{ef}}=\frac{4}{3} \frac{U}{c^{2}} \tag{10.150}
\end{equation*}
$$

This is the famous (or rather infamous :-) $4 / 3$ problem that does not allow to interpret the electron's mass as that of its electric field. The (admittedly, rather formal) resolution of this paradox is possible only in quantum electrodynamics with its renormalization techniques - beyond the framework of this course. Note that these issues are only important for motions with frequencies of the order of $1 / \tau$ $\sim 10^{23} \mathrm{~s}^{-1}$, i.e. at energies $\varepsilon \sim \hbar / \tau \sim 10^{-11} \mathrm{~J} \sim 10^{8} \mathrm{eV}$, while other quantum electrodynamics effects may be observed at much lower frequencies, starting from $\sim 10^{10} \mathrm{~s}^{-1}$. Hence the $4 / 3$ problem is by no means the only motivation for the transfer from classical to quantum electrodynamics.

However, the reader should not think that his or her time spent on this course has been lost: quantum electrodynamics incorporates virtually all classical electrodynamics results, and transition between them is surprisingly straightforward. ${ }^{54}$

### 10.6. Exercise problems

10.1. A point charge $q$ that had been in a stationary position on a circle of radius $R$, is carried over, along the circle, to the opposite position on the same diameter (see Fig. on the right) as fast as only physically possible, and then is kept steady at this new position. Calculate and sketch the time dependence of the
 electric field $\mathbf{E}$ at the center of the circle.

[^452]10.2. Express the total radiation power by a relativistic particle with the electric charge $q$ and the rest mass $m$, moving with velocity $\mathbf{u}$, via the external Lorentz force $\mathbf{F}$ exerted on the particle.
10.3. A relativistic particle with electric charge $q$, initially at rest, is accelerated by a constant force $\mathbf{F}$ until it reaches certain velocity $u$, and then moves by inertia. Calculate the total energy radiated during the acceleration.
10.4. ${ }^{*}$ Calculate the power spectrum of the radiation emitted by a relativistic particle with charge $q$, performing 1D harmonic oscillations with frequency $\omega$ and displacement amplitude $a$.
10.5. Analyze the polarization and the spectral contents of the synchrotron radiation in the direction propagating perpendicular to particle's rotation plane. How do the results change if not one, but $N>1$ similar particles move around the circle, at equal angular distances?
10.6. Calculate the time dependence of the kinetic energy of a charged relativistic particle performing synchrotron motion in a constant and uniform magnetic field $\mathbf{B}$, and hence emitting the synchrotron radiation. Sketch particle's trajectory.

Hint: You may assume that the energy loss is relatively slow $\left(-d \mathcal{E} / d t \ll \omega_{c} \mathcal{E}\right)$, but should spell out the condition of validity of this assumption.
10.7. Find the polarization of the synchrotron radiation propagating within particle's rotation plane.
10.8. The basic quantum theory of radiation shows ${ }^{55}$ that the electric dipole radiation by a particle is allowed only if its angular momentum change at the transition equals $\pm \hbar$.
(i) Estimate the change $\Delta L$ of the orbital momentum of an ultra-relativistic particle due to its emission of a single photon of the synchrotron radiation.
(ii) Does the quantum mechanics forbid such radiation? If not, why?
10.9. A relativistic particle moves along axis $z$, with velocity $u_{z}$, through an undulator - a system of permanent magnets providing (in the simplest model) a perpendicular magnetic field, whose distribution near axis $z$ is sinusoidal: ${ }^{56}$

$$
\mathbf{B}=\mathbf{n}_{y} B_{0} \cos k_{0} z .
$$

Assuming that the field is so weak that it causes only relatively small deviations of particle's trajectory from the straight line, calculate the angular distribution of the resulting radiation. What condition does this assumption impose on system's parameters?

[^453]10.10. Discuss possible effects of the interference of the undulator radiation from different periods of its static field distribution, in particular, calculate the angular positions of maxima of the radiation power density.
10.11. An electron, launched directly toward a plane surface of a perfect conductor, is instantly absorbed by it at the collision. Find the angular distribution and frequency spectrum of the electromagnetic waves radiated at this collision, if the initial kinetic energy $T$ of the particle is much larger than conductor's workfunction $\phi$. Give a semi-quantitative discussion of the limitations of your result.
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# Part QM: Quantum Mechanics 

Last corrections: 2019/05/08

A revised version of this material is now published by the IOP under the title
"Quantum Mechanics: Lecture notes"
(Essential Advanced Physics - Volume 5, ISBN 978-0-7503-1411-4),
with the model solutions of the exercise problems published under the title
"Quantum Mechanics: Problems with solutions"
(Essential Advanced Physics - Volume 6, ISBN 978-0-7503-1414-5)

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## Chapter 1. Introduction

This introductory chapter briefly reviews the major motivations for quantum mechanics. Then its simplest formalism - Schrödinger's wave mechanics - is described, and its main features are discussed Much of this material (perhaps except for the last section) may be found in undergraduate textbooks. ${ }^{1}$

### 1.1. Experimental motivations

By the beginning of the 1900s, physics (which by that time included what we now know as nonrelativistic classical mechanics, classical statistics and thermodynamics, and classical electrodynamics including geometric and wave optics) looked as an almost completed discipline, with a lot of experimental observations explained, and just a couple of mysterious "dark clouds" ${ }^{2}$ on the horizon. However, the rapid technological progress and the resulting fast development of experimental techniques have led to a fast multiplication of observed phenomena that could not be explained on the classical basis. Let me list the most consequential of those experimental findings.
(i) Blackbody radiation measurements, started by G. Kirchhoff in 1859, have shown that the in the thermal equilibrium, the power of electromagnetic radiation by a fully absorbing ("black") surface per unit frequency interval drops exponentially at high frequencies. This is not what could be expected from the combination of the classical electrodynamics and statistics, which predicted an infinite growth of the radiation density with frequency. Indeed, the classical electrodynamics shows ${ }^{3}$ that electromagnetic field modes in free space evolve in time as harmonic oscillators, and that the density of these modes in a large volume $V \gg \lambda^{3}$ per small frequency interval is

$$
\begin{equation*}
d N=2 V \frac{d V_{k}}{(2 \pi)^{3}}=2 V \frac{4 \pi k^{2} d k}{(2 \pi)^{3}}=V \frac{\omega^{2}}{\pi^{2} c^{3}} d \omega \tag{1.1}
\end{equation*}
$$

where $c \approx 3 \times 10^{8} \mathrm{~m} / \mathrm{s}$ is the free-space speed of light, $\omega$ its frequency, $k=\omega / c$ the free-space wave number, and $\lambda=2 \pi / k$ is the radiation wavelength. On the other hand, classical statistics ${ }^{4}$ predicts that in the thermal equilibrium at temperature $T$, the average energy $E$ of each 1D harmonic oscillator should equal $k_{\mathrm{B}} T$, where $k_{\mathrm{B}}$ is the Boltzmann constant. ${ }^{5}$

Combining these two results, we readily get the so-called Rayleigh-Jeans formula for the average electromagnetic wave energy per unit volume:

[^454]\[

$$
\begin{equation*}
u \equiv \frac{1}{V} \frac{d E}{d \omega}=\frac{k_{B} T}{V} \frac{d N}{d \omega}=\frac{\omega^{2}}{\pi^{2} c^{3}} k_{\mathrm{B}} T \tag{1.2}
\end{equation*}
$$

\]

that diverges at $\omega \rightarrow \infty$. On the other hand, the blackbody radiation measurements, improved by O . Lummer and E. Pringsheim, and also H. Rubens and F. Kurlbaum to reach a $1 \%$-scale accuracy, were compatible with the phenomenological law suggested in 1900 by Max Planck:

$$
\begin{equation*}
u=\frac{\omega^{2}}{\pi^{2} c^{3}} \frac{\hbar \omega}{\exp \left(\hbar \omega / k_{\mathrm{B}} T\right)-1} \tag{1.3a}
\end{equation*}
$$

The law may be reconciled with the fundamental Eq. (1) if the following replacement is made for the average energy of each field oscillator:

$$
\begin{equation*}
k_{\mathrm{B}} T \rightarrow \frac{\hbar \omega}{\exp \left(\hbar \omega / k_{\mathrm{B}} T\right)-1}, \tag{1.3b}
\end{equation*}
$$

with a constant factor

$$
\begin{equation*}
\hbar \approx 1.055 \times 10^{-34} \mathrm{~J} \cdot \mathrm{~s}, \tag{1.4}
\end{equation*}
$$

Planck's constant
now called Planck's constant. ${ }^{6}$ At low frequencies $\left(\hbar \omega \ll k_{\mathrm{B}} T\right.$ ), the denominator in Eq. (3) may be approximated as $\hbar \omega / k_{\mathrm{B}} T$, so that the average energy (3b) tends to its classical value $k_{\mathrm{B}} T$, and the Planck law (3a) reduces to the Rayleigh-Jeans formula (2). However, at higher frequencies ( $\hbar \omega \gg k_{\mathrm{B}} T$ ), Eq. (3) describes the experimentally observed rapid decrease of the radiation density - see Fig. 1.


Fig. 1.1. Blackbody radiation density $u$, expressed in units of $u_{0} \equiv\left(k_{\mathrm{B}} T\right)^{3} / \pi^{2} \hbar^{2} c^{3}$, as a function of frequency, according to: the Rayleigh-Jeans formula (blue line) and the Planck law (red line).
(ii) The photoelectric effect, experimentally discovered in 1887 by H. Hertz, shows a sharp lower bound on the frequency of light that may kick electrons out from metallic surfaces, regardless of the light intensity. Albert Einstein, in the first of his three famous 1905 papers, noticed that this

[^455]threshold $\omega_{\min }$ could be readily explained assuming that light consisted of certain particles (now called photons) with energy

with the same Planck's constant that participates in Eq. (3). ${ }^{7}$ Indeed, with this assumption, at the photon absorption by the surface, its energy $E=\hbar \omega$ is divided between a fixed energy $W$ (now called the workfunction) of electron binding inside the metal, and the residual kinetic energy $m v^{2} / 2>0$ of the freed electron - see Fig. 2. In this picture, the frequency threshold finds a natural explanation as $\omega_{\min }=W / \hbar .{ }^{8}$ Moreover, as was shown by S. Bose in 1924, Eq. (5) readily explains ${ }^{9}$ Planck's law (3).


Fig. 1.2. Einstein's explanation of the photoelectric effect's frequency threshold.
(iii) The discrete frequency spectra of radiation by excited atomic gases, known since the 1600 s , could not be explained by classical physics. (Applied to the planetary model of atoms, proposed by E. Rutherford, it predicts the collapse of electrons on nuclei in $\sim 10^{-10}$ s due to electric dipole radiation of electromagnetic waves. ${ }^{10}$ ) Especially challenging was the observation by J. Balmer (in 1885) that the radiation frequencies of simple atoms may be described by simple formulas. For example, for the simplest atom, hydrogen, all radiation frequencies may be numbered with just two positive integers $n$ and $n^{\prime}$ :

$$
\begin{equation*}
\omega_{n, n^{\prime}}=\omega_{0}\left(\frac{1}{n^{2}}-\frac{1}{n^{\prime 2}}\right) \tag{1.6}
\end{equation*}
$$

with $\omega_{0} \equiv \omega_{1, \infty} \approx 2.07 \times 10^{16} \mathrm{~s}^{-1}$. The Balmer series, including the value of $\omega_{0}$, have found its first explanation in the famous 1913 theory by Niels Bohr, which was a semi-phenomenological precursor for quantum mechanics. In this theory, $\omega_{n, n}$, is interpreted as the frequency of a photon that obeys the Einstein's formula (5), with its energy $E_{n, n}$, being the difference between two quantized (discrete) energy levels of the atom (Fig. 3):

$$
\begin{equation*}
E_{n, n^{\prime}}=E_{n^{\prime}}-E_{n}>0 . \tag{1.7}
\end{equation*}
$$

[^456]

Fig. 1.3. Electromagnetic wave radiation at system's transition between its two quantized energy levels.

Bohr showed that the correct ${ }^{11}$ expression for the levels (relative to the free electron energy),

$$
\begin{equation*}
E_{n}=-\frac{E_{\mathrm{H}}}{2 n^{2}}<0 \tag{1.8}
\end{equation*}
$$

and the correct value of the so-called Hartree energy ${ }^{12}$

$$
\begin{equation*}
E_{\mathrm{H}} \equiv 2 \hbar \omega_{0}=\frac{m_{e}}{\hbar^{2}}\left(\frac{e^{2}}{4 \pi \varepsilon_{0}}\right)^{2} \approx 27.2 \mathrm{eV}, \tag{1.9}
\end{equation*}
$$

(where $e \approx 1.602 \times 10^{-19} \mathrm{C}$ is the fundamental electric charge, and $m_{e} \approx 0.911 \times 10^{-30} \mathrm{~kg}$ is electron's rest mass) could be obtained, with a virtually one-line calculation, from the classical mechanics plus just one additional postulate, equivalent to the assumption that the angular momentum $L=m_{e} v r$ of the electron moving on a circular trajectory of radius $r$ about hydrogen's nuclei (i.e. proton, assumed to stay at rest), is quantized as

$$
\begin{equation*}
L=\hbar n \tag{1.10}
\end{equation*}
$$

where $\hbar$ is again the same Planck's constant (4), and $n$ is an integer. Indeed, in order to derive Eq. (8), it is sufficient to solve Eq. (10) together with the $2^{\text {nd }}$ Newton's law for the rotating electron,

$$
\begin{equation*}
m_{e} \frac{v^{2}}{r}=\frac{e^{2}}{4 \pi \varepsilon_{0} r^{2}}, \tag{1.11}
\end{equation*}
$$

for the electron velocity $v$ and radius $r$, and then plug the results into the non-relativistic expression for the full electron's energy

$$
\begin{equation*}
E=\frac{m_{e} v^{2}}{2}-\frac{e^{2}}{4 \pi \varepsilon_{0} r} . \tag{1.12}
\end{equation*}
$$

(This non-relativistic approach to the problem is justified a posteriori by the fact the relevant energy scale $E_{\mathrm{H}}$ is much smaller than electron's rest energy, $m_{e} c^{2} \sim 0.5 \mathrm{MeV}$.) By the way, the value of $r$, corresponding to $n=1$, i.e. to the smallest possible electron orbit,

$$
\begin{equation*}
r_{\mathrm{B}} \equiv \frac{\hbar^{2}}{m_{e}\left(e^{2} / 4 \pi \varepsilon_{0}\right)} \approx 0.053 \mathrm{~nm} \tag{1.13}
\end{equation*}
$$


#### Abstract

Bohr radius


[^457]and called the Bohr radius, defines the most important spatial scale of phenomena in atomic, molecular and condensed matter physics - as well as in chemistry and biochemistry.

Now note that the quantization postulate (10) may be presented as the condition than an integer number $(n)$ of certain waves ${ }^{13}$ fits the circular orbit's perimeter $2 \pi r=n \lambda$. Dividing both parts of this relation by $\lambda$, we see that for this statement to be true, the wave number $k \equiv 2 \pi / \lambda$ of the (then hypothetic) de Broglie waves should be proportional to electron's momentum $p=m v$ :

$$
\begin{equation*}
p=\hbar k \tag{1.14}
\end{equation*}
$$

(iv) The Compton effect ${ }^{14}$ is the reduction of frequency of X-rays at their scattering on free (or nearly-free) electrons - see Fig. 4.


Fig. 1.4. Compton effect.

The effect may be explained assuming that the X-ray photon also has a momentum that obeys the vector-generalized version of Eq. (14):

$$
\begin{equation*}
\mathbf{p}_{\text {photon }}=\hbar \mathbf{k}=\frac{\hbar \omega}{c} \mathbf{n}, \tag{1.15}
\end{equation*}
$$

where $\mathbf{k}$ is the wavevector (whose magnitude is equal to the wave number $k$, and direction coincides with that, $\mathbf{n}$, of the wave propagation), and that momenta $\mathbf{p}$ of both the photon and the electron are related to their energies $E$ by the classical relativistic formula ${ }^{15}$

$$
\begin{equation*}
E^{2}=(c p)^{2}+\left(m c^{2}\right)^{2} \tag{1.16}
\end{equation*}
$$

(For a photon, the rest energy is zero, and this relation is reduced to Eq. (5): $E=c p=c \hbar k=\hbar \omega$.) Indeed, a straightforward solution of the following system of three equations,

$$
\begin{align*}
\hbar \omega+m_{e} c^{2} & =\hbar \omega^{\prime}+\left[(c p)^{2}+\left(m_{e} c^{2}\right)^{2}\right]^{1 / 2},  \tag{1.17}\\
\frac{\hbar \omega}{c} & =\frac{\hbar \omega^{\prime}}{c} \cos \theta+p \cos \varphi,  \tag{1.18}\\
0 & =\frac{\hbar \omega^{\prime}}{c} \sin \theta-p \sin \varphi, \tag{1.19}
\end{align*}
$$

[^458](which describe, respectively, the conservation of the full energy of the photon-electron system, and of two relevant Cartesian components of its full momentum, at the scattering event - see Fig. 4), yields the following result,
\[

$$
\begin{equation*}
\frac{1}{\hbar \omega^{\prime}}=\frac{1}{\hbar \omega}+\frac{1}{m_{e} c^{2}}(1-\cos \theta), \tag{1.20a}
\end{equation*}
$$

\]

which is traditionally represented as the relation between the initial and final values of photon's wavelength $\lambda=2 \pi / k=2 \pi /(\omega / c)$ :

$$
\begin{equation*}
\lambda^{\prime}=\lambda+\frac{2 \pi \hbar}{m_{e} c}(1-\cos \theta)=\lambda+\lambda_{c}(1-\cos \theta), \quad \text { with } \lambda_{c} \equiv \frac{2 \pi \hbar}{m_{e} c}, \tag{1.20b}
\end{equation*}
$$

and is in agreement with experiment. ${ }^{16}$
(v) De Broglie wave diffraction. In 1927, following the suggestion by W. Elassger (who was excited by de Broglie's conjecture of "matter waves"), C. Davisson and L. Germer, and independently G. Thomson succeeded to observe diffraction of electrons on crystals (Fig. 5). Specifically, they have found that the intensity of the elastic reflection from a crystal increases sharply when angle $\theta$ between the incident beam of electrons and crystal's atomic planes, separated by distance $d$, satisfies the following relation:

$$
\begin{equation*}
2 d \sin \theta=n \lambda \tag{1.21}
\end{equation*}
$$

where $\lambda=2 \pi / k=2 \pi \hbar / p$ is the de Broglie wavelength of electrons, and $n$ is an integer. As Fig. 5 shows, this is just the well-known condition ${ }^{17}$ that the optical path difference $\Delta l=2 d \sin \theta$ between the de Broglie waves reflected from two adjacent crystal planes coincides with an integer number of $\lambda$, i.e. of the constructive interference of the waves. ${ }^{18}$


Fig. 1.5. Electron scattering from a crystal lattice.
${ }^{16}$ The constant $\lambda_{c}$, which participates in this relation, is close to $2.46 \times 10^{-12} \mathrm{~m}$ and is called the Compton wavelength of the electron. This term is somewhat misleading: as the reader can see from Eqs. (17)-(19), no wave in the Compton problem has such a wavelength - either before or after the scattering.
${ }^{17}$ Frequently called the Bragg condition, due to the pioneering experiments by W. Bragg with X-ray scattering from crystals (that started in 1912).
${ }^{18}$ Later, spectacular experiments with diffraction and interference of heavier particles, e.g., neutrons and even $\mathrm{C}_{60}$ molecules, have also been performed - see, e.g., a review by A. Zeilinger et al., Rev. Mod. Phys. 60, 1067 (1988) and a later publication by O. Nairz et al., Am. J. Phys. 71, 319 (2003). Nowadays, such interference of heavy particles is used for ultrasensitive measurements of gravity - see, e.g., a popular review by M. Arndt, Phys. Today 67, 30 (May 2014), and recent advanced experiments by P. Hamilton et al., Phys. Rev. Lett. 114, 100405 (2015). Moreover, quantum interference between different parts and different quantum states of such macroscopic objects as superconducting condensates of millions Cooper pairs has been observed - see Sec. 3.1 below for details.

To summarize, all the listed effects may be explained starting from two very simple (and similarly looking) formulas: Eq. (5) for photons, and Eq. (15) for both photons and electrons - both relations involving the same Planck's constant. This might give an impression of sufficient experimental evidence to declare light consisting of discrete particles (photons), and, on the contrary, electrons being some "matter waves" rather than particles. However, by that time (the mid 1920s) physics has accumulated overwhelming evidence of wave properties of light, such as interference and diffraction. In addition, there was also a strong evidence for lumped-particle ("corpuscular") behavior of electrons. It is sufficient to mention the famous oil-drop experiments by R. Millikan and H. Fletcher (1909-1913) in that only single (and whole!) electrons could be added to an oil drop, changing its total electric charge by multiples of electron's charge ( $-e$ ) - and never its fraction. It was apparently impossible to reconcile these observations with a purely wave picture, in which an electron and hence its charge need to be spread over the wave, so that its arbitrary part of it could be cut out using appropriate experimental setups.

Thus the founding fathers of quantum mechanics faced a formidable task of reconciling the wave and corpuscular properties of electrons and photons - and other particles. The decisive breakthrough in that task has been achieved in 1926 by Ervin Schrödinger and Max Born who formulated what is now known as either the Schrödinger picture of non-relativistic quantum mechanics in the coordinate representation, or simply as wave mechanics. I will now formulate that picture, somewhat disregarding the actual history of its development.

### 1.2. Wave mechanics postulates

Let us consider a spinless, ${ }^{19}$ non-relativistic point-like particle whose classical dynamics may be described by a certain Hamiltonian function $H(\mathbf{r}, \mathbf{p}, t),{ }^{20}$ where $\mathbf{r}$ is particle's radius-vector and $\mathbf{p}$ is coordinate. ${ }^{21}$ Wave mechanics of such Hamiltonian particles may based on the following set of postulates ${ }^{22}$ that are comfortingly elegant - though their final justification is given only by the agreement of all their corollaries with experiment.
(i) Wavefunction and probability. Such variables as $\mathbf{r}$ or $\mathbf{p}$ cannot be always measured exactly, even at "perfect conditions" when all external uncertainties, including measurement instrument imperfection, macroscopic fluctuations of the initial state preparation, and unintended particle interactions with its environment, have been removed. ${ }^{23}$ Moreover, $\mathbf{r}$ and $\mathbf{p}$ of the same particle can

[^459]never be measured exactly simultaneously. Instead, even the most detailed description of the particle's state, allowed by Nature, ${ }^{24}$ is given by a certain complex function $\Psi(\mathbf{r}, t)$, called the wavefunction, that generally enables only probabilistic predictions of measured values of $\mathbf{r}, \mathbf{p}$, and other directly measurable variables (in quantum mechanics, called observables).

Specifically, the probability $d W$ of finding a particle inside an infinitesimal volume $d V \equiv d^{3} r$ is proportional to this volume and may be characterized by the probability density $w \equiv d W / d^{3} r$ that in turn is related to the wavefunction as

$$
\begin{equation*}
w=|\Psi(\mathbf{r}, t)|^{2} \equiv \Psi^{*}(\mathbf{r}, t) \Psi(\mathbf{r}, t) \tag{1.22a}
\end{equation*}
$$

where sign * means the complex conjugate. As a result, the total probability of finding the particle somewhere inside a volume $V$ may be calculated as

$$
\begin{equation*}
W=\int_{V} w d^{3} r=\int_{V} \Psi^{*} \Psi d^{3} r \tag{1.22b}
\end{equation*}
$$

In particular, if the volume $V$ contains the particle definitely (i.e. with the $100 \%$ probability, $W=1$ ), Eq. (22b) is reduced to the so-called normalization condition

$$
\begin{equation*}
\int_{V} \Psi^{*} \Psi d^{3} r=1 \tag{1.22c}
\end{equation*}
$$

(ii) Observables and operators. To each observable $A$, quantum mechanics associates a certain linear operator $\hat{A}$, such that, in the perfect conditions mentioned above, the average measured value (also called the expectation value) of $A$ is expressed as ${ }^{25}$

$$
\begin{equation*}
\langle A\rangle=\int_{V} \Psi^{*} \hat{A} \Psi d^{3} r, \tag{1.23}
\end{equation*}
$$

where $\langle\ldots\rangle$ means the statistical average, i.e. the result of averaging the measurement results over a large ensemble (set) of macroscopically similar experiments, and $\Psi$ is the normalized wavefunction - see Eq. (22c). For Eqs. (22) and (23) to be compatible, the identity ("unit") operator $\hat{I}$, defined by relation

$$
\begin{equation*}
\hat{I} \Psi=\Psi \tag{1.24}
\end{equation*}
$$

has to be associated with a particular type of measurement, namely with particle's detection.
(iii) Hamiltonian operator and the Schrödinger equation. Another particular operator, the Hamiltonian $\hat{H}$, whose observable is the particle's energy $E$, also plays in wave mechanics a very special role, because it participates in the Schrödinger equation,

$$
\begin{equation*}
i \hbar \frac{\partial \Psi}{\partial t}=\hat{H} \Psi \tag{1.25}
\end{equation*}
$$

[^460]that determines wavefunction's dynamics, i.e. its time evolution.
(iv) Radius-vector and momentum operators. In the coordinate representation accepted in wave mechanics, the (vector) operator of particle's radius-vector $\mathbf{r}$ just multiples the wavefunction by this

Operators of coordinate and momentum vector, while the operator of particle's momentum ${ }^{26}$ is represented by the spatial derivative:

$$
\begin{equation*}
\hat{\mathbf{p}}=-i \hbar \nabla, \tag{1.26a}
\end{equation*}
$$

where $\nabla$ is the del (or "nabla") vector operator. ${ }^{27}$ Thus in the Cartesian coordinates,

$$
\begin{equation*}
\hat{\mathbf{r}}=\mathbf{r}=\{x, y, z\}, \quad \hat{\mathbf{p}}=-i \hbar\left\{\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right\} \tag{1.26b}
\end{equation*}
$$

(v) Correspondence principle. In the limit when quantum effects are insignificant, e.g., when the characteristic scale of action $S^{28}$ (i.e. the product of the relevant energy and time scales of the problem) is much larger than Planck's constant $\hbar$, all wave mechanics results have to tend to those given by classical mechanics. Mathematically, the correspondence is achieved by duplicating the classical relations between observables by similar relations between the corresponding operators. For example, for a free particle, the Hamiltonian (that in this case corresponds to the kinetic energy alone) has the form

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}=-\frac{\hbar^{2}}{2 m} \nabla^{2}, \tag{1.27a}
\end{equation*}
$$

Free
particle's Hamiltonian
so that, taking into account Eq. (26b), in the Cartesian coordinates,

$$
\begin{equation*}
\hat{H}=-\frac{\hbar^{2}}{2 m}\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial z^{2}}\right) \tag{1.27b}
\end{equation*}
$$

Even before a discussion of physics of the postulates (offered in the next section), we may immediately see that they indeed provide a way toward the resolution of the apparent contradiction between the wave and corpuscular properties of particles. For a free particle, the Schrödinger equation (25), with the substitution of Eq. (27), takes the form

$$
\begin{equation*}
i \hbar \frac{\partial \Psi}{\partial t}=-\frac{\hbar^{2}}{2 m} \nabla^{2} \Psi \tag{1.28}
\end{equation*}
$$

whose particular (but most important) solution is a plane, monochromatic wave, ${ }^{29}$

$$
\begin{equation*}
\Psi(\mathbf{r}, t)=a e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)} \tag{1.29}
\end{equation*}
$$

[^461]where $a$, $\mathbf{k}$ and $\omega$ are constants. Indeed, plugging Eq. (29) into Eq. (28), we immediately see the plane wave, with an arbitrary amplitude $a$, is indeed a solution of the Schrödinger equation, provided a specific dispersion relation between wavevector $\mathbf{k}$ and frequency $\omega$ :
\[

$$
\begin{equation*}
\hbar \omega=\frac{(\hbar k)^{2}}{2 m} \tag{1.30}
\end{equation*}
$$

\]

Constant $a$ may be calculated, for example, assuming that solution (29) is extended over a certain volume $V$, while beyond it, $\Psi=0$. Then from the normalization condition (22c) and Eq. (29), we get ${ }^{30}$

$$
\begin{equation*}
|a|^{2} V=1 \tag{1.31}
\end{equation*}
$$

Now we can use Eqs. (23), (26) and (27) to calculate the expectation value of particle's momentum $\mathbf{p}$ and energy $E$ (which, for a free particle, coincides with its Hamiltonian function $H$ ), The result is

$$
\begin{equation*}
\langle\mathbf{p}\rangle=\hbar \mathbf{k}, \quad\langle E\rangle=\langle H\rangle=\frac{(\hbar k)^{2}}{2 m} \tag{1.32}
\end{equation*}
$$

according to Eq. (30), the last equality may be rewritten as $\langle E\rangle=\hbar \omega$.
Next, Eq. (23) enables one to calculate not only the statistical average (in the math speak, the first moment) of an observable, but also its higher moments, notably the second moment (in physics, usually called either the variance or dispersion):

$$
\begin{equation*}
\left\langle\widetilde{A}^{2}\right\rangle \equiv\left\langle(A-\langle A\rangle)^{2}\right\rangle=\left\langle A^{2}\right\rangle-\langle A\rangle^{2}, \tag{1.33}
\end{equation*}
$$

and hence its root mean square (r.m.s.) fluctuation,

$$
\begin{equation*}
\delta A \equiv\left\langle\tilde{A}^{2}\right\rangle^{1 / 2} \tag{1.34}
\end{equation*}
$$

Observable's variance
that characterizes the scale of deviations $\widetilde{A} \equiv A-\langle A\rangle$ of measurement results from the average, i.e. the uncertainty of observable $A$. In application to wavefunction (29), these relations yield $\delta E=0, \delta \mathbf{p}=0$, while the particle coordinate $\mathbf{r}($ at $V \rightarrow \infty)$ is completely uncertain. This means that in the plane-wave, monochromatic state (29), the energy and momentum of the particle are exactly defined, so that the signs of statistical average in Eqs. (32) might be removed. Thus, these relations are reduced to the experimentally-inferred Eqs. (5) and (15), though the relation of frequency $\omega$ of wavefunction's evolution in time to experimental observations still has to be clarified.

Hence the wave mechanics postulates may indeed explain the observed wave properties of nonrelativistic particles. (For photons, we would need a relativistic formalism - see Ch. 9 below.) On the other hand, due to the linearity of the Schrödinger equation (25), any sum of its solutions is also a solution - the so-called linear superposition principle. For a free particle, this means that a set of plane waves (29) is also a solution of this equation. Such sets, with close values of $\mathbf{k}$ and hence $\mathbf{p}=\hbar \mathbf{k}$ (and, according to Eq. (30), of $\omega$ as well), may be used to describe spatially localized "pulses", called wave packets - see Fig. 6. In Sec. 2.1, I will prove (or rather reproduce H. Weyl's proof :-) that the wave

[^462]packet extension $\delta x$ in any direction (say, $x$ ) is related to the width $\delta k_{x}$ of the corresponding component of its wave vector distribution as $\delta x \delta k_{x} \geq 1 / 2$, and hence, according to Eq. (15), to the width $\delta p_{x}$ of the momentum component distribution as
 relation
\[

$$
\begin{equation*}
\delta x \cdot \delta p_{x} \geq \frac{\hbar}{2} \tag{1.35}
\end{equation*}
$$

\]


(b)

Fig. 1.6. (a) Snapshot of a typical wave packet propagating along axis $x$, and (b) the corresponding distribution of wave numbers $k_{x}$, i.e. momenta $p_{x}$.

This is the famous the famous Heisenberg's uncertainty principle, which quantifies the first postulate's point that coordinate and momentum cannot be defined exactly simultaneously. However, since the Planck's constant is extremely small on the human scale of things, it still allows for the particle's localization in a very small volume even if the momentum spread in the wave packet is also small on that scale. For example, according to Eq. (35), a $0.1 \%$ spread of momentum of a 1 keV electron ( $p \sim 1.7 \times 10^{-24} \mathrm{~kg} \cdot \mathrm{~m} / \mathrm{s}$ ) allows a wave packet to be as small as $\sim 3 \times 10^{-10} \mathrm{~m}$. (For a heavier particle such as a proton, the packet would be even tighter.) As a result, wave packets may be used to describe particles that are point-like from the macroscopic point of view.

In a nutshell, this is the main idea of the wave mechanics, and the first part of this course (Chapters 1-3) will be essentially a discussion of various manifestations of this approach. During this discussion, we will not only evidence wave mechanics' many triumphs within its applicability domain, but will also gradually accumulate evidence for its handicaps, which force the eventual transfer to a more general formalism - to be discussed in Chapter 4 and beyond.

### 1.3. Postulates' discussion

The postulates listed in the previous section look very simple, and they are hopefully familiar to the reader from his or her undergraduate studies. However, the physics of these axioms are very deep, they lead to several counter-intuitive conclusions, and their in-depth discussion requires solutions of several key problems using these axioms. This is why in this section I will give only an initial, admittedly superficial discussion of the postulates, and will be repeatedly returning to the conceptual foundations of quantum mechanics throughout the course, especially in Secs. 7.7, 10.1, and 10.2.

First of all, the fundamental uncertainty of observables, which is in the core of postulate (i), is very foreign to the basic ideas of classical mechanics, and historically has made quantum mechanics so hard to swallow for many star physicists, notably including A. Einstein - despite his 1905 work which essentially launched the whole field! However, this fact has been confirmed by numerous experiments,
and (more importantly) there have not been a single confirmed experiment which would contradict to this postulate, so that quantum mechanics was long ago promoted from a theoretical hypothesis to the rank of a reliable scientific theory.

One more remark in this context is that Eq. (25) itself is deterministic, i.e. conceptually enables an exact calculation of wavefunction's distribution in space at any instant $t$, provided that its initial distribution, and particle's Hamiltonian, are known exactly. In classical kinetics, the probability density distribution $w(\mathbf{r}, t)$ may be also calculated from deterministic differential equations, e.g., the FokkerPlanck equation or the Boltzmann equation. ${ }^{31}$ The quantum-mechanical description differs from those situations in two important aspects. First, in the perfect conditions outlined above (exact initial state preparation, no irreversible interaction with environment, the best possible measurement), the FokkerPlanck equation reduces to the $2^{\text {nd }}$ Newton law, i.e. the statistical uncertainty disappears. In quantum mechanics this is not true: the quantum uncertainly, such as Eq. (35), persists even in this limit. Second, the wavefunction $\Psi(\mathbf{r}, t)$ gives more information than just $w(\mathbf{r}, t)$, because besides the modulus of $\Psi$, involved in Eq. (22), this complex function also has phase $\varphi \equiv \arg \Psi$, and may affect some observables, describing, in particular, the interference and diffraction of the de Broglie waves.

Next, it is very important to understand that the relation between the quantum mechanics to experiment, given by postulate (ii), necessarily involves another key notion: that of the corresponding statistical ensemble. Such ensemble may be defined as a set of many experiments carried out at apparently (macroscopically) similar conditions, which nevertheless may lead to different measurement results (outcomes). Indeed, the probability of a certain ( $n$-th) outcome of an experiment may be only defined for a certain ensemble, as the limit

$$
\begin{equation*}
W_{n} \equiv \lim _{M \rightarrow \infty} \frac{M_{n}}{M}, \quad \text { with } M \equiv \sum_{n=1}^{N} M_{n} \tag{1.36}
\end{equation*}
$$

where $M$ is the total number of experiments, $M_{n}$ is the number of outcomes of the $n$-th type, and $N$ is the number of different outcomes. It is clear that a particular choice of an ensemble may affect probabilities $W_{n}$ very significantly.

For example, if we pull out playing cards at random from a pack of 52 different cards of 4 suits, the probability $W_{n}$ of getting a certain card (e.g., the queen of spades) is $1 / 52$. However, if cards of a certain suit (say, hearts) had been taken out from the pack in advance, the probability of getting the queen of spades is higher, $1 / 39$. It is important that we would also get the last number for probability even if we had used the full 52 -card pack, but by some reason ignored results of all experiments giving us any rank of hearts.

Similarly, in quantum mechanics, the probability distributions (and hence expectation values of particle coordinate and other observables) depend not only on the experiment setup, but also on the set of outcomes we count. Because of the fundamental relation (22) between $w$ and $\Psi$, this means the wavefunction also depends on those factors, i.e. on both the experiment set preparation and the subset of outcomes taken into account. The insistence on the attribution of the wavefunction to a single experiment, both before and after the measurement, may lead to very unphysical interpretations of some experiments, including wavefunction's evolution not described by the Schrödinger equation (the socalled wave packet reduction), subluminal action on distance, etc. Later in the course we will see that minding the statistical nature of the quantum mechanics, and in particular the dependence of the

[^463]wavefunction on statistical ensemble's specification, may readily explain some apparent paradoxes of quantum measurements.

Let me also emphasize that statistics is intimately related to the information theory - and not only via their common mathematical background, the probability theory. For example, the question, "What subset of experimental results we will count?" may be replaced by the question, "What subset of results will we use information about?" As a result, the reader has to be prepared to the use of information theory notions for the discussion quantum mechanics, or at least its relation to experiment - i.e. to the "physical reality". This feature of quantum mechanics makes some physicists uncomfortable, because much of classical mechanics and electrodynamics may be discussed without any reference to information. In quantum mechanics (as in statistical mechanics), such an abstraction is impossible.

Proceeding to postulate (ii) and in particular Eq. (23), a better feeling of this definition may be obtained by its comparison with the general definition of the expectation value (i.e. the statistical average) in the probability theory. Namely, let each of $N$ possible outcomes in a set of $M$ macroscopically similar experiments give a certain value $A_{n}$ of observable $A$; then

Definition of statistical average

$$
\begin{equation*}
\langle A\rangle \equiv \lim _{M \rightarrow \infty} \frac{1}{M} \sum_{n=1}^{N} A_{n} M_{n}=\sum_{n=1}^{N} A_{n} W_{n} . \tag{1.37}
\end{equation*}
$$

Taking into account Eq. (22), which relates $W$ and $\Psi$, the structure of Eq. (23) and the final form of Eq. (37) is similar. Their exact relation will be further discussed in Sec. 4.1.

### 1.4. Continuity equation

The wave mechanics postulates survive one more sanity check: they satisfy the natural requirement that the particle does not appear or vanish in the course of the quantum evolution. ${ }^{32}$ Indeed, let us use Eq. (22) to calculate the rate of change of the probability $W$ to find the particle within a certain volume $V$ :

$$
\begin{equation*}
\frac{d W}{d t}=\frac{d}{d t} \int_{V} \Psi \Psi^{*} d^{3} r \tag{1.38}
\end{equation*}
$$

Assuming for simplicity that the boundaries of volume $V$ do not move, it is sufficient to carry out the partial differentiation of the product $\Psi \Psi^{*}$ inside the integral. Using the time-dependent Schrödinger equation (25), together with its complex conjugate,

$$
\begin{equation*}
-i \hbar \frac{\partial \Psi^{*}}{\partial t}=(\hat{H} \Psi)^{*} \tag{1.39}
\end{equation*}
$$

we get

$$
\begin{equation*}
\frac{d W}{d t}=\int_{V} \frac{\partial}{\partial t}\left(\Psi \Psi^{*}\right) d^{3} r=\int_{V}\left(\Psi^{*} \frac{\partial \Psi}{\partial t}+\Psi \frac{\partial \Psi^{*}}{\partial t}\right) d^{3} r=\frac{1}{i \hbar} \int_{V}\left[\Psi^{*}(\hat{H} \Psi)-\Psi(\hat{H} \Psi)^{*}\right] d^{3} r . \tag{1.40}
\end{equation*}
$$

[^464]Let the particle move in a field of external forces (not necessarily constant in time), so that its classical Hamiltonian function $H$ is a sum of particle's kinetic energy $p^{2} / 2 m$ and its potential energy $U(\mathbf{r}$, $t) .{ }^{33}$ According to the correspondence principle, the Hamiltonian operator may be presented as the sum ${ }^{34,}$

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}+U(\mathbf{r}, t)=-\frac{\hbar^{2}}{2 m} \nabla^{2}+U(\mathbf{r}, t) \tag{1.41}
\end{equation*}
$$

At this stage we should notice that such operator, when acting on a real function, returns a real function. ${ }^{35}$ Hence, the result of its action on an arbitrary complex function $\Psi=a+i b$ (where $a$ and $b$ are real) is

$$
\begin{equation*}
\hat{H} \Psi=\hat{H}(a+i b)=\hat{H} a+i \hat{H} b \tag{1.42}
\end{equation*}
$$

where $\hat{H} a$ and $\hat{H} b$ are also real, while

$$
\begin{equation*}
(\hat{H} \Psi)^{*}=(\hat{H} a+i \hat{H} b)^{*}=\hat{H} a-i \hat{H} b=\hat{H}(a-i b)=\hat{H} \Psi^{*} . \tag{1.43}
\end{equation*}
$$

This means that Eq. (40) may be rewritten as

$$
\begin{equation*}
\frac{d W}{d t}=\frac{1}{i \hbar} \int_{V}\left[\Psi^{*} \hat{H} \Psi-\Psi \hat{H} \Psi^{*}\right] d^{3} r=-\frac{\hbar^{2}}{2 m} \frac{1}{i \hbar} \int_{V}\left[\Psi^{*} \nabla^{2} \Psi-\Psi \nabla^{2} \Psi^{*}\right] d^{3} r \tag{1.44}
\end{equation*}
$$

Now, let us use general rules of vector calculus ${ }^{36}$ to write the following identity:

$$
\begin{equation*}
\nabla \cdot\left(\Psi^{*} \nabla \Psi-\Psi \nabla \Psi^{*}\right)=\Psi^{*} \nabla^{2} \Psi-\Psi \nabla^{2} \Psi^{*} \tag{1.45}
\end{equation*}
$$

A comparison of Eqs. (44) and (45) shows that we may write

$$
\begin{equation*}
\frac{d W}{d t}=-\int_{V}(\nabla \cdot \mathbf{j}) d^{3} r \tag{1.46}
\end{equation*}
$$

where vector $\mathbf{j}$ is defined as

$$
\begin{equation*}
\mathbf{j} \equiv \frac{i \hbar}{2 m}\left(\Psi \nabla \Psi^{*}-\text { c.c. }\right)=\frac{\hbar}{m} \operatorname{Im}\left(\Psi^{*} \nabla \Psi\right), \tag{1.47}
\end{equation*}
$$

Probability
current density

[^465]Hamiltonian of a particle in a field
where $j_{n}$ is the projection of vector $\mathbf{j}$ on the outwardly directed normal to surface $S$ that limits volume $V$, i.e. the scalar product $\mathbf{j} \cdot \mathbf{n}$, where $\mathbf{n}$ is the unit vector along this normal.

Equations (47) and (48) show that if the wavefunction on the surface vanishes, the total probability $W$ of finding the particle within the volume does not change, providing the required sanity check. In the general case, Eq. (48) says that $d W / d t$ equals to flux $I$ of vector $\mathbf{j}$ through the surface, with the minus sign. It is clear that this vector may be interpreted as the probability current density - and $I$, as the total probability current through surface $S$. This interpretation may be further supported by rewriting Eq. (47) for a wavefunction presented in the polar form $\Psi=a e^{i \varphi}$, with real $a$ and $\varphi$ :

$$
\begin{equation*}
\mathbf{j}=a^{2} \frac{\hbar}{m} \nabla \varphi \tag{1.49}
\end{equation*}
$$

- evidently a real quantity. Note that for a real wavefunction, or even for that with an arbitrary but spaceconstant phase $\varphi$, the probability current density vanishes. On the contrary, for the traveling wave (29), with a constant probability density $w=a^{2}$, Eq. (49) yields a nonvanishing (and physically very transparent) result:

$$
\begin{equation*}
\mathbf{j}=w \frac{\hbar}{m} \mathbf{k}=w \frac{\mathbf{p}}{m}=w \mathbf{v} \tag{1.50}
\end{equation*}
$$

where $\mathbf{v}=\mathbf{p} / m$ is particle's velocity. If multiplied by the particle's mass $m$, the probability density $w$ turns into the (average) mass density $\rho$, and the probability current density into the mass flux density $\rho \mathbf{v}$, while if multiplied by the total electric charge $q$ of the particle, with $w$ turning into the charge density $\sigma$, j becomes the electric current density, both satisfying the classical continuity equations similar to Eq. (48). ${ }^{38}$

Finally, let us recast the continuity equation, rewriting Eq. (46) as

$$
\begin{equation*}
\int_{V}\left(\frac{\partial w}{\partial t}+\nabla \cdot \mathbf{j}\right) d^{3} r=0 \tag{1.51}
\end{equation*}
$$

Now we may argue that this equality may is true for any choice of volume $V$ only if the expression under the integral vanishes everywhere, i.e. if

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\nabla \cdot \mathbf{j}=0 \tag{1.52}
\end{equation*}
$$

This differential form of the continuity equation is sometimes more convenient than its integral form (48).

### 1.5. Eigenstates and eigenvalues

Now let us discuss important corollaries of wave mechanics' linearity. First of all, it uses only linear operators. This term means that the operators must obey the following two rules: ${ }^{39}$

[^466]\[

$$
\begin{gather*}
\left(\hat{A}_{1}+\hat{A}_{2}\right) \Psi=\hat{A}_{1} \Psi+\hat{A}_{2} \Psi  \tag{1.53}\\
\hat{A}\left(c_{1} \Psi_{1}+c_{2} \Psi_{2}\right)=\hat{A}\left(c_{1} \Psi_{1}\right)+\hat{A}\left(c_{2} \Psi_{2}\right)=c_{1} \hat{A} \Psi_{1}+c_{2} \hat{A} \Psi_{2} \tag{1.54}
\end{gather*}
$$
\]

where $\Psi_{n}$ are arbitrary wavefunctions, while $c_{n}$ are arbitrary constants (in quantum mechanics, frequently called c-numbers, to distinguish them from operators and wavefunctions). Most important examples of linear operators are given by:
(i) the multiplication by a function, such as for operator $\hat{\mathbf{r}}$ in wave mechanics, and
(ii) the spatial or temporal differentiation of the wavefunction, such as in Eqs. (25)-(27).

Next, it is of key importance that the Schrödinger equation (25) is also linear. (We have already used this fact when we discussed wave packets in the last section.) This means that if each of functions $\Psi_{n}$ are (particular) solutions of Eq. (25) with a certain Hamiltonian, then an arbitrary linear combination

$$
\begin{equation*}
\Psi=\sum_{n} c_{n} \Psi_{n} \tag{1.55}
\end{equation*}
$$

is also a solution of the same equation. ${ }^{40}$
Now let us use the linearity of wave mechanics to accomplish an apparently impossible feat: immediately find the general solution to the Schrödinger equation for the most important case when system's Hamiltonian does not depend on time explicitly - for example, like in Eq. (27), or in Eq. (41) with time-independent $U=U(\mathbf{r})$. First of all, let us prove that the following product,

$$
\Psi_{n}=T_{n}(t) \psi_{n}(\mathbf{r}),
$$

qualifies as a (particular) solution to the Schrödinger equation. Indeed, plugging Eq. (56) into Eq. (25), using the fact that for a time-independent Hamiltonian

$$
\begin{equation*}
\hat{H} T_{n}(t) \psi_{n}(\mathbf{r})=T_{n}(t) \hat{H} \psi_{n}(\mathbf{r}), \tag{1.57}
\end{equation*}
$$

and dividing both parts of the equation by $\Psi_{n}=T_{n} \psi_{n}$, we get

$$
\begin{equation*}
\frac{i \hbar \dot{T}_{n}}{T_{n}}=\frac{\hat{H} \psi_{n}}{\psi_{n}} \tag{1.58}
\end{equation*}
$$

where (here and below) the dot denotes the differentiation over time. The left hand side of this equation may depend only on time, while the right hand one, only on coordinates. These facts may be only reconciled if we assume that each of these parts is equal to (the same) constant of the dimension of energy, which I will denote as $E_{n} .{ }^{41}$ As a result, we are getting two separate equations for the temporal and spatial parts of the wavefunction:

$$
\begin{equation*}
i \hbar \dot{T}_{n}=E_{n} T_{n} \tag{1.59}
\end{equation*}
$$

[^467]Stationary
Schrödinger equation

Stationary state:
evolution

$$
\begin{equation*}
\hat{H} \psi_{n}=E_{n} \psi_{n} \tag{1.60}
\end{equation*}
$$

The first of these equations is readily integrable, giving

$$
\begin{equation*}
T_{n}=\text { const } \times \exp \left\{-i \omega_{n} t\right\}, \quad \text { with } \omega_{n} \equiv \frac{E_{n}}{\hbar}, \tag{1.61}
\end{equation*}
$$

and thus substantiating the fundamental relation (5) between energy and frequency. Plugging Eqs. (56) and (61) into Eq. (22), we see that in such a state, the probability $w$ of finding the particle at a certain location does not depend on time. Doing the same with Eq. (23) shows that the same is true for the expectation value of any operator that does not depend on time explicitly:

$$
\begin{equation*}
\langle A\rangle_{n} \equiv \int \psi_{n}^{*} \hat{A} \psi_{n} d^{3} r=\text { const. } \tag{1.62}
\end{equation*}
$$

Due to this property, the states described by Eqs. (56), (60), and (61), are called stationary. In contrast to the simple and universal time dependence (61), the spatial distributions $\psi_{n}(\mathbf{r})$ of the stationary states are often hard to find, and the solution of the stationary (or "time-independent") Schrödinger equation (60), ${ }^{42}$ which describes the distributions, for various situations is a major focus of wave mechanics.

The stationary Schrödinger equation (60), with time-independent Hamiltonian (41),

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi_{n}+U(\mathbf{r}) \psi_{n}=E_{n} \psi_{n} \tag{1.63}
\end{equation*}
$$

falls into the mathematical category of linear eigenproblems, ${ }^{43}$ in which eigenfunctions $\psi_{n}$ and eigenvalues $E_{n}$ should be found simultaneously - self-consistently. ${ }^{44}$ Mathematics tells us that for the such problems with space-confined eigenfunctions $\psi_{n}$, tending to zero at $r \rightarrow \infty$, the spectrum of eigenvalues is discrete. It also proves that the eigenfunctions corresponding to different eigenvalues are orthogonal, i.e. that space integrals of the products $\psi_{n} \psi^{*}{ }_{n}$, vanish for all pairs with $n \neq n^{\prime}$. Moreover, due to the Schrödinger equation linearity, each of these functions may be multiplied by a constant coefficient to make this set orthonormal:

$$
\int \psi_{n}^{*} \psi_{n^{\prime}} d^{3} r=\delta_{n, n^{\prime}} \equiv \begin{cases}1, & \text { if } n=n^{\prime}  \tag{1.64}\\ 0, & \text { if } n \neq n^{\prime}\end{cases}
$$

Also, the eigenfunctions form a full set, meaning that an arbitrary function $\psi(\mathbf{r})$, in particular the actual wavefunction $\Psi$ of the system in the initial moment of its evolution (which I will take for $t=0$, with a few exceptions), may be presented as a unique expansion over the eigenfunction set:

$$
\begin{equation*}
\Psi(\mathbf{r}, 0)=\sum_{n} c_{n} \psi_{n}(\mathbf{r}) \tag{1.65}
\end{equation*}
$$

The expansion coefficients $c_{k}$ may be readily found by multiplying both parts of Eq. (65) by $\psi^{*}{ }_{n}$, integrating the result over the space, and using Eq. (64). The result is

[^468]\[

$$
\begin{equation*}
c_{n}=\int \psi_{n}^{*}(\mathbf{r}) \Psi(\mathbf{r}, 0) d^{3} r . \tag{1.66}
\end{equation*}
$$

\]

Now let us consider the following wavefunction

$$
\begin{equation*}
\Psi(\mathbf{r}, t)=\sum_{n} c_{n} a_{k}(t) \psi_{k}(\mathbf{r})=\sum_{n} c_{n} \psi_{n}(\mathbf{r}) \exp \left\{-i \frac{E_{n}}{\hbar} t\right\} \tag{1.67}
\end{equation*}
$$

Since each term of the sum has the form (56) and satisfies the Schrödinger equation, so does the sum as the whole. Moreover, if coefficients $c_{n}$ are derived in accordance with Eq. (66), then solution (67) satisfies the initial conditions as well. At this moment we can again use one more help by mathematicians who tell us that the partial differential equation of type (28) with the Hamiltonian operator (41) with fixed initial conditions, may have only one (unique) solution. This means that in our case of motion in a time-independent potential $U=U(\mathbf{r})$, Eq. (67) gives the general solution of the timedependent Schrödinger equation (25) for our case:

$$
\begin{equation*}
i \hbar \frac{\partial \Psi}{\partial t}=-\frac{\hbar^{2}}{2 m} \nabla^{2} \Psi+U(\mathbf{r}) \Psi . \tag{1.68}
\end{equation*}
$$

We will repeatedly use this key fact through the course, though in many cases, following the physical sense of particular problems, will be more interested in certain specific particular solutions of Eq. (68) rather in the whole linear superposition (67).

In order to get some feeling of functions $\psi_{n}$, let us consider perhaps the simplest example, which nevertheless will be the basis for discussion of many less trivial problems: a particle confined in a rectangular quantum well 45 with a flat "bottom" and sharp and infinitely high "hard walls":

The only way to keep the product $U \psi_{n}$ in Eq. (68) finite outside the well, is to have $\psi=0$ in these regions. Also, the function have to be continuous everywhere, to avoid the divergence of its Laplace operator. Hence, we may solve the stationary Schrödinger equation (63) only inside the well, where it takes a simple form ${ }^{46}$

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi_{n}=E_{n} \psi_{n}, \tag{1.70a}
\end{equation*}
$$

with zero boundary conditions on all the walls. For our particular geometry, it is natural to express the Laplace operator in the Cartesian coordinates $\{x, y, z\}$ aligned with the well sides, so that we get the following boundary problem:

[^469]\[

$$
\begin{gather*}
-\frac{\hbar^{2}}{2 m}\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial z^{2}}\right) \psi_{n}=E_{n} \psi_{n}, \quad \text { for } 0<x<a_{x}, 0<y<a_{y}, \text { and } 0<z<a_{z}  \tag{1.70b}\\
\psi_{n}=0, \quad \text { for } x=0 \text { and } a_{x} ; \quad y=0 \text { and } a_{y} ; \quad z=0 \text { and } a_{z} .
\end{gather*}
$$
\]

This problem may be readily solved using the same variable separation method which was used earlier in this section to separate the spatial and temporal variables, now to separate Cartesian spatial variables from each other. Let us look for a particular solution in the form

$$
\begin{equation*}
\psi(\mathbf{r})=X(x) Y(y) Z(z) . \tag{1.71}
\end{equation*}
$$

(It is convenient to postpone taking care of proper indices for a minute.) Plugging this expression into the Eq. (70b) and dividing by $\psi=X Y Z$, we get

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left(\frac{1}{X} \frac{d^{2} X}{d x^{2}}+\frac{1}{Y} \frac{d^{2} Y}{d y^{2}}+\frac{1}{Z} \frac{d^{2} Z}{d z^{2}}\right)=E . \tag{1.72}
\end{equation*}
$$

Now let us repeat the standard argumentation of the variable separation method: since each term in the parentheses may be only a function of the corresponding argument, the equality is possible only if each term is a constant - with the dimensionality of energy. Calling them $E_{x}$, etc., we get three 1D equations

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{1}{X} \frac{d^{2} X}{d x^{2}}=E_{x}, \quad-\frac{\hbar^{2}}{2 m} \frac{1}{Y} \frac{d^{2} Y}{d y^{2}}=E_{y}, \quad-\frac{\hbar^{2}}{2 m} \frac{1}{Z} \frac{d^{2} Z}{d x^{2}}=E_{z}, \tag{1.73}
\end{equation*}
$$

with Eq. (72) turning into the energy-matching condition

$$
\begin{equation*}
E_{x}+E_{y}+E_{z}=E . \tag{1.74}
\end{equation*}
$$

All three ordinary differential equations (73), and their solutions, are similar. For example, for $X(x)$, we have a 1D Helmholtz equation

$$
\begin{equation*}
\frac{d^{2} X}{d x^{2}}+k_{x}^{2} X=0, \quad \text { with } k_{x}^{2} \equiv \frac{2 m E_{x}}{\hbar^{2}}, \tag{1.75}
\end{equation*}
$$

and simple boundary conditions: $X(0)=X\left(a_{x}\right)=0$. Let me hope that the reader knows how to solve this well-known 1D boundary problem - describing, for example, usual mechanical waves on a guitar string, though with a very much different expression for $k_{x}$. The problem allows an infinite number of sinusoidal standing-wave solutions, ${ }^{47}$

Rectangular quantum well: partial eigenfunctions

$$
\begin{equation*}
X=\left(\frac{2}{a_{x}}\right)^{1 / 2} \sin k_{x} x=\left(\frac{2}{a_{x}}\right)^{1 / 2} \sin \frac{\pi n_{x} x}{a_{x}}, \text { with } n_{x}=1,2, \ldots \tag{1.76}
\end{equation*}
$$

corresponding to eigenenergies

$$
\begin{equation*}
E_{x}=\frac{\hbar^{2}}{2 m} k_{x}^{2}=\frac{\pi^{2} \hbar^{2}}{2 m a_{x}^{2}} n_{x}^{2} \equiv E_{x 1} n_{x}^{2} \tag{1.77}
\end{equation*}
$$

[^470]Figure 7 shows this result using a somewhat odd but very graphic and hence common way when the eigenenergy values (frequently called energy levels) are used as horizontal axes for plotting eigenfunctions, despite their different dimensionality.

Due to the similarity of all Eqs. (73), $Y(y)$ and $Z(z)$ are similar functions of their arguments, and may also be numbered by integers (say, $n_{y}$ and $n_{z}$ ) independent of $n_{x}$, so that the spectrum of the total energy (74) is

$$
\begin{equation*}
E_{n_{x}, n_{y}, n_{z}}=\frac{\pi^{2} \hbar^{2}}{2 m}\left(\frac{n_{x}^{2}}{a_{x}^{2}}+\frac{n_{y}^{2}}{a_{y}^{2}}+\frac{n_{z}^{2}}{a_{z}^{2}}\right) . \tag{1.78}
\end{equation*}
$$



Fig. 1.7. Eigenfunctions (solid lines) and eigenvalues (dashed lines) of the 1D wave equation (75) on a finitelength segment. Solid black lines show the potential energy profile of the problem.

Thus, in this 3D problem, the role of index $n$ in Eq. (67) is played by a set of 3 independent integers $\left\{n_{x}, n_{y}, n_{z}\right\}$. In quantum mechanics, such integers play a key role, and thus have a special name, quantum numbers. Now the general solution (67) of our simple problem may be presented as the sum

$$
\begin{equation*}
\Psi(\mathbf{r}, t)=\sum_{n_{x}, n_{y}, n_{z}=1}^{\infty} c_{n_{x}, n_{y}, n_{z}} \sin \frac{\pi n_{x} x}{a_{x}} \sin \frac{\pi n_{y} y}{a_{y}} \sin \frac{\pi n_{z} z}{a_{z}} \exp \left\{-i \frac{E_{n_{x}, n_{y}, n_{z}}^{\hbar}}{\hbar} t\right\} \tag{1.79}
\end{equation*}
$$

with the coefficients which may be readily calculated from the initial wavefunction $\Psi(\mathbf{r}, 0)$, using Eq. (66), again with the replacement $n \rightarrow\left\{n_{x}, n_{y}, n_{z}\right\}$. This simplest problem is a good illustration of the basic features of wave mechanics for a spatially-confined motion, including the discrete energy spectrum, and (in this case, evidently) orthogonal eigenfunctions.

An example of the opposite limit of a continuous spectrum for unconfined motion of a free particle is given by plane waves (29) which, with the account of relations $E=\hbar \omega$ and $\mathbf{p}=\hbar \mathbf{k}$, may be viewed as the product of the time-dependent factor (46) by eigenfunction

$$
\begin{equation*}
\psi_{\mathbf{k}}=a_{\mathbf{k}} \exp \{i \mathbf{k} \cdot \mathbf{r}\} \tag{1.80}
\end{equation*}
$$

Rectangular quantum well: general solution
I-2
that is the solution to the stationary Schrödinger equation (70a) if it is valid in the whole space. ${ }^{48}$
The reader should not be worried too much by the fact that the fundamental solution (80) in free space is a traveling wave (having, in particular, nonvanishing value (50) of the probability current $\mathbf{j}$ ),

[^471]while those inside a quantum well are standing waves, with $\mathbf{j}=0$, even though the free space may be legitimately considered as the ultimate limit of a quantum well with volume $V=a_{x} a_{y} a_{z} \rightarrow \infty$. Indeed, due to the linearity of wave mechanics, two traveling-wave solutions (80) with equal and opposite values of momentum (and hence with the same energy) may be readily combined to give a standingwave solution, for example $\exp \{i \mathbf{k} \cdot \mathbf{r}\}+\exp \{-i \mathbf{k} \cdot \mathbf{r}\}=2 \cos (\mathbf{k} \cdot \mathbf{r})$, with the net current $\mathbf{j}=0$. Thus, depending on convenience for solution of a particular problem, we can present the general solution as a sum of either traveling-wave or standing-wave eigenfunctions.

Since in the free space there are no boundary conditions to satisfy, Cartesian components of the wave vector $\mathbf{k}$ in Eq. (80) can take any real values. (This is why it is more convenient to label the wavefunctions and eigenenergies,
 eigenenergies
 of states

$$
\begin{equation*}
E_{\mathbf{k}}=\frac{\hbar^{2} k^{2}}{2 m} \geq 0 \tag{1.81}
\end{equation*}
$$

by their wave vector $\mathbf{k}$ rather than an integer index.) However, one aspect of systems with continuous spectrum requires a bit more math caution: summation (67) should be replaced by integration over a continuous index or indices (in this case, 3 components of vector $\mathbf{k}$ ). The main rule of such replacement may be readily extracted from Eq. (76): according to this relation, for standing-wave solutions, the eigenvalues of $k_{x}$ are equidistant, i.e. separated by equal intervals $\Delta k_{x}=\pi / a_{x}$ (with the similar relations for other two Cartesian components of vector $\mathbf{k}$ ). Hence the number of different eigenvalues of the standing wave vector $\mathbf{k}$ (with $k_{x}, k_{y}, k_{z} \geq 0$ ), within a volume $d^{3} k \gg 1 / V$ of the $\mathbf{k}$ space is just $d N=$ $d^{3} k /\left(\Delta k_{x} \Delta k_{x} \Delta k_{x}\right)=V / \pi^{3}$. Since in continuum it is more convenient to work with traveling waves, we should take into account that, as was just discussed, there are two different traveling wave vectors ( $\mathbf{k}$ and $\mathbf{k}^{\prime}=-\mathbf{k}$ ) corresponding to each standing wave vector $\mathbf{k}$. Hence the same number of physically different states corresponds to $2^{3}=8$-fold larger $\mathbf{k}$ space (which now is infinite in all directions) or, equivalently, to a smaller number of states per unit volume $d^{3} k$ :

$$
\begin{equation*}
d N=\frac{V}{(2 \pi)^{3}} d^{3} k \tag{1.82}
\end{equation*}
$$

For $d N \gg 1$, this expression is independent on the boundary conditions, ${ }^{49}$ and is frequently presented as the following summation rule

$$
\begin{equation*}
\lim _{k^{3} V \rightarrow \infty} \sum_{\mathbf{k}} f(\mathbf{k})=\int f(\mathbf{k}) d N=\frac{V}{(2 \pi)^{3}} \int f(\mathbf{k}) d^{3} k \tag{1.83}
\end{equation*}
$$

where $f(\mathbf{k})$ is an arbitrary function of $\mathbf{k}$. This rule is very important for statistical physics. Note also that if the same wave vector $\mathbf{k}$ corresponds to several internal quantum states (such as spin - see Chapter 4), the right-hand part of Eq. (83) requires multiplication by the corresponding degeneracy factor.

### 1.6. Dimensionality reduction

To conclude this introductory chapter, let me discuss the conditions when the spatial dimensionality of a wave mechanics problem may be reduced. ${ }^{50}$ For example, following our discussion

[^472]of the 3D rectangular, flat-bottom quantum well in Sec. 5, let us consider an infinitely deep quantum well whose bottom is flat only in one direction, say $z$ :
\[

U(\mathbf{r})=\left\{$$
\begin{array}{lr}
U(x, y), & \text { for } 0<z<a_{z}  \tag{1.84}\\
+\infty, & \text { otherwize }
\end{array}
$$\right.
\]

In this case, we can separate variables only partly, by presenting the eigenfunction as $\psi(x, y) Z(z)$. Plugging such solution into the corresponding form of the stationary Schrödinger equation (63), we see that functions $Z(z)$ are again similar to those given by Eq. (76), while function $\psi(x, y)$ satisfies the following 2D stationary Schrödinger equation:
$-\frac{\hbar^{2}}{2 m} \nabla_{x, y}^{2} \psi+U_{\text {ef }}(x, y) \psi=E_{x, y} \psi$,
where

$$
\begin{equation*}
U_{\mathrm{ef}}(x, y) \equiv U(x, y)+E_{z}=U(x, y)+\frac{\pi^{2} \hbar^{2} n_{z}^{2}}{2 m a_{z}^{2}} \tag{1.86}
\end{equation*}
$$

Thus, we have arrived at the boundary problem similar to the initial one, but with the spatial dimensionality reduced from 3 to 2 , due to what is called the partial confinement ${ }^{51}$ in direction $z$. If all partial functions $Z(z)$ are normalized to unity, the wavefunction normalization condition (22c) becomes

$$
\begin{equation*}
W=\int_{A} \psi(x, y) \psi^{*}(x, y) d x d y \tag{1.87}
\end{equation*}
$$

where $A$ is the total area of the system on the $[x, y]$ plane, and is formally similar to the initial 3D normalization condition. However, the effective 2D potential energy $U_{\text {ef }}(x, y)$ includes term $E_{z}$ depending on quantum number $n_{z},{ }^{52}$ making the physical relevance of such variable separation much less general than might be naively expected. There are three possible cases:
(i) If there is no strong relation between the energy scale $E_{x, y}$ of potential $U_{\text {ef }}(x, y)$ and $E_{z}$, the solution of a typical problem has to be presented as a (typically, large) sum of partial solutions $\psi(x, y) Z(z)$, each with its own $n_{z}, U_{\text {ef }}$, and $E_{z}$. In this general case, the variable separation may not provide much relief at all, because eigenenergies of solutions with different $n_{z}$ may be close, so that several of them would simultaneously participate in realistic processes.
(ii) $E_{z}$ is much smaller than $E_{x, y}$ and may be neglected. This may be the case, for example, if the potential profile is more steep along axes $x$ and $y$, than along direction $z$. Notice, however, that condition, $a_{z} \rightarrow \infty$, does not guarantee the smallness of $E_{z}$, because it may be compensated by large values of $n_{z}$. In this case (typical for solid state problems), either summation or integration over $n_{z}$ still

[^473]may be needed, though sometimes may be carried out analytically, because functions $Z(z)$ are simple sinusoidal waves.
(iii) Counter-intuitively, the most robust dimensionality reduction is possible in the opposite limit, when $a_{z}$ is much smaller than the characteristic scale of motion within the $[x, y]$ plane (Fig. 8a). Indeed, in this case the distance between adjacent levels of the confinement energy $E_{z}$ is much larger than the characteristic energy $E_{x, y}$ of motion within the plane. As a result, if the system was initially prepared to be on the lowest, ground level of $E_{z}$, , a "soft" motion along $x$ and $y$ cannot excite the system to higher levels of $E_{z} \cdot{ }^{53}$ Hence, the system keeps the fixed quantum number $n_{z}=1$, through the motion, so that the confinement energy $E_{z}$ is constant and, according to Eq. (86), may be treated just as a fixed potential energy offset.

The last conclusion is true even if the quantum well's profile in direction $z$ is not rectangular (provided that $E_{z}$ is still much larger than $E_{x, y}$ ). For example, many 2D quantum phenomena, such as the quantum Hall effect, ${ }^{54}$ have been studied experimentally using electrons confined at semiconductor heterojunctions (e.g., epitaxial interfaces $\mathrm{GaAs} / \mathrm{Al}_{\mathrm{x}} \mathrm{Ga}_{1-\mathrm{x}} \mathrm{As}$ ) where the potential well in the direction perpendicular to the interface has a nearly triangular shape, with the splitting of energies $E_{z}$ is the order of $10^{-2} \mathrm{eV} .{ }^{55}$ This splitting energy corresponds to $k_{\mathrm{B}} T$ at temperature $\sim 100 \mathrm{~K}$, so that careful experimentation at liquid helium temperatures ( 4 K and below) may keep the electrons performing purely 2 D motion in the "lowest subband" $\left(n_{z}=1\right)$.

(b)


Fig. 1.8. Partial confinement in: (a) one dimension, and (b) two dimensions.
Now, if a quantum well is formed in two dimensions (say, $y$ and $z$, see Fig. 8b), ${ }^{56}$

$$
U(\mathbf{r})=\left\{\begin{array}{lr}
U(x), & \text { for } 0<y<a_{y} \text { and } 0<z<a_{z}  \tag{1.88}\\
+\infty, & \text { otherwize }
\end{array}\right.
$$

then repeating the variable separation procedure we see that the 3D Schrödinger equation (68) may be satisfied with particular solutions of the type (71), again with sinusoidal standing waves $Y(y)$ and $Z(z)$, but generally a more complex function $X(x)$, which has to satisfy the following $1 D$ Schrödinger equation equation

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} X}{d x^{2}}+U_{\text {ef }}(x) X=E_{x} X \tag{1.89}
\end{equation*}
$$

[^474]with the effective potential energy
\[

$$
\begin{equation*}
U_{\mathrm{ef}}(x)=U(x)+E_{y}+E_{z} . \tag{1.90}
\end{equation*}
$$

\]

> Effective potential energy

Again, if the particle stays in the lowest subband, $n_{y}=n_{z}=1$, both $E_{y}$ and $E_{z}$ retain their constant values $E_{y 1}$ and $E_{z 1}$. Repeating the above discussion of the one-dimensional partial confinement, we can expect that a wave mechanics problem may be substantially simplified if $E_{y 1}$ and $E_{z 1}$ are much larger than the energy scale $E_{x}$ of the motion in direction $x$. Namely, if:
(i) the potential profile within the 2D partial confinement plane $[y, z]$ is arbitrary (provided that it provides partial confinement scales $a_{y}$ and $a_{z}$ much smaller the spatial scale of the motion in direction $x$ ), and
(ii) the potential energy $U$ is either constant in time or changes relatively slowly, at a time scale $\tau$ $\gg \hbar / E_{y z 1}$ (where $E_{y z 1}$ is the lowest eigenenergy of motion within the $[y, z]$ plane),
then a large range of experiments may be adequately described by looking for solution of the general (time-dependent, 3D) Schrödinger equation in the form of the following product

$$
\begin{equation*}
\Psi(x, t) Y Z_{1}(y, z) \exp \left\{-i \frac{E_{y z 1}}{\hbar} t\right\}, \tag{1.91}
\end{equation*}
$$

where $Y Z_{1}$ is the lowest (ground-state) eigenfunction of the 2D problem in the $[y, z]$ plane. Substituting this solution to the equation, and separating variables $\{y, z\}$ from $\{x, t\}$, we obtain the following timedependent, 1D equation

$$
\begin{equation*}
i \hbar \frac{\partial \Psi(x, t)}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi(x, t)}{\partial x^{2}}+U(x, t) \Psi(x, t) \tag{1.92}
\end{equation*}
$$

The next chapter will be devoted to a detailed discussion of the wave mechanics described by this 1 D equation, because it allows to study most basic phenomena and concepts of wave mechanics without involving overly complex math. In that chapter, for the notation simplicity, energy $E_{x}$ 1D motion will be referred to just as $E$. However, one should always remember that each " 1 D problem" has two hidden degrees of freedom and that the genuine energy of the particle also includes a constant shift $E_{y z 1}$ which is typically much larger than $E_{x}$. The Universe is (at least :-) 3-dimensional, and it shows!

Finally, note that in systems with reduced dimensionality, Eq. (82) for the number of states at large $\mathbf{k}$ (i.e., for an essentially free particle motion) should be replaced accordingly: in a 2 D system of area $A \gg 1 / k^{2}$,

$$
\begin{equation*}
d N=\frac{A}{(2 \pi)^{2}} d^{2} k \tag{1.93}
\end{equation*}
$$

2D number of states

[^475]with the corresponding changes of the summation rule (83). This change has important implications for the density of states on the energy scale, $d N / d E$ : it is straightforward (and hence left for the reader :-) to use Eqs. (82), (93), and (94) to show that for free 3D particles the density increases with $E$
(proportionally to $E^{1 / 2}$ ), for free 2D particles it does not depend on energy, while for free 1D particles it scales as $E^{-1 / 2}$, i.e. decreases with energy.

### 1.7. Exercise problems

1.1. The actual postulate made by N. Bohr in his original 1913 paper was not directly Eq. (10), but an assumption that at quantum leaps between adjacent large (quasiclassical) orbits with $n \gg 1$, hydrogen atom either emits or absorbs energy $\Delta E=\hbar \omega$, where $\omega$ is its classical radiation frequency according to classical electrodynamics, equal to the angular velocity of electron's rotation. Prove that this postulate is indeed compatible with Eqs. (8)-(10).
1.2. Use Eq. (53) to prove that linear operators of quantum mechanics are commutative: $\hat{A}_{2}+\hat{A}_{1}=\hat{A}_{1}+\hat{A}_{2}$, and associative: $\left(\hat{A}_{1}+\hat{A}_{2}\right)+\hat{A}_{3}=\hat{A}_{1}+\left(\hat{A}_{2}+\hat{A}_{3}\right)$.
1.3. Prove that for any Hamiltonian operator $\hat{H}$ and two arbitrary complex functions $f(\mathbf{r})$ and $g(\mathbf{r})$,

$$
\int f(\mathbf{r}) \hat{H} g(\mathbf{r}) d^{3} r=\int \hat{H} f(\mathbf{r}) g(\mathbf{r}) d^{3} r
$$

1.4. Prove that the Schrödinger equation (1.25) with Hamiltonian (1.41) is Galilean-invariant, provided that the wave function is transformed as

$$
\Psi^{\prime}\left(\mathbf{r}^{\prime}, t^{\prime}\right)=\Psi(\mathbf{r}, t) \exp \left\{-i \frac{m \mathbf{v} \cdot \mathbf{r}}{\hbar}+i \frac{m v^{2} t}{2 \hbar}\right\},
$$

where the prime sign denotes the variables measured in the reference frame $O$ ' that moves, without rotation, with a constant velocity $\mathbf{v}$ relatively to the "lab" frame $O$. Give a physical interpretation of this transformation.
1.5.* Prove the so-called Hellmann-Feynman theorem: ${ }^{57}$

$$
\frac{\partial E_{n}}{\partial \lambda}=\left\langle\frac{\partial H}{\partial \lambda}\right\rangle_{n},
$$

where $\lambda$ is some parameter, on whom the Hamiltonian $\hat{H}$, and hence its eigenenergies $E_{n}$ depend.
1.6. Calculate $\langle x\rangle,\left\langle p_{x}\right\rangle, \delta x$, and $\delta p_{x}$ for eigenstate $\left\{n_{x}, n_{y}, n_{z}\right\}$ of a rectangular, infinitely deep quantum well (69). Compare product $\delta x \delta p_{x}$ with Heisenberg's uncertainty relation.

[^476]1.7. A particle, placed in a hard-wall, rectangular box with sides $a_{x}, a_{y}$, and $a_{z}$, is in its ground state. Calculate the average force acting on each face of the box. Can the forces be characterized by a certain pressure?
1.8. A 1 D quantum particle was initially in the ground state of a very deep, rectangular quantum well of width $a$ :
\[

U(x)=\left\{$$
\begin{array}{lr}
0, & \text { for }-a / 2<x<+a / 2 \\
+\infty, & \text { otherwise }
\end{array}
$$\right.
\]

At some instant, the well's width is abruptly increased to value $a^{\prime}>a$ (leaving the well symmetric about point $x=0$ ), and then left constant. Calculate the probability that after the change, the particle is still in the ground state of the system.
1.9. At $t=0$, a 1 D particle of mass $m$ is placed into a hard-wall, flat-bottom potential well

$$
U(x)=\left\{\begin{array}{lr}
0, & \text { for } 0<x<a \\
+\infty, & \text { otherwise }
\end{array}\right.
$$

in a $50 / 50$ linear superposition of the lowest (ground) and the first excited states, so that its wavefunction at that instant is

$$
\Psi(x, 0)=C\left[\psi_{g}(x)+\psi_{e}(x)\right]
$$

where $C$ is the normalization constant which ensures that the particle is (somewhere) in the well with probability $W=1$. Calculate:
(i) the normalized wavefunction $\Psi(x, t)$ for arbitrary time $t$, and
(ii) the time evolution of the expectation value $\langle x\rangle$ of particle's coordinate.
1.10. Find the potential profile $U(x)$ for which the following wavefunctions,

$$
\begin{align*}
& \Psi=c \exp \left\{-a x^{2}-i b t\right\}, \text { and }  \tag{i}\\
& \Psi=c \exp \{-a|x|-i b t\},
\end{align*}
$$

(with real coefficients $a>0$ and $b$ ), satisfy the Schrödinger equation for a particle with mass $m$. For each case, calculate $\langle x\rangle,\left\langle p_{x}\right\rangle, \delta x$, and $\delta p_{x}$, and compare the product $\delta x \delta p_{x}$ with Heisenberg's uncertainty relation.
1.11. Calculate the energy density $d N / d E$ of traveling wave states in large rectangular quantum wells of various dimensions: $d=1,2$, and 3 .
1.12.* Use the finite difference method with steps $a / 2$ and $a / 3$ to find as many eigenenergies as possible for a particle in the infinitely deep, hard-wall quantum well of width $a$. Compare the results with each other, with the exact formula. ${ }^{58}$

[^477]
## Chapter 2. 1D Wave Mechanics

The main goal of this chapter is the solution and discussion of a few conceptually most important problems of wave mechanics for the simplest, $1 D$ case. This lowest dimensionality, and a wide use of potential profiles' approximation by sets of Dirac's delta-functions, simplify the necessary calculations considerably without sacrificing the physical essence of the described phenomena. The reader is advised to pay special attention to Sections 6-9, which cover some important material not usually discussed in textbooks.

### 2.1. Probability current and uncertainty relations

As was discussed in the end of Chapter 1, in several cases (most importantly, at strong confinement within the $[y, z]$ plane), the general (3D) Schrödinger equation may be reduced to the 1D equation (1.92):

Schrödinger equation

Probability

Normalization

Expectation value

Probability
current

Continuity equation
耍

$$
\begin{equation*}
i \hbar \frac{\partial \Psi(x, t)}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi(x, t)}{\partial x^{2}}+U(x, t) \Psi(x, t) \tag{2.1}
\end{equation*}
$$

If the transversal factor - say, the function $Y Z_{1}(y, z)$ that participates in Eq. (1.91), is normalized to unity, then the integration of Eq. (1.22a) over a segment $\left[x_{1}, x_{2}\right]$, gives the probability to find the particle on this segment:

$$
\begin{equation*}
W(t) \equiv \int_{x_{1}}^{x_{2}} \Psi(x, t) \Psi^{*}(x, t) d x \tag{2.2}
\end{equation*}
$$

If the particle under analysis is definitely inside the system, the normalization of its 1 D wavefunction $\Psi(x, t)$ is provided by extending integral (2) to the whole axis $x$ :

$$
\begin{equation*}
\int_{-\infty}^{+\infty} w(x, t) d x=1, \quad \text { where } w(x, t) \equiv \Psi(x, t) \Psi *(x, t) \tag{2.3}
\end{equation*}
$$

A similar integration of Eq. (1.23) shows that the expectation value of any operator depending only on coordinate $x$ (and possibly time), may be expressed as

It is also useful to introduce the probability current along the $x$-axis (a scalar):

$$
\begin{equation*}
I(x, t) \equiv \int j_{x} d y d z=\frac{\hbar}{m} \operatorname{Im}\left(\Psi^{*} \frac{\partial}{\partial x} \Psi\right)=\frac{\hbar}{m}|\Psi(x, t)|^{2} \frac{\partial \varphi}{\partial x} \tag{2.5}
\end{equation*}
$$

where $j_{x}$ is $x$-component of the probability current density vector $\mathbf{j}(\mathbf{r}, t)$. Then the continuity equation (1.48) for the segment $\left[x_{1}, x_{2}\right]$ takes the form

$$
\begin{equation*}
\frac{d W}{d t}+I\left(x_{2}\right)-I\left(x_{1}\right)=0 \tag{2.6}
\end{equation*}
$$

The above formulas are the basis for the analysis of 1D problems of wave mechanics, but before proceeding to particular cases, let me deliver on my earlier promise to prove that Heisenberg's uncertainty relation (1.35) is indeed valid for any wavefunction $\Psi(x, t)$. For that, let us consider an evidently positive (or at least non-negative) integral

$$
\begin{equation*}
J(\lambda) \equiv \int_{-\infty}^{+\infty}\left|x \Psi+\lambda \frac{\partial \Psi}{\partial x}\right|^{2} d x \geq 0 \tag{2.7}
\end{equation*}
$$

where $\lambda$ is an arbitrary real constant, and assume that at the at $x \rightarrow \pm \infty$ the wavefunction vanishes, together with its first derivative. The left-hand part of Eq. (7) may be recast as

$$
\begin{align*}
& \int_{-\infty}^{+\infty} x \Psi+\left.\lambda \frac{\partial \Psi}{\partial x}\right|^{2} d x=\int_{-\infty}^{+\infty}\left(x \Psi+\lambda \frac{\partial \Psi}{\partial x}\right)\left(x \Psi+\lambda \frac{\partial \Psi}{\partial x}\right)^{*} d x  \tag{2.8}\\
& =\int_{-\infty}^{+\infty} x^{2} \Psi \Psi^{*} d x+\lambda \int_{-\infty}^{+\infty} x\left(\Psi \frac{\partial \Psi *}{\partial x}+\frac{\partial \Psi}{\partial x} \Psi^{*}\right) d x+\lambda^{2} \int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^{*}}{\partial x} d x
\end{align*}
$$

According to Eq. (4), the first term in the last form of Eq. (8) is just $\left\langle x^{2}\right\rangle$. The second and the third integrals may be worked out by parts:

$$
\begin{align*}
& \int_{-\infty}^{+\infty} x\left(\Psi \frac{\partial \Psi^{*}}{\partial x}+\frac{\partial \Psi}{\partial x} \Psi^{*}\right) d x=\int_{-\infty}^{+\infty} x \frac{\partial}{\partial x}\left(\Psi \Psi^{*}\right) d x=\int_{x=-\infty}^{x=+\infty} x d\left(\Psi \Psi^{*}\right)=\left.\Psi \Psi^{*} x\right|_{x=-\infty} ^{x=+\infty}-\int_{-\infty}^{+\infty} \Psi \Psi^{*} d x=-1  \tag{2.9}\\
& \int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^{*}}{\partial x} d x=\int_{x=-\infty}^{x=+\infty} \frac{\partial \Psi}{\partial x} d \Psi^{*}=\frac{\partial \Psi}{\partial x} \Psi^{*} \left\lvert\, \begin{array}{l}
x=+\infty \\
x=-\infty \\
x-\int_{-\infty}^{+\infty} \Psi^{*} \frac{\partial^{2} \Psi}{\partial x^{2}} d x=\frac{1}{\hbar^{2}} \int_{-\infty}^{+\infty} \Psi^{*} \hat{p}_{x}^{2} \Psi d x=\frac{\left\langle p_{x}^{2}\right\rangle}{\hbar^{2}}
\end{array} .\right. \tag{2.10}
\end{align*}
$$

As a result, Eq. (7) takes the following form:

$$
\begin{equation*}
J(\lambda)=\left\langle x^{2}\right\rangle-\lambda+\lambda^{2} \frac{\left\langle p_{x}^{2}\right\rangle}{\hbar^{2}} \geq 0, \quad \text { i.e. } \lambda^{2}+a \lambda+b \geq 0, \quad \text { with } a \equiv-\frac{\hbar^{2}}{\left\langle p_{x}^{2}\right\rangle} \text { and } b \equiv \frac{\hbar^{2}\left\langle x^{2}\right\rangle}{\left\langle p_{x}^{2}\right\rangle} . \tag{2.11}
\end{equation*}
$$

This inequality should be valid for any real $\lambda$, i.e. the corresponding quadratic equation, $\lambda^{2}+a \lambda+b=0$, can have either one (degenerate) real root - or no real roots at all. This is only possible if its determinant, Det $=a^{2}-4 b$, is non-positive, leading to the following requirement:

$$
\begin{equation*}
\left\langle x^{2}\right\rangle\left\langle p_{x}^{2}\right\rangle \geq \frac{\hbar^{2}}{4} \tag{2.12}
\end{equation*}
$$

In particular, if $\langle x\rangle=0$ and $\left\langle p_{x}\right\rangle=0,{ }^{1}$ then according to Eq. (1.33), Eq. (12) takes the form

$$
\begin{equation*}
\left\langle\tilde{x}^{2}\right\rangle\left\langle\tilde{p}_{x}^{2}\right\rangle \geq \frac{\hbar^{2}}{4} \tag{2.13}
\end{equation*}
$$

which, according to the definition (1.34) of r.m.s. uncertainties, is equivalent to Eq. (1.35).

[^478]Now let us notice that the Heisenberg's uncertainty relation looks very similar to the commutation relation between the corresponding operators:

$$
\begin{equation*}
\left[\hat{x}, \hat{p}_{x}\right] \Psi \equiv\left(\hat{x} \hat{p}_{x}-\hat{p}_{x} \hat{x}\right) \Psi=-i \hbar x \frac{\partial \Psi}{\partial x}+i \hbar \frac{\partial}{\partial x}(x \Psi)=i \hbar \Psi . \tag{2.14a}
\end{equation*}
$$

Coordinate/ momentum operators' commutator

Since this relation is valid for arbitrary wavefunction $\Psi(x, \mathrm{t})$, we may present it as an operator equality:

$$
\begin{equation*}
\left[\hat{x}, \hat{p}_{x}\right]=i \hbar \neq 0 \tag{2.14b}
\end{equation*}
$$

In Sec. 4.5 we will see that the relation between Eqs. (13) and (14) is just a particular case of a general relation between the expectation values of non-commuting operators and their commutators.

### 2.2. Free particle: Wave packets

Let us start our discussion of particular problems with free the 1D motion, with $U(x, t)=0$. From our discussion of Eq. (1.29) in Chapter 1, it is clear that in the 1D case, a similar "fundamental" (i.e. a particular but the most important) solution of the Schrödinger equation (1) is a monochromatic wave

$$
\begin{equation*}
\Psi_{0}(x, t)=\mathrm{const} \times e^{i\left(k_{0} x-\omega_{0} t\right)} . \tag{2.15}
\end{equation*}
$$

According to Eqs. (1.32), it corresponds to a particle with an exactly defined momentum ${ }^{2} p_{0}=\hbar k_{0}$ and energy $E_{0}=\hbar \omega_{0}=\hbar^{2} k_{0}^{2} / 2 m$. However, for this wavefunction, product $\Psi * \Psi$ does not depend on either $x$ or $t$, so that the particle is completely delocalized, i.e. its probability is spread all over axis $x$, at all times. (As a result, such state is still compatible with Heisenberg's uncertainty relation (13), despite the exact value $p_{0}$ of momentum $p$.)

In order to describe a space-localized particle, let us form, at the initial moment of time $(t=0)$, a wave packet of the type shown in Fig. 1.6, by multiplying the sinusoidal waveform (15) by some smooth envelope function $A(x)$. As the most important particular example, consider a Gaussian packet

Initial Gaussian wave packet

$$
\begin{equation*}
\Psi(x, 0)=A(x) e^{i k_{0} x}, \quad \text { with } A(x)=\frac{1}{(2 \pi)^{1 / 4}(\delta x)^{1 / 2}} \exp \left\{-\frac{x^{2}}{(2 \delta x)^{2}}\right\} \tag{2.16}
\end{equation*}
$$

(By the way, Fig. 1.6 shows exactly such a packet.) The pre-exponential factor in this envelope function has been selected in the way to have the initial probability density,

$$
\begin{equation*}
w(x, 0)=\Psi^{*}(x, 0) \Psi(x, 0)=A^{*}(x) A(x)=\frac{1}{(2 \pi)^{1 / 2} \delta x} \exp \left\{-\frac{x^{2}}{2(\delta x)^{2}}\right\}, \tag{2.17}
\end{equation*}
$$

normalized according to Eq. (3), for any parameters $\delta x$ and $k_{0} \cdot{ }^{3}$
In order to explore the evolution of this packet in time, we could try to solve Eq. (1) with the initial condition (16) directly, but in the spirit of the discussion in Sec. 1.5, it is easier to proceed

[^479]differently. Let us first present the initial wavefunction (16) as a sum (1.65) of eigenfunctions $\psi_{k}(x)$ of the corresponding stationary 1D Schrödinger equation (1.60), in our current case
\[

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi_{k}}{d x^{2}}=E_{k} \psi_{k}, \quad \text { with } E_{k} \equiv \frac{\hbar^{2} k^{2}}{2 m} \tag{2.18}
\end{equation*}
$$

\]

that are simply monochromatic waves,

$$
\begin{equation*}
\psi_{k}=a_{k} e^{i k x} \tag{2.19}
\end{equation*}
$$

with a continuum spectrum of possible wave numbers $k$. For that, sum (1.65) should be replaced with an integral: ${ }^{4}$

$$
\begin{equation*}
\Psi(x, 0)=\int a_{k} \psi_{k}(x) d p=\int a_{k} e^{i k x} d k \tag{2.20}
\end{equation*}
$$

Now let us notice that from the point of view of mathematics, Eq. (20) is just the usual Fourier transform from variable $k$ to the "conjugate" variable $x$, and we can use the well-known formula of the reciprocal Fourier transform to calculate

$$
\begin{equation*}
a_{k}=\frac{1}{2 \pi} \int \Psi(x, 0) e^{-i k x} d x=\frac{1}{2 \pi} \frac{1}{(2 \pi)^{1 / 4}(\delta x)^{1 / 2}} \int \exp \left\{-\frac{x^{2}}{(2 \delta x)^{2}}-i \widetilde{k} x\right\} d x, \quad \text { where } \tilde{k} \equiv k-k_{0} \tag{2.21}
\end{equation*}
$$

This Gaussian integral may be worked out by the following standard method. Let us complement the exponent to the full square of a linear combination of $x$ and $k$, plus a term independent of $x$ :

$$
\begin{equation*}
-\frac{x^{2}}{(2 \delta x)^{2}}-i \widetilde{k} x=-\frac{1}{(2 \delta x)^{2}}\left[x+2 i \widetilde{k}(\delta x)^{2}\right]^{2}-\widetilde{k}^{2}(\delta x)^{2} \tag{2.22}
\end{equation*}
$$

Since the integration in the right-hand part of Eq. (20) should be performed at constant $\widetilde{k}$, in the infinite limits, its result would not change if we replace $d x$ by $d x{ }^{\prime} \equiv d\left[x+2 i(\delta x)^{2} \widetilde{k}\right] .{ }^{5}$ As a result, we get,

$$
\begin{equation*}
a_{k}=\frac{1}{2 \pi} \frac{1}{(2 \pi)^{1 / 4}(\delta x)^{1 / 2}} \exp \left\{-\widetilde{k}^{2}(\delta x)^{2}\right\} \int \exp \left\{-\frac{x^{\prime 2}}{(2 \delta x)^{2}}\right\} d x^{\prime}=\left(\frac{1}{2 \pi}\right)^{1 / 2} \frac{1}{(2 \pi)^{1 / 4}(\delta k)^{1 / 2}} \exp \left\{-\frac{\widetilde{k}^{2}}{(2 \delta k)^{2}}\right\} \cdot( \tag{2.23}
\end{equation*}
$$

so that $a_{k}$ also has a Gaussian distribution, now along axis $k$, centered to value $k_{0}$ (Fig. 1.6b), with constant $\delta k$ defined as

$$
\begin{equation*}
\delta k \equiv 1 / 2 \delta x \tag{2.24}
\end{equation*}
$$

Thus we may present the initial wave packet (16) as

$$
\begin{equation*}
\Psi(x, 0)=\left(\frac{1}{2 \pi}\right)^{1 / 2} \frac{1}{(2 \pi)^{1 / 4}(\delta k)^{1 / 2}} \int \exp \left\{-\frac{\left(k-k_{0}\right)^{2}}{(2 \delta k)^{2}}\right\} e^{i k x} d k \tag{2.25}
\end{equation*}
$$

From comparison of this formula with Eq. (16), it is evident that the r.m.s. uncertainty of the wave number $k$ in this packet is indeed equal to $\delta k$ defined by Eq. (24), thus justifying the notation. The

[^480]comparison of that relation with Eq. (1.35) shows that the Gaussian packet presents the ultimate case in which the product $\delta x \delta p=\delta x(\hbar \delta k)$ has the lowest possible value ( $\hbar / 2$ ); for any other envelope's shape the uncertainty product may only be larger. We could of course get the same result for $\delta k$ from Eq. (16) using definitions (1.23), (1.33), and (1.34); the real advantage of Eq. (24) is that it can be readily generalized to $t>0$.

Indeed, we already know that the time evolution of the wavefunction is given by Eq. (1.67), for our case giving ${ }^{6}$


$$
\begin{equation*}
\Psi(x, t)=\left(\frac{1}{2 \pi}\right)^{1 / 2} \frac{1}{(2 \pi)^{1 / 4}(\delta k)^{1 / 2}} \int \exp \left\{-\frac{\left(k-k_{0}\right)^{2}}{(2 \delta k)^{2}}\right\} e^{i k x} \exp \left\{-i \frac{\hbar k^{2}}{2 m} t\right\} d k \tag{2.26}
\end{equation*}
$$

Fig. 1 shows several snapshots of the real part of wavefunction (26), for a particular case $\delta k=0.1 k_{0}$.


The plots clearly show the following effects:
(i) the wave packet as a whole (as characterized by its envelope) moves along the $x$ axis with a certain group velocity $\mathrm{v}_{\mathrm{gr}}$,

[^481](ii) the "carrier" wave inside the packet moves with a different, phase velocity $v_{\mathrm{ph}}$, which may be defined as the velocity the spatial points where wave's phase $\varphi(x, t) \equiv \arg \Psi$ takes a certain fixed value (say, $\varphi=\pi / 2$, where $\operatorname{Re} \Psi$ vanishes), and
(iii) the packet's spatial width gradually increases with time - the packet spreads.

All these effects are common for waves of any physical nature. ${ }^{7}$ Indeed, let us consider a 1D wave packet of the type (26),

$$
\begin{equation*}
\Psi(x, t)=\int a_{k} e^{i(k x-\omega t)} d k \tag{2.27}
\end{equation*}
$$

propagating in a media with an arbitrary (but smooth!) dispersion relation $\omega(k)$, and assume that the wave number distribution $a_{k}$ is arbitrary but narrow: $\delta k \ll\langle k\rangle \equiv k_{0}$ - see Fig. 1.6b. Then we may expand function $\omega(k)$ into the Taylor series near the central point $k_{0}$, and keep only two of its leading terms:

$$
\begin{equation*}
\omega(k) \approx \omega_{0}+\frac{d \omega}{d k} \widetilde{k}+\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} \widetilde{k}^{2}, \quad \text { where } \widetilde{k} \equiv k-k_{0}, \omega_{0} \equiv \omega\left(k_{0}\right) \tag{2.28}
\end{equation*}
$$

and both derivatives are also evaluated at point $k=k_{0}$. In this approximation, ${ }^{8}$ the expression in parentheses in the right-hand part of Eq. (27) may be rewritten as

$$
\begin{equation*}
k x-\omega t=k_{0} x+\widetilde{k} x-\left(\omega_{0}+\frac{d \omega}{d k} \widetilde{k}+\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} \widetilde{k}^{2}\right) t=\left(k_{0} x-\omega_{0} t\right)+\widetilde{k}\left(x-\frac{d \omega}{d k} t\right)-\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} \widetilde{k}^{2} t \tag{2.29}
\end{equation*}
$$

so that Eq. (27) is reduced to integral

$$
\begin{equation*}
\Psi(x, t)=e^{i\left(k_{0} x-\omega_{0} t\right)} \int a_{k} \exp \left\{i\left[\widetilde{k}\left(x-\frac{d \omega}{d k} t\right)-\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} \widetilde{k}^{2} t\right]\right\} d \widetilde{k} . \tag{2.30}
\end{equation*}
$$

First, let neglect the last term in square brackets (which is much smaller than the first term if the dispersion relation is smooth enough and/or the time interval $t$ is sufficiently small), and compare the result with the initial form of the wave packet (27)

$$
\begin{equation*}
\Psi(x, 0)=\int a_{k} e^{i k x} d k=A(x) e^{i k_{0} x}, \quad \text { with } A(x) \equiv \int a_{k} e^{i \tilde{k} x} d \tilde{k} \tag{2.31}
\end{equation*}
$$

The comparison shows that Eq. (30) is reduced to

$$
\begin{equation*}
\Psi(x, t)=A\left(x-v_{\mathrm{gr}} t\right) e^{i k_{0}\left(x-v_{\mathrm{ph}} t\right)} \tag{2.32}
\end{equation*}
$$

where $v_{\mathrm{gr}}$ and $v_{\mathrm{ph}}$ are two constants with the dimension of velocity:

$$
\begin{equation*}
\left.v_{\mathrm{gr}} \equiv \frac{d \omega}{d k}\right|_{k=k_{0}}, \quad \text { and }\left.\quad v_{\mathrm{ph}} \equiv \frac{\omega}{k}\right|_{k=k_{0}} \tag{2.33}
\end{equation*}
$$

It is clear that Eq. (32) describes effects (i) and (ii) listed above. Let us calculate the group and phase velocities for the particular case of de Broglie waves whose dispersion law is given by Eq. (1.30):

[^482]\[

$$
\begin{equation*}
\omega=\frac{\hbar k^{2}}{2 m},\left.\quad v_{\mathrm{gr}} \equiv \frac{d \omega}{d k}\right|_{k=k_{0}}=\frac{\hbar k_{0}}{m} \equiv v_{0},\left.\quad v_{\mathrm{ph}} \equiv \frac{\omega}{k}\right|_{k=k_{0}}=\frac{\hbar k_{0}}{2 m}=\frac{v_{g r}}{2} . \tag{2.34}
\end{equation*}
$$

\]

We see that (very fortunately!) the velocity of the wave packet envelope is constant and equals to that of the classical particle moving by inertia, in accordance with the correspondence principle.

The remaining term in the square brackets of Eq. (30) describes effect (iii), the wave packet's spread. It may be readily evaluated if the packet (27) is initially Gaussian, as in our example (25):

$$
\begin{equation*}
a_{k}=\text { const } \times \exp \left\{-\frac{\widetilde{k}^{2}}{(2 \delta k)^{2}}\right\} . \tag{2.34}
\end{equation*}
$$

In this case integral (30) is Gaussian, and may be worked out exactly as integral (20), i.e. merging the exponents under the integral, and presenting them as a full square of linear combination of $x$ and $k$ :

$$
\begin{equation*}
-\frac{\widetilde{k}^{2}}{(2 \delta k)^{2}}+i \widetilde{k}\left(x-v_{\mathrm{gr}} t\right)-\frac{i}{2} \frac{d^{2} \omega}{d k^{2}} \widetilde{k}^{2} t=-\Delta(t)\left(\widetilde{k}+i \frac{x-v_{\mathrm{gr}} t}{2 \Delta(t)}\right)^{2}-\frac{\left(x-v_{\mathrm{gr}} t\right)^{2}}{4 \Delta(t)}+i k_{0} x-\frac{i}{2} \frac{d^{2} \omega}{d k^{2}} k_{0}^{2} t \tag{2.35}
\end{equation*}
$$

where I have introduced the following complex function of time:

$$
\begin{equation*}
\Delta(t) \equiv \frac{1}{4(\delta k)^{2}}+\frac{i}{2} \frac{d^{2} \omega}{d k^{2}} t=(\delta x)^{2}+\frac{i}{2} \frac{d^{2} \omega}{d k^{2}} t \tag{2.36}
\end{equation*}
$$

and have used Eq. (24) in the second equality. Now integrating over $\widetilde{k}$, we get

$$
\begin{equation*}
\Psi(x, t) \propto \exp \left\{-\frac{\left(x-v_{\mathrm{gr}} t\right)^{2}}{4 \Delta(t)}+i\left(k_{0} x-\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} k_{0}^{2} t\right)\right\} . \tag{2.37}
\end{equation*}
$$

The imaginary part of ratio $1 / \Delta(t)$ in the exponent gives just an additional contribution to wave's phase, and does not affect the resulting probability distribution

$$
\begin{equation*}
w(x, t)=\Psi^{*} \Psi \propto \exp \left\{-\frac{\left(x-v_{\mathrm{gr}} t\right)^{2}}{2} \operatorname{Re} \frac{1}{\Delta(t)}\right\} \tag{2.38}
\end{equation*}
$$

This is again a Gaussian bell curve spread over axis $x$, centered to point $\langle x\rangle=v_{\mathrm{gr}} t$, with the r.m.s. width

$$
\begin{equation*}
\left(\delta x^{\prime}\right)^{2} \equiv\left\{\operatorname{Re}\left[\frac{1}{\Delta(t)}\right]\right\}^{-1}=(\delta x)^{2}+\left(\frac{1}{2} \frac{d^{2} \omega}{d k^{2}} t\right)^{2} \frac{1}{(\delta x)^{2}} . \tag{2.39a}
\end{equation*}
$$

In the particular case of de Broglie waves, $d^{2} \omega / d k^{2}=\hbar / m$, so that

Wave packet's spread with time

$$
\begin{equation*}
\left(\delta x^{\prime}\right)^{2}=(\delta x)^{2}+\left(\frac{\hbar t}{2 m}\right)^{2} \frac{1}{(\delta x)^{2}} \tag{2.39b}
\end{equation*}
$$

The physics of the spreading is very simple: if $d^{2} \omega / d k^{2} \neq 0$, the group velocity $d \omega / d k$ of each small group $d k$ of monochromatic components of the wave packet is different, resulting in the gradual (eventually, linear) accumulation of the differences of the distances traveled by the groups. The most curious feature of Eq. (39) is that the packet width at $t>0$ depends on its initial width $\delta x{ }^{\prime}(0)=\delta x$ in a
non-monotonic way, tending to infinity at both $\delta x \rightarrow 0$ and $\delta x \rightarrow \infty$. Because of that, for a fixed $t$, there is an optimal value of $\delta x$ with minimizes $\delta x$ ':

$$
\begin{equation*}
\left(\delta x^{\prime}\right)_{\min }=\sqrt{2}(\delta x)_{\mathrm{opt}}=\left(\frac{\hbar t}{m}\right)^{1 / 2} \tag{2.40}
\end{equation*}
$$

This expression may be used for spreading effect estimates. Due to the smallness of the Planck constant $\hbar$ on the human scale of things, for macroscopic bodies this effect is extremely small even for very long time intervals; however, for light particles it may be very noticeable: for the electron ( $\mathrm{m}=\mathrm{m}_{e} \approx 10^{-30}$ kg ), and $t=1 \mathrm{~s}$, Eq. (40) yields ( $\left.\delta x^{\prime}\right)_{\min } \sim 1 \mathrm{~cm}$ !

Note also that for any $t \neq 0$, the wave packet retains its Gaussian envelope, but the ultimate relation (24) is not satisfied, $\delta x$ ' $\delta p>\hbar / 2$ - due to a gradually accumulated phase shift between the component monochromatic waves. The last remark on this topic: in quantum mechanics, the wave packet spreading is not an ubiquitous effect! For example, in Chapter 5 we will see that in a quantum oscillator, the spatial width of a Gaussian packet (for that system, called the Glauber state) does not grow monotonically but rather either stays constant or oscillates in time.

Now let us briefly discuss the case when the initial wave packet is not Gaussian, but is described by an arbitrary initial wavefunction. In order to make the forthcoming result more appealing, it is beneficial to generalize out calculations to an arbitrary initial time $t_{0}$; it is evident that if $U$ does not depend on time explicitly, it is sufficient to replace $t$ with $\left(t-t_{0}\right)$ in all above formulas. With this replacement, Eq. (27) becomes

$$
\begin{equation*}
\Psi(x, t)=\int a_{k} e^{i\left[k x-\omega\left(t-t_{0}\right)\right]} d k \tag{2.41}
\end{equation*}
$$

and the reciprocal transform (21) reads

$$
\begin{equation*}
a_{k}=\frac{1}{2 \pi} \int \Psi\left(x, t_{0}\right) e^{-i k x} d x \tag{2.42}
\end{equation*}
$$

If we want to express these two formulas with one relation, i.e. plug Eq. (42) into Eq. (41), we should give the integration variable $x$ some other name, e.g., $x_{0}$. The result is

$$
\begin{equation*}
\Psi(x, t)=\frac{1}{2 \pi} \int d k \int d x_{0} \Psi\left(x_{0}, t_{0}\right) e^{i\left[k\left(x-x_{0}\right)-\omega\left(t-t_{0}\right)\right]} . \tag{2.43}
\end{equation*}
$$

Changing the order of integration, this expression may be rewritten in the following general form:

$$
\begin{equation*}
\Psi(x, t)=\int G\left(x, t ; x_{0}, t_{0}\right) \Psi\left(x_{0}, t_{0}\right) d x_{0} \tag{2.44}
\end{equation*}
$$

where function $G$, usually called kernel in mathematics, in quantum mechanics is called the propagator. ${ }^{9}$ According to Eq. (43), in our particular case of a free particle the propagator is equal to

[^483]\[

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\frac{1}{2 \pi} \int e^{i\left[k\left(x-x_{0}\right)-\omega\left(t-t_{0}\right)\right]} d k, \tag{2.45}
\end{equation*}
$$

\]

The physical sense of the propagator may be understood by considering the following special initial conditions: ${ }^{10}$

$$
\begin{equation*}
\Psi\left(x_{0}, t_{0}\right)=\delta\left(x_{0}-x^{\prime}\right), \tag{2.46}
\end{equation*}
$$

where $x$ ' is a certain point within the domain of particle's motion. In this particular case, Eq. (44) evidently gives

$$
\begin{equation*}
\Psi(x, t)=G\left(x, t ; x^{\prime}, t_{0}\right) . \tag{2.47}
\end{equation*}
$$

Hence, the propagator, considered as a function of $x$ and $t$ only, is just the solution of the linear differential equation with $\delta$-functional initial conditions. Thus while Eq. (41) may be understood as a mathematical expression of the linear superposition principle in the momentum (i.e., reciprocal) space domain, Eq. (44) is an expression of this principle in the direct space domain: the system's "response" $\Psi(x, t)$ to an arbitrary initial condition $\Psi\left(x_{0}, t_{0}\right)$ is just a sum of its responses to its thin spatial "slices", with propagator $G\left(x, t ; x_{0}, t_{0}\right)$ representing the weight of each slice in the final sum.

Calculating integral (45), one should remember that $\omega$ is not a constant but a function of $k$, given by the dispersion relation for particular waves. In particular, for the de Broglie waves

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right) \equiv \frac{1}{2 \pi} \int \exp \left\{i\left[k\left(x-x_{0}\right)-\frac{\hbar k^{2}}{2 m}\left(t-t_{0}\right)\right]\right\} d k \tag{2.48}
\end{equation*}
$$

This is a Gaussian integral again, and may be readily calculated just it was done (twice) above, by completing the exponent to the full square. The result is

Free
particle's propagator

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\left(\frac{m}{2 \pi i \hbar\left(t-t_{0}\right)}\right)^{1 / 2} \exp \left\{-\frac{m\left(x-x_{0}\right)^{2}}{2 i \hbar\left(t-t_{0}\right)}\right\} \tag{2.49}
\end{equation*}
$$

Please note the following features of this complex function (plotted in Fig. 2):


[^484](i) It depends only on differences $\left(x-x_{0}\right)$ and $\left(t-t_{0}\right)$. This is natural, because the free-particle propagation problem is uniform (translation-invariant) both in space and time.
(ii) The function shape does not depend on its arguments - they just rescale the same function: its snapshot (Fig. 2), if plotted as a function of un-normalized $x$, just becomes broader and lower with time. It is curious that the spatial broadening scales as $\left(t-t_{0}\right)^{1 / 2}-$ just as at the classical diffusion, as a result of a deep analogy between quantum mechanics and classical statistics - to be discussed further in Chapter 7.
(iii) In accordance with the uncertainty relation, the ultimately compressed wave packet (46) has an infinite width of momentum distribution, and the quasi-sinusoidal tails of the free-particle propagator, clearly visible in Fig. 2, are the results of the free propagation of the fastest (highestmomentum) components of that distribution, in both directions from the packet center. In the following sections, we will mostly focus on the spatial distribution of stationary, monochromatic wavefunctions (that, for unconfined motion, may be interpreted as wave packets of very large spatial width $\delta x$ ), only rarely coming back to the wave packet discussion. Our excuse is the linear superposition principle, i.e. our conceptual ability to restore the general solution from that of monochromatic waves of all possible energies. However, the reader should not forget that, as the above discussion has illustrated, mathematically this restoration is not always trivial.

### 2.3. Particle motion in simple potential profiles

Now, let us proceed to the cases in which the potential energy $U(x, t)$ is not identically equal to zero. The easiest case is that of spatially-uniform but time-dependent potential: $U=U(t)=$ const. Indeed, the corresponding Schrödinger equation (1.25) with Hamiltonian

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}+U(t)=-\frac{\hbar^{2}}{2 m} \nabla^{2}+U(t) \tag{2.50}
\end{equation*}
$$

allows the variable separation similar to that performed in Sec. 1.5, besides that the time-dependent function $T(t)$ obeys an equation of motion that is slightly more general than Eq. (1.59):

$$
\begin{equation*}
i \hbar \dot{T}=[E-U(t)] T \tag{2.51}
\end{equation*}
$$

whose solution may be expressed as an evident generalization of Eq. (1.61):

$$
\begin{equation*}
T(t)=T(0) e^{-i[\omega t+\varphi(t)]}, \quad \text { with } \omega=\frac{E}{\hbar} \text { and } \quad \frac{d \varphi}{d t}=-\frac{U(t)}{\hbar} . \tag{2.52}
\end{equation*}
$$

Looking at the basic relations (1.22) and (1.23) of wave mechanics, it seems that this additional phase factor does not affect the particle probability distribution, or even any observable (including energy it is referred to the instant value of $U$ ), and hence the phase increment $\varphi$, associated with $U(t)$, is just a mathematical artifact. This is certainly true for a single particle, however, the situation changes as soon as we recall that the Universe consists of more that one of them.

For example, consider two similar, independent particles, each in the same (say, ground) eigenstate, but with the potential energies (and hence eigenenergies $E_{1,2}$ ) different by a constant $\Delta U \equiv U_{1}$ $-U_{2}$. Then, the difference $\varphi \equiv \varphi_{1}-\varphi_{2}$ of their wavefunction phases evolves in time as

Quantum phase difference's evolution

$$
\begin{equation*}
\frac{d \varphi}{d t}=-\frac{\Delta U}{\hbar} \tag{2.53}
\end{equation*}
$$

If the particles are in different worlds (or at least in different laboratories :-), this evolution is unobservable; however, it should be intuitively clear that a very weak coupling of a certain detector to each particle may allow it to observe phase $\varphi$, while keeping the particle dynamics virtually unperturbed, i.e. Eq. (53) intact.

Perhaps the most dramatic demonstration of this phenomenon is the Josephson effect in superconductors. ${ }^{11}$ Experimentally, the easiest way to observe the effect is by connecting two bulk superconductor samples with a weak, short electric contact (called either the weak link or the Josephson junction) and bias them with a constant (dc) voltage $V$, typically in a few-microvolt range - see Fig. 3.


Fig. 2.3. Josephson effect in a weak link between two bulk superconductor electrodes.

Superconductivity may be explained by a specific coupling between its conduction electrons, that leads, at low temperatures, to formation of the so-called Cooper pairs. Such pairs, each consisting of two electrons with opposite spins and momenta, behave as Bose particles, and form coherent BoseEinstein condensate. ${ }^{12}$ Most properties of such a condensate may be described by a single wavefunction, evolving in time as that of a free particle with the effective potential energy $U=q \phi=-2 e \phi$, where $\phi$ is the electrochemical potential, ${ }^{13}$ and $q=-2 e$ is the total charge of the Cooper pair. As a result, for the situation shown in Fig. 3, Eq. (53) takes the form

$$
\begin{equation*}
\frac{d \varphi}{d t}=\frac{2 e}{\hbar} V, \tag{2.54}
\end{equation*}
$$

Josephson effect: basic equations
where $V=\phi_{1}-\phi_{2}$ is the applied voltage. B. Josephson has predicted that, in a particular case when a weal link is a tunnel junction, electric current $I$ of Cooper pairs through it should have a simple form: ${ }^{14}$

$$
\begin{equation*}
I=I_{c} \sin \varphi \tag{2.55}
\end{equation*}
$$

[^485]where $I_{c}$ is some constant (scaling as the weak link strength). Combining Eqs. (53) and (54), we see that if the applied voltage is constant in time, the current oscillates with the so-called Josephson frequency
\[

$$
\begin{equation*}
f_{J}=\frac{\omega_{J}}{2 \pi}, \quad \text { where } \omega_{J} \equiv \frac{2 e}{\hbar} \bar{V}, \tag{2.56}
\end{equation*}
$$

\]

as high as $\sim 484 \mathrm{MHz}$ per each microvolt of applied dc voltage. This effect is now well documented, though a direct detection of the Josephson radiation is tricky; it is much easier to observe the phase locking (synchronization) ${ }^{15}$ of the radiation by external microwave signal, which results in formation of nearly flat dc current steps at dc voltages

$$
\begin{equation*}
\bar{V}_{n}=n \frac{\hbar \omega}{2 e}, \tag{2.57}
\end{equation*}
$$

where $\omega$ is the external signal frequency and $n$ is an integer. ${ }^{16}$ This effect is now being used in highly accurate standards of dc voltage. ${ }^{17}$

Now, let us move on to a discussion of the opposite case, when a 1D particle modes in various potential profiles $U(x)$ that are constant in time. Conceptually, the simplest of such profiles is a potential step - see Fig. 4.


Fig. 2.4. Classical 1D motion in a potential profile $U(x)$.

As I am sure the reader knows, in classical mechanics, if a particle is incident on such a step (in Fig. 4, from the left), its kinetic energy $p^{2} / 2 m$ cannot be negative, so that it can only travel through the classically accessible region where its (conserved) full energy,

$$
\begin{equation*}
E=\frac{p^{2}}{2 m}+U(x) \tag{2.58}
\end{equation*}
$$

is larger than the local value $U(x)$. Let the initial velocity $v=p / m$ be positive, i.e. directed toward the step. Before it has reached the classical turning point $x_{c}$, defined by equation

$$
\begin{equation*}
U\left(x_{c}\right)=E, \tag{2.59}
\end{equation*}
$$

[^486]kinetic energy $p^{2} / 2 m$ never turns to zero, so that the particle continues to move in the initial direction. On the other hand, the particle cannot penetrate that classically forbidden region $x>x_{c}$, because there its kinetic energy would be negative there. At the point $x=x_{c}$, particle's velocity changes sign, i.e. it is reflected back from the classical turning point.

In order to see what the wave mechanics says about this situation, let us start from the simplest, sharp potential step shown with bold black lines in Fig. 5:

$$
U(x)=U_{0} \theta(x)= \begin{cases}0, & \text { at } x<0,  \tag{2.60}\\ U_{0}, & \text { at } 0<x .\end{cases}
$$

For this choice, and any energy within the interval $0<E<U_{0}$, the classical turning point is $x_{c}=0$.


Fig. 2.5. Reflection of a monochromatic wave from a potential step $U_{0}>E$. (This particular wavefunction's shape is for $U_{0}=5 E$.) The wavefunction is plotted with the same schematic vertical offset by $E$, as those in Fig. 1.7.

Let us represent an incident particle with a wave packet so long that the spread $\delta k \sim 1 / \delta x$ of its wave number spectrum, and hence the energy uncertainty $\delta E=\hbar \delta \omega=\hbar(d \omega / d k) \delta k$ is negligible in comparison with its average value $E<U_{0}$, as well as with ( $U_{0}-E$ ). In this case, $E$ may be considered a given constant, and the time dependence of the solution is given by Eq. (1.61), and we can limit ourselves to the solution of the 1D version of the stationary Schrödinger equation (1.63), in this case

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi}{d x^{2}}+U(x) \psi=E \psi \tag{2.61}
\end{equation*}
$$

for the spatial part $\psi(x)$ of the wavefunction. ${ }^{18}$
At $x<0$, i.e. at $U=0$, the equation is reduced to the Helmholtz equation (1.75), and may be satisfied with two traveling waves, proportional to $\exp \{+i k x\}$ and $\exp \{-i k x\}$ correspondingly, with $k$ satisfying the dispersion equation (1.30):

$$
\begin{equation*}
k^{2} \equiv \frac{2 m E}{\hbar^{2}} . \tag{2.62}
\end{equation*}
$$

Thus the general solution of Eq. (61) in this region may be presented as

[^487]\[

$$
\begin{equation*}
\psi_{-}(x)=A e^{+i k x}+B e^{-i k x} \tag{2.63}
\end{equation*}
$$

\]

The second term in the right-hand part evidently describes an (infinitely long) wave packet traveling to the left, which represents particle's reflection from the potential step. If $B=-A$, this solution is reduced to Eq. (1.76) for the potential well with infinitely high walls, but as we will see in a minute, for our current case of finite step height $U_{0}$, the relation between coefficients $B$ and $A$ may be different.

To show this, let us solve Eq. (61) for $x>0$, where $U=U_{0}>E$. In this region the equation may be rewritten as

$$
\begin{equation*}
\frac{d^{2} \psi_{+}}{d x^{2}}=\kappa^{2} \psi_{+} \tag{2.64}
\end{equation*}
$$

where $\kappa$ is a real constant defined by the relation similar to Eq. (62):

$$
\begin{equation*}
\kappa^{2} \equiv \frac{2 m\left(U_{0}-E\right)}{\hbar^{2}}>0 \tag{2.65}
\end{equation*}
$$

The general solution of Eq. (64) is the sum of $\exp \{+\kappa x\}$ and $\exp \{-\kappa x\}$, with arbitrary coefficients. However, the wavefunction should be finite at $x \rightarrow \infty$, so only the latter exponent is acceptable:

$$
\begin{equation*}
\psi_{+}(x)=C e^{-\kappa x} \tag{2.66}
\end{equation*}
$$

This penetration of the wavefunction into the classically forbidden region, and hence a finite probability to find the particle there, is one of the most fascinating predictions of quantum mechanics, and has been repeatedly observed in experiment, e.g., via tunneling experiments - see below. From Eq. (66), it is evident that the constant $\kappa$, defined by Eqs. (65), may be interpreted as the reciprocal penetration depth. Even for the lightest particles this depth is usually very small. Indeed, for $E \ll U_{0}$ that equation yields

$$
\begin{equation*}
\left.\delta \equiv \frac{1}{\kappa}\right|_{E=0}=\frac{\hbar}{\left(2 m U_{0}\right)^{1 / 2}} . \tag{2.67}
\end{equation*}
$$

For example, for a conduction electron in a typical metal, that runs, at its surface, into a sharp potential step $U_{0}$, whose height equals to metal's workfunction $W \approx 5 \mathrm{eV}$ (see the discussion of the photoelectric effect in Sec. 1.1), $\delta$ is close to 0.1 nm , i.e. is close to a typical size of an atom. For heavier elementary particles (e.g., protons) the penetration depth is correspondingly lower, and for macroscopic bodies it is hardly measurable.

Returning to our problem, we still should find coefficients $A, B$, and $C$ from the boundary conditions at $x=0$. Since $E$ is a finite constant, and $U(x)$ is a finite function, Eq. (61) says that $d^{2} \psi / d x^{2}$ should be finite as well. This means that the first derivative should be continuous:

$$
\begin{equation*}
\lim _{\varepsilon \rightarrow 0}\left(\left.\frac{d \psi}{d x}\right|_{x=+\varepsilon}-\left.\frac{d \psi}{d x}\right|_{x=-\varepsilon}\right)=\lim _{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{+\varepsilon} \frac{d^{2} \psi}{d x^{2}} d x=\frac{2 m}{\hbar^{2}} \lim _{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{+\varepsilon}[U(x)-E] \psi d x=0 \tag{2.68}
\end{equation*}
$$

Repeating such calculation for function $\psi(x)$ itself, we see that it also should be continuous at all points, including $x=0$, so that

$$
\begin{equation*}
\psi_{-}(0)=\psi_{+}(0), \quad \frac{d \psi_{-}}{d x}(0)=\frac{d \psi_{+}}{d x}(0) . \tag{2.69}
\end{equation*}
$$

Plugging solutions (63) and (66) into these two boundary conditions, we get a system of two linear equations

$$
\begin{equation*}
A+B=C, \quad i k A-i k B=-\kappa C \tag{2.70}
\end{equation*}
$$

whose (elementary) solution enables us to express $B$ and $C$ via $A$ :

$$
\begin{equation*}
B=A \frac{k-i \kappa}{k+i \kappa}, \quad C=A \frac{2 k}{k+i \kappa} . \tag{2.71}
\end{equation*}
$$

We immediately see that since the numerator and denominator in the first of these formulas have equal moduli, so that $|B|=|A|$. This means that, as we could expect, a particle with energy $E<U_{0}$ is totally reflected from the step. As a result, at $x<0$ our solution (63) may be presented by a standing wave

$$
\begin{equation*}
\psi_{-}=2 i A e^{i \theta} \sin (k x-\theta), \quad \text { with } \theta \equiv \tan ^{-1} \frac{k}{\kappa} . \tag{2.72}
\end{equation*}
$$

Notice that the shift $\Delta x \equiv \theta / k=\left(\tan ^{-1} k / \kappa\right) / k$ of the standing wave to the right, due to the partial penetration of the wavefunction under the potential step, is commensurate with, but generally not equal to $\delta \equiv 1 / \kappa$. Figure 5 shows the full behavior of the wavefunction, for a particular case $E=U_{0} / 5$, at which $k / \kappa=\left[E /\left(U_{0}-E\right)\right]^{1 / 2}=1 / 2$.

According to Eq. (65), as the particle's energy $E$ is increased to approach $U_{0}$, the penetration depth $1 / \kappa$ diverges. This raises an important issue: what happens at $E>U_{0}$, i.e. if there is no classically forbidden region in the problem? Again, in classical mechanics the incident particle would continue to move to the right, though with a reduced velocity, corresponding to the new kinetic energy $E-U_{0}$, so there would be no reflection. In quantum mechanics, however, the situation is different. In order to analyze it, it is not necessary to re-solve the whole problem; it is sufficient to note that all our calculations, and hence Eqs. (71) are still valid if we take ${ }^{19}$

$$
\begin{equation*}
\kappa=-i k^{\prime}, \quad \text { with } \quad k^{\prime 2} \equiv \frac{2 m\left(E-U_{0}\right)}{\hbar^{2}}>0 . \tag{2.73}
\end{equation*}
$$

With this replacement, Eq. (71) becomes ${ }^{20}$

$$
\begin{equation*}
B=A \frac{k-k^{\prime}}{k+k^{\prime}}, \quad C=A \frac{2 k}{k+k^{\prime}} . \tag{2.74}
\end{equation*}
$$

The most important result of this change is that now the reflection is not complete: $|B|<|A|$. In order to evaluate this effect qualitatively, it is more fair to use not the $B / A$ or $C / A$ ratios, but rather that

[^488]of the probability currents (5) corresponding to traveling waves with amplitudes $C$ and $A$, in the corresponding regions (respectively, $x>0$ and $x<0$ ):
\[

$$
\begin{equation*}
T \equiv \frac{I_{C}}{I_{A}}=\frac{k^{\prime}|C|^{2}}{k|A|^{2}}=\frac{4 k k^{\prime}}{\left(k+k^{\prime}\right)^{2}}=\frac{4\left[E\left(E-U_{0}\right)\right]^{1 / 2}}{\left[E^{1 / 2}+\left(E-U_{0}\right)^{1 / 2}\right]^{2}} . \tag{2.75}
\end{equation*}
$$

\]

( $T$ so defined is called the transparency of the inhomogeneity, in our current case of the potential step.) The result given by Eq. (75) is plotted in Fig. 6a. Notice its most important features:
(i) At $U_{0}=0$, the transparency is full, $T=1$ - naturally, for having no step at all.
(ii) At $U_{0} \rightarrow E$, the transparency tends to zero - giving a proper connection with the case $E<U_{0}$.
(iii) We can use result (75) even for $U_{0}<0$, i.e. for the step-down (or "cliff") profile - see Fig. 6 b. Very counter-intuitively, the particle is (partly) reflected even from such a cliff, and the transmission diminishes (rather slowly) at $U_{0} \rightarrow-\infty$.



Fig. 2.6. (a) Transparency of a potential step with $U_{0}<E$ as a function of its height, according to Eq. (75), and (b) the potential profile at $U_{0}<0$.

The most important conceptual conclusion of our analysis is that the quantum particle is partly reflected from a potential step with $U_{0}<E$, in the sense that there is a nonvanishing probability $T<1$ to find it passed over the step, while there is also probability $(1-T)$ to have it reflected.

The same property is exhibited, for any relation between $E$ and $U_{0}$, by another simple potential profile $U(x)$, the famous tunnel barrier. Figure 7 shows its simple, "rectangular" version:

$$
U(x)=\left\{\begin{array}{lr}
0, & \text { for } x<-d / 2  \tag{2.76}\\
U_{0}, & \text { for }-d / 2<x<+d / 2 \\
0, & \text { for }+d / 2<x
\end{array}\right.
$$



Fig. 2.7. Rectangular tunnel barrier.

In order to analyze this problem, it is sufficient to look for the solution to the Schrödinger equation in the form (63) at $x \leq-d / 2$. At $x>+d / 2$, i.e., behind the barrier, we may use the arguments presented above (no wave packet source on the right!) to keep just one traveling wave,

$$
\begin{equation*}
\psi_{+}(x)=F e^{i k x} . \tag{2.77}
\end{equation*}
$$

However, under the barrier, i.e. at $-d / 2 \leq x \leq+d / 2$, we should generally keep both exponential terms,

$$
\begin{equation*}
\psi_{b}(x)=C e^{-\kappa x}+D e^{+\kappa x} \tag{2.78}
\end{equation*}
$$

because our previous argument, used in the potential step problem's solution, is no longer valid. (Here $k$ and $\kappa$ are still defined, respectively, by Eqs. (62) and (65).) In order to find the relation between coefficients $A, B, C, D$, and $F$, we need to plug in the solutions into the boundary conditions similar to Eqs. (69), but now at two boundary points, $x= \pm d / 2$.

Solving the resulting system of 4 linear equations for five amplitudes $(A, B, C, D$, and $F$ ), we can readily calculate four ratios $B / A, C / A$, etc., in particular,

$$
\begin{equation*}
\frac{F}{A}=\frac{\exp \{-i k d\}}{\cosh \kappa d+\frac{i}{2}\left(\frac{\kappa}{k}-\frac{k}{\kappa}\right) \sinh \kappa d} \tag{2.79a}
\end{equation*}
$$

and hence barrier's transparency

Rectangular tunnel barrier's transparency

$$
\begin{equation*}
T \equiv\left|\frac{F}{A}\right|^{2}=\left[\cosh ^{2} \kappa d+\left(\frac{\kappa^{2}-k^{2}}{2 \kappa k}\right)^{2} \sinh ^{2} \kappa d\right]^{-1} \tag{2.79b}
\end{equation*}
$$

Figure 8 a shows the transparency as a function of particle energy $E$, for several characteristic values of the barrier thickness $d$, or rather of the ratio $d / \delta$, where $\delta$ is defined by Eq. (67).


Fig. 2.8. Transparency of the rectangular tunnel barrier as a function of particle's energy $E$.

The plots show that for a thin barrier $(d<\delta)$ the transparency grows gradually with particle's energy. This growth is natural, because the penetration constant $\kappa$ decreases with the growth of $E$, i.e., the wavefunction penetrates more and more into the barrier, so that more and more of it is "picked up" at the second interface $(x=+d / 2)$ and transferred into the wave $F \exp \{i k x\}$ propagating behind the barrier. As Eq. (79b) shows, for thick barriers ( $d \gg \delta$ ), this dependence is dominated by an exponent,

$$
\begin{equation*}
T \approx\left(\frac{4 k \kappa}{k^{2}+\kappa^{2}}\right)^{2} e^{-2 \kappa d} \tag{2.80}
\end{equation*}
$$

Thick
tunnel
barrier's transparency
that may be clearly seen as a straight segments in semi-log plots (Fig. 8b) of $T$ as a function of the combination $\left(1-E / U_{0}\right)^{1 / 2}$ which is proportional to $\kappa$ - see Eq. (65).

Equation (80) also clearly shows the exponential dependence of the barrier transparency of its thickness at $d \gg \delta$. This dependence is the most important factor for various applications of the quantum-mechanical tunneling - from the field emission ${ }^{21}$ of electrons to scanning tunneling microscopy. ${ }^{22}$ Also noted should be substantial negative implications of the effect for modern electronic engineering, most importantly imposing a limit for scaling down of field effect transistors in semiconductor integrated circuits (and hence the circuit density increase according to the well-known Moore's law), due to increase of tunneling both through the gate oxide and along transistor's channel. ${ }^{23}$

Another interesting effect visible in Fig. 8a (for case $d=0.3 \delta$ ) are the oscillations of $T$ at $E>U_{0}$. This is our first glimpse at one more interesting quantum effect: resonant tunneling. I will discuss this effect in detail in Sec. 5 below.

### 2.4. The WKB approximation

Before moving on to exploring more complex potentials, let us see whether the results discussed in the previous section hold on in the opposite limit of so-called soft, gradual potential profiles, like that sketched in Fig. 4. (The quantitative conditions of the "softness" will be derived below). The most efficient analytical tool in this limit is the $W K B$ (or "quasiclassical") approximation developed by H. Jeffrey, G. Wentzel, A. Kramers, and L. Brillouin in 1926-27.

In order to derive its 1D version, let us rewrite the Schrödinger equation (61) as

$$
\begin{equation*}
\frac{d^{2} \psi}{d x^{2}}+k^{2}(x) \psi=0 \tag{2.81}
\end{equation*}
$$

where the local value of wave number $k(x)$ is defined similarly to Eq. (73),

$$
\begin{equation*}
k^{2}(x) \equiv \frac{2 m[E-U(x)]}{\hbar^{2}} \tag{2.82}
\end{equation*}
$$

Local wave
number
but now it may be a function of $x$. We already know that for $k(x)=$ const, the fundamental solutions of this equation have form $A \exp \{+i k x\}$ and $B \exp \{-i k x\}$. Any of them may be presented in a simple form

[^489]\[

$$
\begin{equation*}
\psi(x)=e^{i \Phi(x)} \tag{2.83}
\end{equation*}
$$

\]

where $\Phi(x)$ is a complex function, in this simplest case equal to either $(k x-i \ln A)$ or $(-k x-i \ln B)$. This is why we may try use Eq. (83) to look for solution of Eq. (81) even in the general case, $k(x) \neq$ const. Differentiating Eq. (83) twice, we get

$$
\begin{equation*}
\frac{d \psi}{d x}=i \frac{d \Phi}{d x} e^{i \Phi}, \quad \frac{d^{2} \psi}{d x^{2}}=\left[i \frac{d^{2} \Phi}{d x^{2}}-\left(\frac{d \Phi}{d x}\right)^{2}\right] e^{i \Phi} \tag{2.84}
\end{equation*}
$$

Plugging the last expression into Eq. (81) and requiring the factor before $\exp \{i \Phi(x)\}$ to vanish, we get

$$
\begin{equation*}
i \frac{d^{2} \Phi}{d x^{2}}-\left(\frac{d \Phi}{d x}\right)^{2}+k^{2}(x)=0 \tag{2.85}
\end{equation*}
$$

This is still an exact, general result. At the first sight, it looks worse than the initial equation (81), because Eq. (85) is nonlinear. However, it is more ready for simplification in the limit when the potential profile is very smooth, $d U / d x \rightarrow 0$. Indeed, we know that for a uniform potential, $\Phi$ " $=0$. Hence, in the " $0^{\text {th" }}$, approximation, $\Phi(x) \rightarrow \Phi_{0}(x)$, we may try to keep that result, so that Eq. (85) yields

$$
\begin{equation*}
\left(\frac{d \Phi_{0}}{d x}\right)^{2}=k^{2}(x) \tag{2.86a}
\end{equation*}
$$

Just as in the uniform case, this equation has two roots,

$$
\begin{equation*}
\frac{d \Phi_{0}}{d x}= \pm k(x) \tag{2.86b}
\end{equation*}
$$

so that its general solution is

$$
\begin{equation*}
\psi_{0}(x)=A \exp \left\{+i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}+B \exp \left\{-i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}, \tag{2.87}
\end{equation*}
$$

where $x$ ' is the lower limits of integration affect only constants $A$ and $B$. The physical sense of this result is simple: it is a sum of forward- and back-propagating waves, with the coordinate-dependent local wave number $k(x)$ that self-adjusts to the potential profile.

Let me emphasize the non-trivial nature of this approximation. ${ }^{24}$ First, any attempt to address the problem with a standard perturbation approach (say, $\psi=\psi_{0}+\psi_{1}+\ldots$, with $\psi_{n}$ proportional to $n^{\text {th }}$ power of some small parameter, ${ }^{25}$ in this case scaling $d^{2} U / d^{2} x$ ) would fail for most potentials, because even a slight but persisting deviation of $U(x)$ from a constant leads to a gradual accumulation of phase $\Phi_{0}$, impossible to describe by any small perturbation of $\psi$. Second, the dropping of term $d^{2} \Phi / d x^{2}$ in Eq. (85) is not too easy to justify. Indeed, since we are committed to the "soft potential limit" $d U / d x \rightarrow 0$, we should be ready to assume the characteristic length $a$ of spatial variation of $\Phi$ to be large, and neglect

[^490]the terms that are the smallest ones in the limit $a \rightarrow \infty$. However, both first terms in Eq. (85) are apparently of the same order in $a$, namely $O\left(a^{-2}\right)$; why have we neglected just one of them?

The price we have paid for such a "sloppy" treatment is high: Eq. (87) does not satisfy the fundamental property of the Schrödinger equation, the probability current conservation. Indeed, since Eq. (81) describes a fixed-energy (stationary) spatial part of the general Schrödinger equation, its probability density $w=\Psi \Psi^{*}=\psi \psi^{*}$, and should not depend on time. Hence, according to Eq. (6), we should have $I(x)=$ const. However, this is not true for each component of Eq. (87); for example for the forward-propagating component of its right-hand part, Eq. (5) yields

$$
\begin{equation*}
I_{0}(x)=\frac{\hbar}{m}|A|^{2} k(x), \tag{2.88}
\end{equation*}
$$

evidently not a constant if $k(x) \neq$ const.
The brilliance of the WKB theory is that the problem may be fixed without revising the $0^{\text {th }}$ approximation. Indeed, let us explore the next, $1^{\text {st }}$ approximation instead:

$$
\begin{equation*}
\Phi(x) \rightarrow \Phi_{\mathrm{WKB}}(x) \equiv \Phi_{0}(x)+\Phi_{1}(x) \tag{2.89}
\end{equation*}
$$

where $\Phi_{0}$ still obeys Eq. (85), while $\Phi_{1}$ describes a small correction to the $0^{\text {th }}$ approximation, in the following sense: ${ }^{26}$

$$
\begin{equation*}
\left|\frac{d \Phi_{1}}{d x}\right| \ll\left|\frac{d \Phi_{0}}{d x}\right|=k(x) . \tag{2.90}
\end{equation*}
$$

Plugging Eq. (89) into Eq. (85), with the account of the definition (86), we get

$$
\begin{equation*}
i\left(\frac{d^{2} \Phi_{0}}{d x^{2}}+\frac{d^{2} \Phi_{0}}{d x^{2}}\right)-\frac{d \Phi_{1}}{d x}\left(2 \frac{d \Phi_{0}}{d x}+\frac{d \Phi_{1}}{d x}\right)=0 \tag{2.91}
\end{equation*}
$$

Using condition (90), we may neglect $d^{2} \Phi_{1} / d x^{2}$ in comparison with $d^{2} \Phi_{0} / d x^{2}$ in the first parenthesis, and $d \Phi_{1} / d x$ in comparison with $2 d \Phi_{0} / d x$ in the second parenthesis. As a result, we get the following approximate result:

$$
\begin{gather*}
\frac{d \Phi_{1}}{d x}=\frac{i}{2} \frac{d^{2} \Phi_{0}}{d x^{2}} / \frac{d \Phi_{0}}{d x}=\frac{i}{2} \frac{d}{d x}\left(\ln \frac{d \Phi_{0}}{d x}\right)=\frac{i}{2} \frac{d}{d x}[\ln k(x)]=i \frac{d}{d x}\left[\ln k^{1 / 2}(x)\right],  \tag{2.92}\\
\left.i \Phi\right|_{\mathrm{WKB}} \equiv i \Phi_{0}+i \Phi_{1}= \pm i \int^{x} k\left(x^{\prime}\right) d x^{\prime}+\ln \frac{1}{k^{1 / 2}(x)},  \tag{2.93}\\
\psi_{\mathrm{WKB}}(x)=\frac{a}{k^{1 / 2}(x)} \exp \left\{i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}+\frac{b}{k^{1 / 2}(x)} \exp \left\{-i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}, \text { for } k^{2}(x)>0 . \tag{2.94}
\end{gather*}
$$

(Again, the lower integration limit is arbitrary, but its choice may be incorporated into complex constants $a$ and $b$.) This modification of the $0^{\text {th }}$ approximation (87) overcomes the problem of current continuity; for example, for the forward-propagating wave, Eq. (5) gives

[^491]\[

$$
\begin{equation*}
I_{\mathrm{WKB}}(x)=\frac{\hbar}{m}|a|^{2}=\mathrm{const} \tag{2.95}
\end{equation*}
$$

\]

Physically, factor $k^{1 / 2}$ in the denominator of the WKB wavefunction's pre-exponent is easy to understand. The smaller the local group velocity (34) of the wave packet, $v_{\mathrm{gr}}(x)=\hbar k(x) / m$, the "easier" (more probable) it should be to find the particle within a certain interval $d x$. This is exactly the result that WKB gives: $d W / d x=w(x)=\psi \psi^{*} \propto 1 / k(x) \propto 1 / v_{\mathrm{gr}}$.

Another value of the $1^{\text {st }}$ approximation is a clarification of WKB theory's validity condition: it is given by Eq. (90). Plugging into this relation the first form of Eq. (92), and estimating $\left|\Phi_{0}{ }^{\prime}\right|$ as $\left|\Phi_{0}{ }^{\prime}\right| / a$, where $a$ is the spatial scale of a substantial change of $\left|\Phi_{0}{ }^{\prime}\right|=k(x)$, we can rewrite the condition as

$$
\begin{equation*}
k a \gg 1 \tag{2.96}
\end{equation*}
$$

In plain English, this means that the region where $U(x)$, and hence $k(x)$, change substantially should contain many de Broglie wavelengths $\lambda=2 \pi / k$.

So far I have implied that $k^{2}(x) \propto E-U(x)$ is positive, i.e. particle moves in the classically accessible region. Now let us extend the WKB approximation to the situation where the difference $E$ $U(x)$ may change sign, for example to the reflection problem sketched in Fig. 4. Just as we did for the sharp potential step, we first need to find the appropriate solution for the classically forbidden region, in this case $x>x_{c}$. For that, there is no need to redo our calculations, because they are still valid if we, just as in the sharp step problem, take $k(x)=i \kappa(x)$, where

$$
\begin{equation*}
\kappa^{2}(x) \equiv \frac{2 m[U(x)-E]}{\hbar^{2}}>0, \quad \text { for } x>x_{c} \tag{2.97}
\end{equation*}
$$

and keep just one of two possible solutions (with $\kappa>0$ ), in analogy with Eq. (66). The result is

$$
\begin{equation*}
\psi_{\mathrm{WKB}}(x)=\frac{c}{\kappa^{1 / 2}(x)} \exp \left\{-\int^{x} \kappa\left(x^{\prime}\right) d x^{\prime}\right\}, \quad \text { for } k^{2}<0, \text { i.e. } \kappa^{2}>0, \tag{2.98}
\end{equation*}
$$

with the lower limit at some point with $\kappa^{2}>0$ as well. This is a really wonderful formula! It describes the quantum-mechanical penetration of the particle into the classically forbidden region, and provides a natural generalization of Eq. (66) - leaving intact, of course, our estimates of the depth $\delta \sim 1 / \kappa$ of such penetration.

Now we have to do what we have done for the sharp-step problem in Sec. 2: use the boundary conditions in the interface point $x=x_{c}$ to relate constants $a, b$, and $c$. However, now this operation is a tad more complex, because both WKB functions (94) and (98) diverge, albeit weakly, at the classical turning point, were both $k(x)$ and $\kappa(x)$ tend to zero. This connection problem may be however, solved in the following way. ${ }^{27}$ Let us use the commitment of potential "softness", assuming that it allows us to keep just two leading terms in the Taylor expansion of function $U(x)$ at point $x_{c}$ :

$$
\begin{equation*}
U(x) \approx U\left(x_{c}\right)+\left.\frac{d U}{d x}\right|_{x=x_{c}}\left(x-x_{c}\right)=E+\left.\frac{d U}{d x}\right|_{x=x_{c}}\left(x-x_{c}\right) . \tag{2.99}
\end{equation*}
$$

[^492]Using this truncated expansion, and introducing a dimensionless variable for coordinate's deviation from the classical turning point,

$$
\begin{equation*}
\zeta \equiv \frac{x-x_{c}}{x_{0}}, \quad x_{0} \equiv\left(\frac{\hbar^{2}}{2 m(d U / d x)}\right)^{1 / 3}, \tag{2.100}
\end{equation*}
$$

we reduce the Schrödinger equation (61) to the simple Airy equation

$$
\begin{equation*}
\frac{d^{2} \psi}{d \zeta^{2}}-\zeta \psi=0 \tag{2.101}
\end{equation*}
$$

Airy equation

As for all linear, ordinary differential equations of the second order, the general solution of Eq. (101) may be presented as a linear combination of two fundamental solutions, in this case called Airy functions $\operatorname{Ai}(\zeta)$ and $\operatorname{Bi}(\zeta)$, shown in Fig. 9a.
(a)

(b)


Fig. 2.9. (a) Airy functions Ai and Bi , and (b) the WKB approximation for function $\mathrm{Ai}(\varsigma)$.

The latter function diverges at $\zeta \rightarrow \infty$, and thus is not suitable for our current problem (Fig. 4), while the former function has the following asymptotic behaviors at $|\zeta| \gg 1: 28$

$$
\operatorname{Ai}(\zeta) \rightarrow \frac{1}{\pi^{1 / 2}|\zeta|^{1 / 4}} \times \begin{cases}\frac{1}{2} \exp \left\{-\frac{2}{3} \zeta^{3 / 2}\right\}, & \text { for } \zeta \rightarrow+\infty  \tag{2.102}\\ \sin \left\{\frac{2}{3}(-\zeta)^{3 / 2}+\frac{\pi}{4}\right\}, & \text { for } \zeta \rightarrow-\infty\end{cases}
$$

Now let us apply the WKB approximation to the Airy equation (101). Taking the classical turning point $(\zeta=0)$ for the lower limit, for $\zeta>0$ we get (in dimensionless units)

[^493]are often convenient for practical calculation of Airy functions at intermediate values of the argument, $\mid \varsigma \sim 1$.
\[

$$
\begin{equation*}
\kappa^{2}(\zeta)=\zeta, \quad \kappa(\zeta)=\zeta^{1 / 2}, \int_{0}^{\zeta} \kappa\left(\zeta^{2}\right) d \zeta^{\prime}=\frac{2}{3} \zeta^{3 / 2}, \tag{2.103}
\end{equation*}
$$

\]

i.e. exactly the exponent in the first line of Eq. (102). Making a similar calculation for $\zeta<0$, with the natural assumption $|b|=|a|$ (full reflection from the potential step), we arrive at the following result:

$$
\mathrm{Ai}_{\mathrm{WKB}}(\zeta)=\frac{1}{|\zeta|^{1 / 4}} \times \begin{cases}c \exp \left\{-\frac{2}{3} \zeta^{3 / 2}\right\}, & \text { for } \zeta>0  \tag{2.104}\\ a \sin \left\{\frac{2}{3}(-\zeta)^{3 / 2}+\varphi\right\}, & \text { for } \zeta<0\end{cases}
$$

This approximation differs from the exact solution at small values of $\zeta$, i.e. close to the classical turning point - see Fig. 9b. However, at $|\zeta| \gg 1$, Eqs. (104) describe the Airy function exactly if

$$
\begin{equation*}
\varphi=\frac{\pi}{4} \quad \text { and } \quad c=\frac{a}{2} . \tag{2.105}
\end{equation*}
$$

Hence we can use these connection formulas to express the relations between coefficients $a, b$, and $c$ of the general WKB solutions (94) and (98). In particular, the first of them yields $b=-a \exp \{i \pi / 2\}$, so that Eq. (94) becomes

$$
\begin{equation*}
\psi_{\mathrm{WKB}}\left(x<x_{c}\right)=\frac{a^{\prime}}{k^{1 / 2}(x)}\left[\exp \left\{+i \int_{x_{c}}^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}-\exp \left\{-i \int_{x_{c}}^{x} k\left(x^{\prime}\right) d x^{\prime}+i \frac{\pi}{2}\right\}\right] . \tag{2.106}
\end{equation*}
$$

This result may be also described by a simple mnemonic rule: reflecting from a "soft" potential step, the wavefunction acquires an additional phase shift $\Delta \varphi=\pi / 2$, if compared with the reflection from a "hard" (vertical) potential wall located at $x=x_{c}$, for which, according to Eq. (1.76), we would have $b=-a$.

Let us quantify the condition of validity of the connection formulas (105) - in other words, the criterion of the step "softness". For that, within the region where the WKB approximation differs from for the exact Airy equation $\left(|\zeta| \sim 1\right.$, i.e. $\left|x-x_{c}\right| \sim x_{0}$ ), the deviation from the linear approximation (99) of the potential profile should be relatively small. This deviation may be estimated using the next term of the Taylor expansion, $d^{2} U /\left.d^{2} x\right|_{x=x c}\left(x-x_{c}\right)^{2} / 2$. As a result, the softness condition may be expressed as $\left|d^{2} U / d^{2} x\right|_{x=x c} x_{0} \ll|d U / d x|_{x=x c}$. With the account of Eq. (100) for $x_{0}$, the condition becomes

WKB:
second condition of validity

$$
\begin{equation*}
\left|\frac{d^{2} U}{d x^{2}}\right|_{x=x c}^{3} \ll \frac{2 m}{\hbar^{2}}\left(\frac{d U}{d x}\right)_{x=x c}^{4} \tag{2.107}
\end{equation*}
$$

As an example of a very useful application of the WKB approximation, let us use it to calculate the energy spectrum of 1D particle in a soft 1D quantum well (Fig. 10). As was discussed above, we may always consider the standing wave describing an eigenstate $\psi_{n}$ (corresponding to eigenenergy $E_{n}$ ) as a traveling wave going back and forth between the walls, being sequentially reflected by each of them. Let us apply the WKB approximation to such a traveling wave. First, according to Eq. (94), propagating from the left classical turning point $x_{L}$ to the right point $x_{R}$, it acquires phase change

$$
\begin{equation*}
\Delta \varphi_{\rightarrow}=\int_{x_{L}}^{x_{R}} k(x) d x \tag{2.108}
\end{equation*}
$$

At the reflection from the soft wall at $x_{R}$, according to the connection formula (106), the wave acquires an additional shift $\pi / 2$. Now, traveling back from $x_{R}$ to $x_{L}$ the wave gets a shift similar to one given by Eq. (108): $\Delta \varphi_{\leftarrow}=\Delta \varphi_{\rightarrow}$. Finally, at the reflection from $x_{L}$ it gets one more $\pi / 2$. Summing up all these contributions, we may write the self-consistency condition (that the wavefunction "catches its own tail with its teeth"), in the form

$$
\begin{equation*}
\Delta \varphi_{\text {total }} \equiv \Delta \varphi_{\rightarrow}+\frac{\pi}{2}+\Delta \varphi_{\leftarrow}+\frac{\pi}{2}=2 \int_{x_{L}}^{x_{R}} k(x) d x+\pi=2 \pi n, \quad \text { with } n=1,2, \ldots \tag{2.109}
\end{equation*}
$$

Rewriting this result in terms of particle's momentum $p(x)=\hbar k(x)$, we arrive at the famous 1D BohrSommerfeld quantization rule

$$
\begin{equation*}
\oint_{C} p(x) d x=2 \pi \hbar\left(n-\frac{1}{2}\right) \tag{2.110}
\end{equation*}
$$

Bohr-
Sommerfeld quantization rule
where the closed path $C$ means the full period of classical motion. ${ }^{29}$


Fig. 2.10. Quasiclassical treatment of eigenstates in a soft 1D potential well.

Let us see what does this rule give for the very important particular case of a quadratic potential profile of a harmonic oscillator of frequency $\omega_{0}$. In this case,

$$
\begin{equation*}
U(x)=\frac{m}{2} \omega_{0}^{2} x^{2}, \tag{2.111}
\end{equation*}
$$

and the classical turning points are the roots of a simple equation

$$
\begin{equation*}
\frac{m}{2} \omega_{0}^{2} x_{c}^{2}=E_{n} \tag{2.112}
\end{equation*}
$$

so that $x_{R}=x_{n} \equiv\left(2 E_{n} / m\right)^{1 / 2} / \omega_{0}>0, x_{L}=-x_{n}<0$. Due to potential's symmetry, the integration required by Eq. (110) is also simple:

$$
\begin{equation*}
\int_{x_{L}}^{x_{R}} p(x) d x=\int_{-x_{c}}^{+x_{c}}\left\{2 m\left[E_{n}-U(x)\right]\right\}^{1 / 2} d x=\left(2 m E_{n}\right)^{1 / 2} \int_{-x_{c}}^{+x_{c}}\left(1-\frac{x^{2}}{x_{n}^{2}}\right)^{1 / 2} d x=\left(2 m E_{n}\right)^{1 / 2} x_{n} \frac{\pi}{2}=\frac{2 E_{n}}{\omega_{0}} \frac{\pi}{2} \tag{2.113}
\end{equation*}
$$

[^494]so that Eq. (110) is satisfied if
\[

$$
\begin{equation*}
E_{n}=\hbar \omega_{0}\left(n^{\prime}+\frac{1}{2}\right), \quad \text { with } n^{\prime} \equiv n-1=0,1,2, \ldots \tag{2.114}
\end{equation*}
$$

\]

In order to estimate the validity of this result, we have to check condition (96) at all points of the classically allowed region, and Eq. (107) at the turning points. A straightforward calculation shows that both conditions are valid for $n \gg 1$. However, we will see below that Eq. (114) is actually exactly correct for all energy levels - thanks to special properties of potential profile (111).

Now, let us look at the second of connection formulas (105), $c=a / 2$. Again, it differs from the result (71) for a sharp potential step, that may be rewritten as

$$
\begin{equation*}
C=A \frac{2 k}{k+i \kappa}=A \frac{2}{\left[1+(\kappa / k)^{2}\right]^{1 / 2}} \exp \{-i 2 \theta\}, \tag{2.115}
\end{equation*}
$$

by both the modulus and phase factor. (In the WKB approximation, the latter factor always equals $\pi / 4$.) Hence, again, the WKB approximation's prediction is not exact for sharp potentials; nevertheless, it is broadly used for practical calculations. One of the most important of them is the transparency of an arbitrary but smooth potential barrier (Fig. 11).


Fig. 2.11. 1D potential barrier of an arbitrary (but smooth) shape.

Here, just as in the case of a rectangular barrier, we need to take unto consideration five partial "waves" (or rather fundamental solutions of the Schrödinger equation): ${ }^{30}$

$$
\psi_{\mathrm{WKB}}= \begin{cases}\frac{a}{k^{1 / 2}(x)} \exp \left\{i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}+\frac{b}{k^{1 / 2}(x)} \exp \left\{-i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}, & \text { for } x<x_{c},  \tag{2.116}\\ \frac{c}{\kappa^{1 / 2}(x)} \exp \left\{-\int^{x} \kappa\left(x^{\prime}\right) d x^{\prime}\right\}+\frac{d}{\kappa^{1 / 2}(x)} \exp \left\{\int^{x} \kappa\left(x^{\prime}\right) d x^{\prime}\right\}, & \text { for } x_{c}<x<x_{c}{ }^{\prime}, \\ \frac{f}{k^{1 / 2}(x)} \exp \left\{i \int^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}, & \text { for } x_{c}{ }^{\prime}<x,\end{cases}
$$

where lower limits of integrals are arbitrary (each within the corresponding range of $x$ ). Since on the right of the left classical point we have two exponents rather than one, and on the right of the second

[^495]point, one traveling waves rather than two, the connection formulas (105) have to be generalized, using asymptotic formulas not only for $\operatorname{Ai}(\zeta)$, but also for the second Airy function, $\mathrm{Bi}(\zeta)$. The analysis, absolutely similar to that carried out above (though naturally a bit more bulky), ${ }^{31}$ gives a remarkably simple result:
\[

$$
\begin{equation*}
T_{\mathrm{WKB}} \equiv\left|\frac{f}{a}\right|^{2}=\exp \left\{-2 \int_{x_{c}}^{x_{c}^{\prime}} \kappa(x) d x\right\}=\exp \left\{-\frac{2}{\hbar} \int_{x_{c}}^{x_{c}^{\prime}}(2 m[U(x)-E])^{1 / 2} d x\right\}, \tag{2.117}
\end{equation*}
$$

\]

with no pre-exponential factor. This formula is broadly used in applied quantum mechanics, despite the approximate character of its pre-exponential coefficient for insufficiently soft barriers that do not satisfy Eq. (107). For example, Eq. (80) shows that for a thick rectangular barrier with $k=\kappa$, i.e. $U_{0}=2 E$, the WKB approximation (117) underestimates $T$ by a factor of 4 . However, on the logarithmic scale of Fig. 8 b , such factor, about half an order of magnitude, still looks as a small correction.

Notice that when $E$ approaches the barrier top $U_{\max }$ (Fig. 11), points $x_{c}$ and $x_{c}{ }^{\prime}$ merge, so that, according to Eq. (117), $T_{\mathrm{WKB}} \rightarrow$ 1, i.e. the particle reflection vanishes at $E=U_{\max }$. However, this conclusion is incorrect even for smooth barriers where one could naively expect the WKB approximation to work perfectly. Indeed, near point $x=x_{m}$ where the potential reaches maximum (i.e. $U\left(x_{m}\right)=U_{\max }$, we may always approximate a smooth function $U(x)$ by an inverted parabola,

$$
\begin{equation*}
U(x) \approx U_{\max }-\frac{m \omega_{0}^{2}\left(x-x_{m}\right)^{2}}{2} \tag{2.118}
\end{equation*}
$$

Calculating the derivatives $d U / d x$ and $d^{2} U / d x^{2}$ of this function and plugging them into condition (107), we see that the WKB approximation is only valid if $\left|U_{\max }-E\right| \gg \hbar \omega_{0}$. An exact analysis ${ }^{32}$ of tunneling through barrier (118) gives the following Kemble formula:

$$
\begin{equation*}
T=\frac{1}{1+\exp \left\{-2 \pi\left(E-U_{\max }\right) / \hbar \omega_{0}\right\}}, \tag{2.119}
\end{equation*}
$$

valid for any sign of difference $\left(E-U_{\max }\right)$. This formula describes a gradual approach of $T$ to 1 , i.e. a gradual reduction of reflection at particle energy's increase, with $T=1 / 2$ (rather than 1 ) at $E=U_{\text {max }}$.

Now the last remark of this section: our discussions of the propagator and the WKB approximation open a straight way toward an alternative formulation of quantum mechanics, based on the Feynman path integral, but I will postpone its discussion until a more compact ("bra-ket") notation has been introduced in Chapter 4.

### 2.5. Transfer matrix, resonant tunneling, and metastable states

Let us now explore motion in more complex potential profiles. The piecewise-constant and smooth-potential models of $U(x)$ are not too convenient here, because they both require "stitching" local

[^496]solutions in each classical turning point, which may lead to very cumbersome calculations. However, we may get a very good insight of the physics phenomena in such profiles, using their approximation by a set of Dirac's delta-functions. For that, let us have a look at what our old result (79) gives in the limit of a very thin and high rectangular barrier, $d \ll \delta, E \ll U_{0}$ (giving $k \ll \kappa \ll 1 / d$ ):
\[

$$
\begin{equation*}
T \equiv\left|\frac{F}{A}\right|^{2} \rightarrow \frac{1}{|1+i \alpha|^{2}}=\frac{1}{1+\alpha^{2}}, \tag{2.120}
\end{equation*}
$$

\]

where parameter $\alpha$ is defined as

$$
\begin{equation*}
\alpha \equiv \frac{1}{2}\left(\frac{\kappa^{2}-k^{2}}{\kappa k}\right) \kappa d \approx \frac{1}{2} \frac{\kappa^{2} d}{k} \approx \frac{m}{\hbar^{2} k} U_{0} d . \tag{2.121}
\end{equation*}
$$

The last product, $U_{0} d$, is just the "area"

$$
\begin{equation*}
w \equiv \int_{U(x)>E} U(x) d x \tag{2.122}
\end{equation*}
$$

of the barrier. This fact implies that the very simple result (120) for the transparency may be correct for a barrier of any shape, provided that it is sufficiently thin and high.

Indeed, let us consider the tunneling problem for a very thin barrier with $\kappa d, k d \ll 1$ (Fig. 12), approximating it by Dirac's $\delta$-function:

$$
\begin{equation*}
U(x)=w \delta(x) . \tag{2.123}
\end{equation*}
$$



Fig. 2.12. Delta-functional tunnel barrier.

We already know the solutions in all points but $x=0-$ see Eqs. (63) and (77) - so we only need to analyze boundary conditions in that point to find coefficients $A, B$, and $F$ - or rather the ratios $B / A$ and $F / A$. However, due to the special character of the $\delta$-function, we should be careful here. Indeed, instead of Eq. (68) we now get

$$
\begin{equation*}
\frac{d \psi_{+}}{d x}(0)-\frac{d \psi_{-}}{d x}(0)=\lim _{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{+\varepsilon} \frac{d^{2} \psi}{d x^{2}} d x=\lim _{\varepsilon \rightarrow 0} \frac{2 m}{\hbar^{2}} \int_{-\varepsilon}^{+\varepsilon}[U(x)-E] \psi d x=\frac{2 m}{\hbar^{2}} w_{\psi}(0) . \tag{2.124}
\end{equation*}
$$

On the other hand, the wavefunction itself is still continuous:

$$
\begin{equation*}
\psi_{+}(0)-\psi_{-}(0)=\lim _{\varepsilon \rightarrow 0} \int_{-\varepsilon}^{+\varepsilon} \frac{d \psi}{d x} d x=0 \tag{2.125}
\end{equation*}
$$

Using these boundary conditions, we readily get the following system of two linear equations,

$$
\begin{equation*}
A+B=F, \quad i k F-(i k A-i k B)=\frac{2 m w}{\hbar^{2}} F, \tag{2.126}
\end{equation*}
$$

whose solution yields

$$
\begin{equation*}
\frac{B}{A}=\frac{-i \alpha}{1+i \alpha}, \quad \frac{F}{A}=\frac{1}{1+i \alpha}, \quad \text { where } \alpha \equiv \frac{m w}{\hbar^{2} k} . \tag{2.127}
\end{equation*}
$$

For the barrier transparency $T \equiv|F / A|^{2}$, this result again gives Eq. (120). That formula may be recast to give a simple expression (valid only for $E \ll U_{\max }$ ) for the transmission coefficient,

$$
\begin{equation*}
T=\frac{1}{1+\alpha^{2}}=\frac{E}{E+E_{0}}, \quad \text { where } E_{0} \equiv \frac{m w^{2}}{2 \hbar^{2}} \tag{2.128}
\end{equation*}
$$

that shows that as energy becomes larger than parameter $E_{0}$, the barrier's transparency approaches unity.
However, the most important application of Eqs. (126) is for deriving transparency of more complex potential profiles. For that, let us first introduce very general notions of the scattering and transfer matrices, currently for the 1D case. Consider an arbitrary but finite-length potential "bump" (more formally called a scatterer), localized somewhere between points $x_{1}$ and $x_{2}$, on the flat potential background, say $U=0$ (Fig. 13). We know the general solution, with a certain energy $E$, outside the interval are a set of two sinusoidal waves. Let us present them in the form

$$
\begin{equation*}
\psi_{j}=A_{j} e^{i k\left(x-x_{j}\right)}+B_{j} e^{-i k\left(x-x_{j}\right)}, \tag{2.129}
\end{equation*}
$$

where (for now) $j=1$ or 2 , and $(\hbar k)^{2} / 2 m=E$. Note that each of the wave pairs (129) has, in this notation, its own reference point $x_{j}$, because this is very convenient for the calculations which follow.


Fig. 2.13. A single 1D scatterer.

As we have already discussed, if the wave/particle is incident from the left, the linear Schrödinger equation within the scatterer range ( $x_{1}<x<x_{2}$ ), can provide only linear expressions of the transmitted $\left(A_{2}\right)$ and reflected $\left(B_{1}\right)$ wave amplitudes via the incident wave amplitude $A_{1}$ :

$$
\begin{equation*}
A_{2}=S_{21} A_{1}, \quad B_{1}=S_{11} A_{1} \tag{2.130}
\end{equation*}
$$

where $S_{11}$ and $S_{21}$ are certain (generally, complex) coefficients. In this case, $B_{2}=0$. Alternatively, if a wave, with amplitude $B_{2}$, is incident from the right, it also may induce a transmitted wave $\left(B_{1}\right)$ and reflected wave $\left(A_{2}\right)$ with amplitudes

$$
\begin{equation*}
B_{1}=S_{12} B_{2}, \quad A_{2}=S_{22} B_{2}, \tag{2.131}
\end{equation*}
$$

where coefficients $S_{22}$ and $S_{12}$ are generally different from $S_{11}$ and $S_{21}$. Now we can use the linear superposition principle to argue that if waves $A_{1}$ and $B_{2}$ are simultaneously incident on the scatterer (say,
because wave $B_{2}$ has been partly reflected back by some other scatterer located at $x>x_{2}$ ), the resulting scattered wave amplitudes $A_{2}$ and $B_{1}$ are just the sums of their values for separate incident waves:

$$
\begin{align*}
& B_{1}=S_{11} A_{1}+S_{12} B_{2}  \tag{2.132}\\
& A_{2}=S_{21} A_{1}+S_{22} B_{2}
\end{align*}
$$

These linear relations may be conveniently presented by the so-called scattering matrix (frequently called just "S-matrix"):

Scattering
matrix: definition

$$
\binom{B_{1}}{A_{2}}=\mathrm{S}\binom{A_{1}}{B_{2}}, \quad \mathrm{~S} \equiv\left(\begin{array}{ll}
S_{11} & S_{12}  \tag{2.133}\\
S_{21} & S_{22}
\end{array}\right) .
$$

Scattering matrices, duly generalized, are an important tool for the analysis of wave scattering in more than one dimensions; for 1D problems, however, another matrix is more convenient to present the same linear relations (132). Indeed, let us solve this system for $A_{2}$ and $B_{2}$. The result is

Transfer
matrix: definition

$$
\left.\begin{array}{l}
A_{2}=T_{11} A_{1}+T_{12} B_{1}, \quad \text { i.e. } \quad\binom{A_{2}}{B_{2}}=T_{21} A_{1}+T_{22} B_{1}, \tag{2.134}
\end{array}\right)=\mathrm{T}\binom{A_{1}}{B_{1}}
$$

where T is the transfer matrix with elements

$$
\begin{equation*}
T_{11}=S_{21}-\frac{S_{11} S_{22}}{S_{12}}, \quad T_{12}=\frac{S_{22}}{S_{12}}, \quad T_{21}=-\frac{S_{11}}{S_{21}}, \quad T_{22}=\frac{1}{S_{12}} . \tag{2.135}
\end{equation*}
$$

One can wonder whether matrices $S$ and $T$ obey any universal properties that would be valid for an arbitrary (but time-independent) scatterer. Such universal equations may be readily found from the probability current conservation and the time-reversal symmetry of the Schrödinger equation. Let me leave finding these relations for reader's exercise. The results show, in particular, that the scattering matrix may be rewritten in the following form:

$$
\mathrm{S}=e^{i \theta}\left(\begin{array}{cc}
r e^{i \varphi} & t  \tag{2.136a}\\
t & -r e^{-i \varphi}
\end{array}\right)
$$

where 4 real parameters $r, t, \theta$, and $\varphi$ satisfy just one universal relation:

$$
\begin{equation*}
r^{2}+t^{2}=1 \tag{2.136b}
\end{equation*}
$$

(so that only 3 of the parameters are independent). As a result of this symmetry, $T_{11}$ may be also presented in a simpler form, similar to $T_{22}: T_{11}=\exp \{i \theta\} / t=1 / S_{12}{ }^{*}=1 / S_{21}{ }^{*}$. The last form allows a ready expression of scatterer's transparency via just one coefficient of the transfer matrix:

$$
\begin{equation*}
T \equiv\left|\frac{A_{2}}{A_{1}}\right|_{B_{2}=0}^{2}=\left|S_{21}\right|^{2}=\left|T_{11}\right|^{-2} \tag{2.137}
\end{equation*}
$$

In our current context, the most important property of 1D transfer matrices is that in order to find the total transfer matrix T of a system consisting of several (say, $N$ ) sequential arbitrary scatterers (Fig. 14), it is sufficient to multiply their matrices. Indeed, extending the definition (134) to other points $x_{j}(j$ $=1,2, \ldots, N+1$ ), we can write

$$
\begin{equation*}
\binom{A_{2}}{B_{2}}=\mathrm{T}_{1}\binom{A_{1}}{B_{1}}, \quad\binom{A_{3}}{B_{3}}=\mathrm{T}_{2}\binom{A_{2}}{B_{2}}=\mathrm{T}_{2} \mathrm{~T}_{1}\binom{A_{1}}{B_{1}}, \tag{2.138}
\end{equation*}
$$

etc. (where the matrix indices indicate the scatterers' order on axis $x$ ), so that

$$
\begin{equation*}
\binom{A_{N+1}}{B_{N+1}}=\mathrm{T}_{N} \mathrm{~T}_{N-1} \ldots \mathrm{~T}_{1}\binom{A_{1}}{B_{1}} . \tag{2.139}
\end{equation*}
$$



Fig. 2.14. A sequence of several 1D scatterers.

But we can also define the total transfer matrix similarly to Eq. (134), i.e. as

$$
\begin{equation*}
\binom{A_{N+1}}{B_{N+1}} \equiv \mathrm{~T}\binom{A_{1}}{B_{1}}, \tag{2.140}
\end{equation*}
$$

so that finally

$$
\begin{equation*}
\mathrm{T}=\mathrm{T}_{N} \mathrm{~T}_{N-1} \ldots \mathrm{~T}_{1} \tag{2.141}
\end{equation*}
$$

This formula is valid even if the flat-potential gaps between component scatterers vanish, so that it may be applied to a scatterer with an arbitrary profile $U(x)$, by fragmenting its length into small segments $\Delta x=x_{j+1}-x_{j}$, and treating each fragment as a rectangular barrier of height $\left(U_{j}\right)_{\text {ef }}=\left[U\left(x_{j+1}\right)-\right.$ $\left.U\left(x_{j}\right)\right] / 2$ - see Fig. 15. Since very efficient numerical algorithms are readily available for fast multiplication of matrices (especially as small as $2 \times 2$ ), this approach is broadly used in practice for the computation of transparency of tunnel barriers with complicated profiles $U(x)$. (This is much more efficient then the direct numerical solution of the Schrödinger equation.)

Fig. 2.15. The transfer matrix approach to a long tunnel barrier of an arbitrary

In order to use this approach for several conceptually important systems, let us calculate the transfer matrices for a few elementary scatterers, starting from the delta-functional barrier located at $x=$ 0 . Taking $x_{1}=x_{2}=0$, we can merely change the notation of wave amplitudes in Eq. (127) to get

Transfer matrix of a composite scatterer
profile.


$$
\begin{equation*}
S_{11}=\frac{-i \alpha}{1+i \alpha}, \quad S_{21}=\frac{1}{1+i \alpha} . \tag{2.142a}
\end{equation*}
$$

An absolutely similar analysis of the wave incidence from the left yields

$$
\begin{equation*}
S_{22}=\frac{-i \alpha}{1+i \alpha}, \quad S_{12}=\frac{1}{1+i \alpha}, \tag{2.142b}
\end{equation*}
$$

and using Eqs. (135), we get

Identity matrix

$$
\mathrm{T}_{\alpha}=\left(\begin{array}{cc}
1-i \alpha & -i \alpha  \tag{2.143}\\
i \alpha & 1+i \alpha
\end{array}\right)
$$

The next example may seem strange at the first glance: what if there is no scatterer at all between points $x_{1}$ and $x_{2}$ ? If points $x_{1}$ and $x_{2}$ coincide, the answer is indeed trivial and can be obtained, e.g., from Eq. (143) by taking $W=0$, i.e. $\alpha=0$ :

$$
\mathrm{T}_{0}=\left(\begin{array}{ll}
1 & 0  \tag{2.144}\\
0 & 1
\end{array}\right) \equiv \mathrm{I}
$$

- the so-called identity matrix. However, we are free to choose the reference points $x_{1,2}$ participating in Eq. (129) as we wish. For example, what if $x_{2}-x_{1}=a$ ? Let us first take the forward-propagating wave alone: $B_{2}=0$ (and hence $B_{1}=0$ ); then

$$
\begin{equation*}
\psi_{2}=\psi_{1}=A_{1} e^{i k\left(x-x_{1}\right)}=A_{1} e^{i k\left(x_{2}-x_{1}\right)} e^{i k\left(x-x_{2}\right)} . \tag{2.145}
\end{equation*}
$$

Comparison of this expression with the definition (129) for $j=2$ shows that $A_{2}=A_{1} \exp \left\{i k\left(x_{2}-x_{1}\right)\right\}=A_{1}$ $\exp \{i k a\}$, i.e. $T_{11}=\exp \{i k a\}$. Repeating the calculation for the back-propagating wave, we see that $T_{22}=$ $\exp \{-i k a\}$, and since this "no-potential" (space interval) provides no particle reflection, we finally get

$$
\mathrm{T}_{a}=\left(\begin{array}{cc}
e^{i k a} & 0  \tag{2.146}\\
0 & e^{-i k a}
\end{array}\right)
$$

independently of the mutual position of points $x_{1}$ and $x_{2}$. At $a=0$, we naturally recover the special case (143).

Now let us use these results to analyze the double-barrier system shown in Fig. 16. We could of course calculate its properties as before, writing down explicit expressions for all 5 traveling waves shown by arrows in Fig. 16, and then using boundary conditions (124) and (125) at each of points $x_{1,2}$ to get a system of 4 linear equations, and then solving it for 4 amplitude ratios.


Fig. 2.16. Double-barrier system. Dashed lines show (schematically) the position of metastable energy levels.

However, the transfer matrix approach simplifies the calculations, because we may immediately use Eqs. (141), (143), and (146) to write

$$
\mathrm{T}=\mathrm{T}_{\alpha} \mathrm{T}_{a} \mathrm{~T}_{\alpha}=\left(\begin{array}{cc}
1-i \alpha & -i \alpha  \tag{2.147}\\
i \alpha & 1+i \alpha
\end{array}\right)\left(\begin{array}{cc}
e^{i k a} & 0 \\
0 & e^{-i k a}
\end{array}\right)\left(\begin{array}{cc}
1-i \alpha & -i \alpha \\
i \alpha & 1+i \alpha
\end{array}\right) .
$$

Let me hope that the reader remembers the "row by column" rule of the multiplication of square matrices; ${ }^{33}$ using it for two last matrices, we reduce Eq. (147) to

$$
\mathrm{T}=\left(\begin{array}{cc}
1-i \alpha & -i \alpha  \tag{2.148}\\
i \alpha & 1+i \alpha
\end{array}\right)\left(\begin{array}{cc}
(1-i \alpha) e^{i k a} & -i \alpha e^{i k a} \\
i \alpha e^{-i k a} & (1+i \alpha) e^{-i k a}
\end{array}\right)
$$

Now there is no need to calculate all elements of the full product T, because, according to Eq. (137), for the calculation of barrier transparency $T$ we need only one its element, $T_{11}$ :

$$
\begin{equation*}
T=\frac{1}{\left|T_{11}\right|^{2}}=\frac{1}{\left|\alpha^{2} e^{-i k a}+(1-i \alpha)^{2} e^{i k a}\right|^{2}} . \tag{2.149}
\end{equation*}
$$

This result is similar to that following from Eq. (79) for $E>U_{0}$ : the transparency is a $\pi$-periodic function of the product $k a$, reaching the maximum $(T=1)$ at some point of each period - see Fig. 17a.

(a)

(b)


Fig. 2.17. Resonant tunneling through a quantum well with delta-functional walls :
(a) transparency a function of $k a$, and (b) calculating resonance's FWHM at $\alpha \gg 1$.

However, the new result is different in that for $\alpha \gg 1$, the resonance peaks of transparency are very narrow, reaching their maxima at $k a \approx k_{n} a \equiv n \pi$, with $n=1,2, \ldots$ Physics of this effect is immediately clear from the comparison of this result with our analysis of the simplest quantum well see Fig. 1.7 and its discussion. At $k \approx k_{n}$, the incident wave, which undertakes multiple sequential reflections from the semi-transparent walls of the well, forms a nearly standing wave, which at $\alpha \gg 1$ virtually coincides with one of eigenfunctions of the well with infinite walls, with the standing wave amplitude much larger that that of the incident wave. As a result, the transmitted wave amplitude is
${ }^{33}$ In the analytical form: $(\mathrm{AB})_{i j^{\prime}}=\sum_{j^{\prime \prime}=1}^{N} A_{i j^{\prime \prime}} B_{j^{\prime \prime j^{\prime}}}$, where $N$ is the matrix rank (in our current case, $N=2$ ).
proportionately increased. This is the famous effect of resonant tunneling, ${ }^{34}$ in mathematical description identical to the resonant transmission of light through an optical Fabry-Perot resonator formed by two parallel semi-transparent mirrors. ${ }^{35}$

Probably, the most surprising feature of this system is the fact that its maximum transparency is perfect $\left(T_{\max }=1\right)$ even at $\alpha \rightarrow \infty$, i.e. in the case of a very low transparency of each of two component barriers. ${ }^{36}$ Indeed, the denominator in Eq. (149) may be interpreted as the squared length of the difference between two vectors, one of length $\alpha^{2}$, and another of length $\left|(1-i \alpha)^{2}\right|=1+\alpha^{2}$, with angle $\theta=2 k a+$ const between them. At the resonance, the vectors are aligned, and the difference is smallest (equal to 1 ) - see Fig. 17b, so that $T_{\max }=1$.

We can use the same vector diagram to calculate the so-called FWHM, the common acronym for the Full Width [of the resonance curve at] Half-Maximum, i.e. the difference $\Delta k=k_{+}-k$. between such two points on the opposite slopes of the same resonance, at which $T=T_{\max } / 2-$ see arrows in Fig. 17a. Let the vectors in Fig. 17b be slightly misaligned, by an angle $\theta \sim 1 / \alpha^{2} \ll 1$, so that the length of the difference vector ( of the order of $\alpha^{2} \theta \sim 1$ ) is still much smaller than the length of each vector. In order to double its length squared, and hence reduce $T$ by a factor of 2 in comparison with its maximum value 1 , the arc, $\alpha^{2} \theta$, between the vectors should also become equal $\pm 1$, i.e. $\alpha^{2}\left(2 k_{ \pm} a+\right.$ const $)= \pm 1$. Subtracting these two equations from each other, we finally get

$$
\begin{equation*}
\Delta k \equiv\left(k_{+}-k_{-}\right)=\frac{1}{a \alpha^{2}} \ll k_{ \pm} . \tag{2.150}
\end{equation*}
$$

Now let us use the simple potential shown in Fig. 16 to discuss an issue of large conceptual importance. For that, consider what would happen if at some initial moment (say, $t=0$ ) we have placed a 1D quantum particle inside the double-barrier well with $\alpha \gg 1$, and left it there alone, without any incident wave. To simplify the analysis, let us prepare the initial state so that it coincides with the ground state of the infinite-wall well - see Eq. (1.76):

$$
\begin{equation*}
\Psi(x, 0)=\psi_{1}(x)=\left(\frac{2}{a}\right)^{1 / 2} \sin \left[k_{1}\left(x-x_{1}\right)\right], \quad \text { where } k_{1}=\frac{\pi}{a} \tag{2.151}
\end{equation*}
$$

At $\alpha \rightarrow \infty$, this is an eigenstate of the system, and from our analysis in Sec. 1.5 we know its time evolution:

$$
\begin{equation*}
\Psi(x, t)=\psi_{1}(x) e^{-i \omega_{1} t}, \quad \text { with } \omega_{1}=\frac{E_{1}}{\hbar}=\frac{\hbar k_{1}^{2}}{2 m}=\frac{\hbar \pi^{2}}{2 m a^{2}}, \tag{2.152}
\end{equation*}
$$

telling us that the particle remains in the well at all times with constant probability $W(t)=W(0)=1.37$
However, if parameter $\alpha$ is large but finite, the de Broglie wave should slowly "leak out" from the well, so that $W(t)$ would slowly decrease. Let us consider this effect approximately, assuming that

[^497]the slow leakage, with a characteristic time $\tau \gg 1 / \omega_{1}$, does not affect the instant wave distribution inside the well, besides the reduction of $W .{ }^{38}$ Then we can generalize Eqs. (151), (152) as follows:
\[

$$
\begin{equation*}
\left.\Psi(x, t)=\left(\frac{2 W}{a}\right)^{1 / 2} \sin \left[k_{1}\left(x-x_{1}\right)\right]\right] e^{-i \omega_{1} t} \tag{2.153}
\end{equation*}
$$

\]

making the probability of finding the particle in the well equal to $W$. This solution may be presented as a sum of two traveling waves:

$$
\begin{equation*}
\Psi(x, t)=A e^{i\left(k_{1} x-\omega_{1} t\right)}+B e^{-i\left(k_{1} x+\omega_{1} t\right)} \tag{2.154}
\end{equation*}
$$

with equal magnitudes of their amplitudes and probability currents

$$
\begin{equation*}
|A|=|B|=\left(\frac{W}{2 a}\right)^{1 / 2}, \quad I_{A}=\frac{\hbar}{m}|A|^{2} k_{1}=\frac{\hbar}{m} \frac{W}{2 a} \frac{\pi}{a}, \quad I_{B}=-I_{A} . \tag{2.155}
\end{equation*}
$$

But we already know from Eq. (128) that at $\alpha \gg 1$ the delta-functional wall transparency $T$ approximately equals $1 / \alpha^{2}$, so that the wave carrying current $I_{A}$, incident on the right wall from inside, induces an outcoming waves outside of the well (Fig. 18) with the following probability current:

$$
\begin{equation*}
I_{R}=\frac{1}{\alpha^{2}} I_{A}=\frac{1}{\alpha^{2}} \frac{\pi \hbar W}{2 m a^{2}} . \tag{2.156a}
\end{equation*}
$$

Absolutely similarly,

$$
\begin{equation*}
I_{L}=\frac{1}{\alpha^{2}} I_{B}=-I_{R} \tag{2.156b}
\end{equation*}
$$



Fig. 2.18. Metastable state's decay in the simple model of a 1D potential well with low-transparent walls - schematically.

Now we may combine the 1D version (6) of the probability conservation law for well's interior,

$$
\begin{equation*}
\frac{d W}{d t}+I_{R}-I_{L}=0 \tag{2.157}
\end{equation*}
$$

with Eqs. (156) to write

$$
\begin{equation*}
\frac{d W}{d t}=-\frac{1}{\alpha^{2}} \frac{\pi \hbar}{m a^{2}} W \tag{2.158}
\end{equation*}
$$

[^498]This is just the standard differential equation,

state's decay law

$$
\begin{equation*}
\frac{d W}{d t}=-\frac{1}{\tau} W \tag{2.159}
\end{equation*}
$$

of the exponential decay, with solution $W(t)=W(0) \exp \{-t / \tau\}$, where constant $\tau$, in our case equal to

$$
\begin{equation*}
\tau=\frac{m a^{2}}{\pi \hbar} \alpha^{2} \tag{2.160}
\end{equation*}
$$

is called the metastable state's lifetime. Using expression (2.34) for the de Broglie waves' group velocity, in our particular wave vector giving $v_{\mathrm{gr}}=\hbar k_{1} / m=\pi \hbar / m a$, Eq. (159) may be rewritten as

Metastable state's lifetime

$$
\begin{equation*}
\tau=\frac{t_{A}}{T} \tag{2.161}
\end{equation*}
$$

where in our case the attempt time $t_{A}$ is equal to $a / v_{\mathrm{gr}}$, and $T=1 / \alpha^{2}$. Relation (161), that is valid for a large class of metastable systems, ${ }^{39}$ may be interpreted in the following semi-classical way. The confined particle travels back and forth between the confining walls, with time intervals $t_{A}$ between the moments of incidence, each time making an attempt to leak through the wall, with a success probability of $T$, so the reduction of $W$ per each incidence is $\Delta W=-W T$, immediately leading to Eq. (161).

Another important look at Eq. (160) may be taken by returning to the resonant tunneling problem and expressing the resonance width (150) in terms of incident particle's energy:

$$
\begin{equation*}
\Delta E=\Delta\left(\frac{\hbar^{2} k^{2}}{2 m}\right) \approx \frac{\hbar^{2} k_{1}}{m} \Delta k=\frac{\hbar^{2} k_{1}}{m} \frac{1}{a \alpha^{2}}=\frac{\pi \hbar^{2}}{m a^{2} \alpha^{2}} . \tag{2.162}
\end{equation*}
$$

Comparing Eqs. (160) and (162), we get a remarkably simple formula

Energy-time uncertainty relation

$$
\begin{equation*}
\Delta E \cdot \tau=\hbar \tag{2.163}
\end{equation*}
$$

This so-called energy-time uncertainty relation is certainly more general than our simple model; for example, it is valid for the lifetime and resonance tunneling width of any metastable state. This seems very natural, since because of the energy identification with frequency, $E=\hbar \omega$, typical for quantum mechanics, Eq. (163) may be rewritten as $\Delta \omega \cdot \tau=1$ and seems to follow directly from the Fourier transform in time, just as the Heisenberg's uncertainty relation (1.35) follows from the Fourier transform in space. In some cases, these two relations are indeed interchangeable; for example, Eq. (24) for the Gaussian wave packet width may be rewritten as $\delta E \cdot \Delta t=\hbar$, where $\delta E=\hbar(d \omega / d k) \delta k=\hbar v_{\mathrm{gr}} \delta k$ is the r.m.s. spread of energies of monochromatic components of the packet, while $\Delta t \equiv \delta x / v_{\mathrm{gr}}$ is the time scale of the packet passage through a fixed observation point $x$.

However, Eq. (163) it is much less general than Heisenberg's uncertainty relation (1.35). Indeed, in non-relativistic quantum mechanics, Cartesian coordinates (say, $x$ ) of a particle, components of its momentum (say, $p_{x}$ ), and energy $E$ are regular observables, presented by operators. In contract, time is treated as a $c$-number argument, and is not presented by an operator, so that Eq. (163) cannot be derived

[^499]in such general assumptions as Eq. (1.35). Thus the time-energy uncertainty relation should be applied with great caution. Unfortunately, not everybody is so careful. One can find, for example, wrong claims that due to this relation, the energy dissipated by any system performing an elementary (single-bit) calculation during time interval $\Delta t$ has to be larger than $\hbar / \Delta t$. ${ }^{40}$ Another incorrect statement is that the energy of a system cannot be measured, during time $\Delta t$, with an accuracy better than $\hbar / \Delta t .^{41}$

Now let us use our simple model of metastable state's decay for a preliminary discussion of one aspect of quantum measurements. Figure 18 shows (schematically) the traveling wave packets emitted by the quantum well after its initial state (152) had been prepared at $t=0$. At $t \gg \tau$, the well becomes essentially empty ( $W \ll 1$ ), and the whole probability distribution is localized in two clearly separated wave packets of equal amplitudes, moving from away with speed $v_{\mathrm{gr}}$, each "carrying the particle away" with a probability of $50 \%$. Now assume an experiment has detected the particle on the left side of the well. Though the formalisms suitable for a quantitative analysis of the detection process will not be discussed until Sec. 7.7, due to the wide separation of the packets, we may safely assume that the detection may be done without any actual physical effect on the counterpart wave packet. ${ }^{42}$ But if we know that the particle has been found on the left, there is no chance to find it on the right.

If we attributed the wavefunction to all stages of this particular experiment, this situation might be rather confusing. Indeed, this would mean that the wavefunction within the right packet should instantly turn into zero - the so-called wave packet reduction - a process that could not be described by either Schrödinger equation or any other law of physics. However, if (as was already discussed in Sec. 1.3) we attribute the wavefunction to a statistical ensemble of similar experiments, there is no paradox here at all. While the two-packet picture we have calculated (Fig. 18) describes the full initial ensemble (regardless of the particle detection results), the "reduced packet" picture (with no wave packet on the right of the well) describes only a sub-ensemble of experiments with the particle detected on the left side. As was discussed on completely classical examples in Sec. 1.3, for such sub-ensemble the probability distribution, and hence the wavefunction, may be dramatically different.

### 2.6. Coupled quantum wells

Let us now move on to tunneling through a more complex potential profile shown in Fig. 19: a sequence of $(N-1)$ similar quantum wells separated by $N$ similar delta-functional tunnel barriers. According to Eq. (141), its transfer matrix is the following product

$$
\begin{equation*}
\mathrm{T}=\underbrace{\mathrm{T}_{\alpha} \mathrm{T}_{a} \mathrm{~T}_{\alpha} \ldots \mathrm{T}_{a} \mathrm{~T}_{\alpha}}_{(N-1)+N \text { terms }}, \tag{2.164}
\end{equation*}
$$

with the component matrices given by Eqs. (143) and (146), and the barrier height parameter $\alpha$ defined by the last of Eqs. (127).

[^500]Remarkably, this multiplication may be carried out analytically, ${ }^{43}$ giving


Fig. 2.19. Resonant tunneling through a system of $N$ similar, equidistant barriers, i.e. $(N-1)$ similar quantum wells.

Transparency of $N$
equidistant tunnel barriers

$$
\begin{equation*}
T \equiv\left|T_{11}\right|^{-2}=\left[(\cos N q a)^{2}+\left(\frac{\sin k a-\alpha \cos k a}{\sin q a} \sin N q a\right)^{2}\right]^{-1} \tag{2.165}
\end{equation*}
$$

where $q$ is a new parameter, with the wave number dimensionality, defined by the following relation:

$$
\begin{equation*}
\cos q a \equiv \cos k a+\alpha \sin k a . \tag{2.166}
\end{equation*}
$$

For $N=1$, Eqs. (165) and (166) immediately yield our old result (128), while for $N=2$ they may be reduced to Eq. (149) - see Fig. 17a. Figure 20 shows its predictions for two larger numbers $N$, and several values of parameter $\alpha$.


Fig. 2.20. Transparency of the system shown in Fig. 19 as a function of product $k a$. Since the function $T(\mathrm{ka}$ ) is $\pi$-periodic (just like for $N=2$, see Fig. 17a), only one period is shown.

Let us start discussion of the plots from case $N=3$, i.e. two coupled quantum wells. The comparison of Fig. 20a and Fig. 17a shows that the transmission patterns, and their dependence on parameter $\alpha$, are very similar, besides that in the coupled wells each resonant tunneling peak splits into two, with the $k a$-difference between them scaling as $1 / \alpha$. In order to comprehend the physics of this important result, let us analyze an auxiliary system shown in Fig. 21: two similar quantum wells

[^501]confined by infinitely high potential walls at $x= \pm a$, and coupled via a transparent, short tunnel barrier at $x=0$.


Fig. 2.21. Two lowest eigenfunctions and eigenenergies of a system of two coupled quantum wells - schematically.

The barrier may be again, for calculation simplicity, approximated by a delta-function:

$$
U(x)= \begin{cases}+\infty, & \text { for }|x|>a  \tag{2.167}\\ w \delta(x), & \text { for }|x|<a .\end{cases}
$$

We already know that the standing-wave eigenfunctions $\psi_{n}$ of the Schrödinger equation in regions with $U(x)=0$, in our current case, segments $-a<x<0$ and $0<x<+a$, may be always presented as linear superpositions of $\sin k x$ and $\cos k x$. In order to immediately satisfy the boundary conditions $\psi=0$ at $x=$ $\pm a$, we can take these solutions in the form

$$
\psi_{n}(x)= \begin{cases}C_{-} \sin k(x+a), & \text { for }-a<x<0  \tag{2.168}\\ C_{+} \sin k(x-a), & \text { for } 0<x<+a\end{cases}
$$

What remains is to satisfy the boundary conditions at $x=0$. Plugging Eq. (167) into Eqs. (124) and (125), we get the following system of two linear equations:

$$
\begin{align*}
k\left(C_{+}-C_{-}\right) \cos k a & =\frac{2 m w}{\hbar^{2}} C_{-} \sin k a  \tag{2.169}\\
C_{-} \sin k a & =-C_{+} \sin k a \tag{2.170}
\end{align*}
$$

The system has two types of solutions, with the two lowest-energy eigenfunctions sketched in Fig. 21:
(i) Antisymmetric solutions (which will be marked with index $A$ ),

$$
\begin{equation*}
\left(C_{+}\right)_{A}=\left(C_{-}\right)_{A} \text {, i.e. } \psi_{A}=C_{A} \sin k_{A} x \text {, } \tag{2.171}
\end{equation*}
$$

with eigenvalues independent of $W$,

$$
\begin{equation*}
\sin k_{A} a=0, \quad \text { i.e. } k_{A} a=k n a \equiv \pi n, \quad n=1,2, \ldots \tag{2.172}
\end{equation*}
$$

Notice that these values of $k$, and hence eigenenergies of these antisymmetric states,

$$
\begin{equation*}
E_{A}=\frac{\hbar^{2} k_{A}^{2}}{2 m}=\frac{\pi^{2} n^{2}}{2 m a^{2}}, \tag{2.173}
\end{equation*}
$$

coincide with those of the simple quantum well of width $a$ - see Fig. 1.7 and its discussion.
(ii) Symmetric solutions (index S):

$$
\begin{equation*}
\left(C_{+}\right)_{S}=-\left(C_{-}\right)_{S} \text {, i.e. } \psi_{S}=C_{S}\left|\sin k_{S}(x-a)\right|, \tag{2.174}
\end{equation*}
$$

with Eq. (169) giving the following characteristic equation for constant $k_{S}$ :

Characteristic equation for two coupled quantum wells

$$
\begin{equation*}
\tan k_{S} a=-\frac{1}{\alpha} \tag{2.175}
\end{equation*}
$$

Figure 22 shows the graphic solution of this equation for three values of parameter $\alpha$, i.e. for various quantum well coupling strength. For each solution, $k_{S} a$ is confined within interval

$$
\begin{equation*}
\pi n<k_{S} a<\pi n-\frac{\pi}{2} \tag{2.176}
\end{equation*}
$$

so that the antisymmetric and symmetric states alternate on the scale of $k$ (and hence of the energy), with the difference $k_{A}-k_{S}$, for each pair of adjacent states, smaller then $\pi / 2 a$ for any value of $\alpha$. The physics of the splitting between eigenenergies corresponding to the symmetric and antisymmetric states is very simple: it is the change of kinetic energy of the particle due to different confinement types - see Fig. 21. In each antisymmetric mode, $\psi_{n}(0)=\psi_{n}( \pm a)=0$, i.e. the wavefunction is essentially confined within a segment of length $a$; as a result, its energy (173) does not depend on the barrier height. On the contrary, in the symmetric mode, that does engage the potential barrier, the wavefunction effectively spreads into the counterpart well. As a result, it changes slower, and hence its kinetic energy is also lower that that of the adjacent antisymmetric mode.


Fig. 2.22. Graphical solution of the characteristic equation (175) for the eigenvalue of $k a$ in the symmetric mode, for 3 values of parameter $\alpha$, considering it independent of $k a$. The dashed line shows approximation (178).

By the way, this problem may serve as a toy model of the strongest (and most important) type of atom cohesion - the covalent (or "chemical") bonding in molecules, liquids, and solids. The classical example of such bonding is that of hydrogen atoms in a $\mathrm{H}_{2}$ molecule. ${ }^{44}$ Each of two electrons of this system ${ }^{45}$ reduces its kinetic energy very substantially by spreading its wavefunction around both nuclei

[^502]protons, rather that being confined near one of them - as it had to be in a single atom. As a result, the bonding is very strong: in chemical units, $429 \mathrm{~kJ} / \mathrm{mol}$, i.e. 18.6 eV per molecule. ${ }^{46}$ Somewhat counterintuitive, this energy is substantially larger than the strongest classical (ionic) bonding due to electron transfer between atoms, leading to the Coulomb attraction of the resulting ions. (For example, the atomic cohesion in the NaCl molecule is just 3.28 eV .)

In the limit $\alpha \rightarrow 0$ (no partition between the wells), $k_{s} a \rightarrow \pi(n-1 / 2)$, i.e. the eigenstates approach the shape and energy of symmetric states of a quantum well of width $2 a$. In the opposite limit $\alpha \gg 1, k_{S} a \rightarrow \pi n$, and in the vicinity of each such point we may approximate $\tan k_{S} a$ with $\left(k_{S} a-\pi n\right)-$ see the dashed line in Fig. 22. As a result, the characteristic equation (175) is reduced to

$$
\begin{equation*}
k_{S} a \approx \pi n-\frac{1}{\alpha} \tag{2.177}
\end{equation*}
$$

so that the splitting between the wave numbers and eigenenergies of the adjacent symmetric and antisymmetric states is small:

$$
\begin{equation*}
k_{A}-k_{S} \approx \frac{1}{\alpha a} \ll k_{n}, \quad 2 \delta_{n} \equiv E_{A}-E_{S} \approx \frac{d E}{d k}\left(k_{A}-k_{S}\right)=\frac{\pi n \hbar^{2}}{m a} \frac{1}{\alpha a}=\frac{2 E_{A}}{\pi n \alpha} . \tag{2.178}
\end{equation*}
$$

(By construction, this result is valid only if $\alpha \gg 1$, i.e. $\delta_{n} \ll E_{A} \approx E_{S}$.)
Let us analyze properties of the system in this limit in much more detail - first, because the results will help us to develop the important tight binding approximation in the band theory, and second, because the weakly coupled quantum wells will be our first example of very important two-level (or "spin- $1 / 2$-like") systems. Let us focus on one couple of symmetric and antisymmetric states, corresponding to virtually the same $E_{n}$. According to Eqs. (171) and (174), in the limit $\alpha \rightarrow \infty$, system's eigenfunctions may be approximately represented as follows:

$$
\begin{equation*}
\psi_{S}(x) \approx \frac{1}{\sqrt{2}}\left[\psi_{R}(x)+\psi_{L}(x)\right], \quad \psi_{A}(x)=\frac{1}{\sqrt{2}}\left[\psi_{R}(x)-\psi_{L}(x)\right], \tag{2.179}
\end{equation*}
$$

where $\psi_{R, L}$ are the normalized ground states of the completely insulated wells:

$$
\psi_{R}(x)=\left\{\begin{array}{ll}
0, & \text { for }-a<x<0,  \tag{2.180}\\
(2 / a)^{1 / 2} \sin k_{n} x, & \text { for } 0<x<+a,
\end{array} \quad \psi_{L}(x)= \begin{cases}-(2 / a)^{1 / 2} \sin k_{n} x, & \text { for }-a<x<0 \\
0, & \text { for } 0<x<+a\end{cases}\right.
$$

Let us perform the following conceptually important thought experiment: place the particle, at $t$ $=0$, into one of the localized states, say $\psi_{R}(x)$, and leave the system alone to evolve. Solving Eqs (180) for $\psi_{R}$, we may present the initial state as a linear superposition of eigenfunctions:

$$
\begin{equation*}
\Psi(x, 0)=\psi_{R}(x) \approx \frac{1}{\sqrt{2}}\left[\psi_{S}(x)+\psi_{A}(x)\right] . \tag{2.181}
\end{equation*}
$$

Now, according to the general solution (1.67) of the time-independent Schrödinger equation, time dynamics may be obtained by just multiplying each eigenfunction by the corresponding factor (1.61):

[^503]\[

$$
\begin{equation*}
\Psi(x, t)=\frac{1}{\sqrt{2}}\left[\psi_{S}(x) \exp \left\{-i \frac{E_{S}}{\hbar} t\right\}+\psi_{A}(x) \exp \left\{-i \frac{E_{A}}{\hbar} t\right\}\right] . \tag{2.182}
\end{equation*}
$$

\]

Now, introducing the following natural notation,

$$
\begin{equation*}
E_{n} \equiv \frac{E_{A}+E_{S}}{2}, \quad \delta_{n} \equiv \frac{E_{A}-E_{S}}{2} . \tag{2.183}
\end{equation*}
$$

And using Eqs. (179), this expression may be rewritten as

$$
\begin{align*}
\Psi(x, t) & =\frac{1}{\sqrt{2}}\left[\psi_{S}(x) \exp \left\{i \frac{\delta_{n}}{\hbar} t\right\}+\psi_{A}(x) \exp \left\{-i \frac{\delta_{n}}{\hbar} t\right\}\right] \exp \left\{-i \frac{E_{n}}{\hbar} t\right\}  \tag{2.184}\\
& =\left[\psi_{R}(x) \cos \frac{\delta_{n}}{\hbar} t+i \psi_{L}(x) \sin \frac{\delta_{n}}{\hbar} t\right] \exp \left\{-i \frac{E_{n}}{\hbar} t\right\} .
\end{align*}
$$

This result implies, in particular, that the probabilities $W_{R}$ and $W_{L}$ to find the particle, correspondingly, in the right and left wells change with time as

$$
\begin{equation*}
W_{R}=\cos ^{2} \frac{\delta_{n}}{\hbar} t, \quad W_{L}=\sin ^{2} \frac{\delta_{n}}{\hbar} t \tag{2.185}
\end{equation*}
$$

mercifully leaving the total probability constant $W_{R}+W_{L}=1$. (If our calculation had not passed this sanity check, we would be in a big trouble.)

This is the famous effect of periodic quantum oscillations, with frequency $\omega_{n}=2 \delta_{n} / \hbar=\left(E_{A}-\right.$ $\left.E_{S}\right) / \hbar$, of the particle between two similar quantum wells, due to their coupling through via tunneling through the tunnel barrier. The physics of this effect is straightforward: just as in the single well problem discussed in Sec. 5, the particle initially placed into a certain quantum well tries to escape from it via tunneling through the semi-transparent wall. However, in our current situation (Fig. 21) the particle can only escape into the adjacent well. After the tunneling into that second well, the tries to escape from it, and hence comes back, etc. - just as a classical 1D oscillator, initially deflected from its equilibrium position.

Maybe the most surprising feature of this effect is its relatively high frequency: according to Eq. (178), the time period of the quantum oscillations,

$$
\begin{equation*}
\Delta t_{n} \equiv \frac{2 \pi}{\omega_{n}}=\frac{2 \pi \hbar}{\left(E_{A}-E_{S}\right)} \approx \frac{2 \pi}{n} \frac{m a^{2}}{\pi \hbar} \alpha, \quad \text { for } \alpha \gg 1, \tag{2.186}
\end{equation*}
$$

is a factor of $\alpha / 2 \pi \gg 1$ shorter than the lifetime $\tau(160)$ of the metastable state of the particle in a similar but single quantum well limited by delta-functional walls with similar parameter $\alpha$. This is a very counterintuitive result indeed: the speed of particle tunneling into a similar adjacent well is much higher than that, through a similar barrier, to the free space!

To see whether this result is an artifact of the delta-functional model of the tunnel barrier, let us calculate splitting $2 \delta_{n}$ for system of two similar, symmetric, soft quantum wells formed by a smooth potential profile $U(x)=U(-x)-$ see Fig. 23.


Fig. 2.23. Weak coupling between two similar, soft quantum wells.

If the barrier transparency is low, the quasi-localized wavefunctions $\psi_{R}(x)$ and $\psi_{L}(x)=\psi_{R}(-x)$ and their eigenenergies may be found approximately by solving the Schrödinger equations in one of the wells, neglecting tunneling through the barrier, but finding $\delta_{n}$ requires a little bit more care. Let us write the stationary Schrödinger equations for the symmetric and antisymmetric solutions in the form

$$
\begin{equation*}
\left[E_{A}-U(x)\right] \psi_{A}=-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi_{A}}{d x^{2}}, \quad\left[E_{S}-U(x)\right] \psi_{S}=-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi_{S}}{d x^{2}} \tag{2.187}
\end{equation*}
$$

then multiply the former equation by $\psi_{S}$, the latter one by $\psi_{A}$, subtract them from each other, and integrate the result from 0 to $\infty$ :

$$
\begin{equation*}
\left(E_{A}-E_{S}\right) \int_{0}^{\infty} \psi_{S} \psi_{A} d x=\frac{\hbar^{2}}{2 m} \int_{0}^{\infty}\left[\frac{d^{2} \psi_{S}}{d x^{2}} \psi_{A}-\frac{d^{2} \psi_{A}}{d x^{2}} \psi_{S}\right] d x \tag{2.188}
\end{equation*}
$$

If $U(x)$, and hence $d^{2} \psi_{A, S} / d x^{2}$, are finite for all $x,{ }^{47}$ we may integrate the right-hand side by parts to get

$$
\begin{equation*}
\left(E_{A}-E_{S}\right) \int_{0}^{\infty} \psi_{S} \psi_{A} d x=\frac{\hbar^{2}}{2 m}\left[\frac{d \psi_{S}}{d x} \psi_{A}-\frac{d \psi_{A}}{d x} \psi_{S}\right]_{0}^{\infty} \tag{2.189}
\end{equation*}
$$

So far, this is an exact equation. For weakly coupled wells, we can do more. In this case, the left hand side may be approximated as $\left(E_{A}-E_{S}\right) / 2 \equiv \delta_{n}$, because the integral is dominated by the vicinity of point $a$, where the second terms in each of Eqs. (179) are negligible, and the integral is equal to $1 / 2$, due to the proper normalization of function $\psi_{R}(x)$. In the right-hand side, the substitution at $x=\infty$ vanishes (due to the wavefunction decay in the classically forbidden region), and so does the first term at $x=0$, because for the antisymmetric solution $\psi_{A}(0)=0$. As a result, we get

$$
\begin{equation*}
\delta_{n}=\frac{\hbar^{2}}{2 m} \psi_{S}(0) \frac{d \psi_{A}}{d x}(0)=\frac{\hbar^{2}}{m} \psi_{R}(0) \frac{d \psi_{R}}{d x}(0)=\frac{\hbar^{2}}{m} \psi_{L}(0) \frac{d \psi_{R}}{d x}(0)=-\frac{\hbar^{2}}{m} \psi_{L}(0) \frac{d \psi_{L}}{d x}(0) . \tag{2.190}
\end{equation*}
$$

It is straightforward to show that within the limits of the WKB approximation validity, Eq. (190) may be reduced to

$$
\begin{equation*}
\delta_{n}=\frac{\hbar}{t_{A}} \exp \left\{-\int_{x_{c}}^{x_{c}^{\prime}} \kappa\left(x^{\prime}\right) d x^{\prime}\right\} \tag{2.191}
\end{equation*}
$$

[^504][^505]where $t_{A}$ is the time period of classical motion of the particle inside one of the wells, function $\kappa(x)$ is defined by Eq. (97), and $x_{c}$ and $x_{c}{ }^{\prime}$ are the classical turning points limiting the potential barrier at the level $E_{n}$ of particle's energy - see Fig. 23. Comparing this result with Eq. (117), we can notice that again, just as in the case of the delta-functional barriers, the transmission coefficient $T$ of a tunnel barrier (and hence the reciprocal lifetime of a metastable state in a potential well separated by such a barrier from a continuum) scales as the square of the WKB exponent participating in Eq. (191), so that the period of quantum oscillations between the well is much smaller than the lifetime. We will return to the discussion of this result, in a more general form, in Chapter 5.

Returning for a second to Fig. 20a, we may now readily interpret the results for tunneling through the double quantum well: each pair of resonance peaks of transparency corresponds to the alignment of incident particle's energy with the pair of energy levels $E_{A}, E_{S}$ of the symmetric and antisymmetric states of the system.

### 2.7. 1 D band theory

Let us now return to Eqs. (165) and (166) describing the resonant tunneling, and discuss their predictions for larger $N$ - see, for example, Fig. 20b. We see that the increase of $N$ results in the increase of the number of resonant peaks per period to $(N-1)$, and at $N \rightarrow \infty$ the peaks merge into the so-called allowed energy bands (frequently called just the "energy bands") of relatively high transparency, separated from similar bands in the adjacent periods of function $T(k a)$ by energy gaps ${ }^{48}$ where $T \rightarrow 0$. Notice the following important features of the pattern:
(i) at $N \rightarrow \infty$, the band/gap edges become sharp for any $\alpha$, and tend to fixed positions (determined by $\alpha$ but independent of $N$ );
(ii) the larger interwell coupling $(\alpha \rightarrow 0)$, the broader the allowed energy bands and narrower the gaps between them.

Our discussion of resonant tunneling in the previous section gives us an evident clue for a semiquantitative interpretation of this pattern: if $(N-1)$ quantum wells are weakly coupled by tunneling through the tunnel barriers separating them, system's energy spectrum consists of groups ( $N-1$ ) energy levels. Each level corresponds to an eigenfunction that is the set of similar local functions in each well, but with certain phase shifts $\Delta \varphi$ between them. It is natural to expect that, just as for 2 coupled wells ( $N$ $-1=2$ ), that at the upper level, $\Delta \varphi=\pi$ (thus providing the highest confinement), with $k a \rightarrow \pi n$ at $\alpha \rightarrow$ $\infty$, while at the lowest level all $\Delta \varphi=0$, providing the most loose confinement. ${ }^{49}$ However, what about $\Delta \varphi$ for other levels?

Answers to all these questions are easy to get in the most important limit $N \rightarrow \infty$, i.e. for periodic structures - which are, in particular, good 1D approximations for solid state crystals, whose samples may feature more than $10^{10}$ similar atoms or molecules in each direction of the crystal lattice. It is almost self-evident that at $N \rightarrow \infty$, due to the translational invariance of $U(x)$,

$$
\begin{equation*}
U(x+a)=U(x) \tag{2.192}
\end{equation*}
$$

[^506]the phase shift $\Delta \varphi$ between local wavefunctions in all adjacent quantum wells should be the same for each period of the system, i.e.
\[

$$
\begin{equation*}
\psi(x+a)=\psi(x) e^{i \Delta \varphi} \tag{2.193a}
\end{equation*}
$$

\]

for all $x$. (A reasonably fair classical image of $\Delta \varphi$ is the geometric angle between similar objects - e.g., similar paper clips - attached at equal distances to a long, uniform rubber band. If the band's ends are twisted, the twist is equally distributed between the structure's periods, representing the constancy of $\Delta \varphi{ }^{50}$ )

Equation (193a) is the (1D version of the) much-celebrated Bloch theorem. ${ }^{51}$ Mathematical rigor aside, ${ }^{52}$ it is a virtually evident fact, because the particle's density $w(x)=\psi^{*}(x) \psi(x)$, that has to be periodic in this $a$-periodic system, may be so only $\Delta \varphi$ is constant. For what follows, it is more convenient to present the real number $\Delta \varphi$ in the form $q a$ (there is no loss of generality here, because parameter $q$ may depend on $a$ as well as other parameters of the system), so that the Bloch theorem takes the form

$$
\begin{equation*}
\psi(x+a)=\psi(x) e^{i q a} \tag{2.193b}
\end{equation*}
$$

1D Bloch theorem

The physical sense of parameter $q$ will be discussed in detail below; for now just note that according to Eq. (193b), an addition of ( $2 \pi / a$ ) to it yields the same wavefunction; hence all observables have to be ( $2 \pi / a$ )-periodic functions of $q .{ }^{53}$

Now let us use the Bloch theorem to find eigenfunctions and eigenenergies for a particular, and probably the simplest periodic function $U(x)$ : an infinite set of similar quantum wells separated by deltafunctional tunnel barriers (Fig. 24).


Fig. 2.24. The simplest periodic potential: an infinite set of similar, equidistant, delta-functional tunnel barriers.

[^507]To start, consider two points separated by distance $a$ : one of them, $x_{j}$, just left of position of one of the barriers, and another one, $x_{j+1}$, just left of the following barrier. Eigenfunctions in each of the points may be presented as linear superpositions of two simple waves $\exp \{ \pm i k x\}$, and amplitudes of their components should be related by a $2 \times 2$ transfer matrix T of the potential fragment separating them. According to Eq. (141), this matrix may be found as the product of the matrix (146) of one interval $a$ and the matrix (143) of one barrier:

$$
\binom{A_{j+1}}{B_{j+1}}=\mathrm{T}_{\mathbf{a}} \mathrm{T}_{\alpha}\binom{A_{j}}{B_{j}}=\left(\begin{array}{cc}
e^{i k a} & 0  \tag{2.194}\\
0 & e^{-i k a}
\end{array}\right)\left(\begin{array}{cc}
1-i \alpha & -i \alpha \\
i \alpha & 1+i \alpha
\end{array}\right)\binom{A_{j}}{B_{j}} .
$$

However, according to the Bloch theorem (193b), the component amplitudes should be also related as

$$
\binom{A_{j+1}}{B_{j+1}}=e^{i q a}\binom{A_{j}}{B_{j}}=\left(\begin{array}{cc}
e^{i q a} & 0  \tag{2.195}\\
0 & e^{i q a}
\end{array}\right)\binom{A_{j}}{B_{j}} .
$$

The condition of self-consistency of these two equations leads to the following characteristic equation:

$$
\left(\begin{array}{cc}
e^{i k a} & 0  \tag{2.196}\\
0 & e^{-i k a}
\end{array}\right)\left(\begin{array}{cc}
1-i \alpha & -i \alpha \\
i \alpha & 1+i \alpha
\end{array}\right)-\left(\begin{array}{cc}
e^{i q a} & 0 \\
0 & e^{i q a}
\end{array}\right)=0
$$

In Sec. 5, we have already calculated the matrix product participating in this equation - see Eq. (148). Using it, we see that Eq. (196) is reduced to the same simple Eq. (166) that has already jumped at us from the solution of the different (resonant tunneling) problem. Let us explore that simple result in detail. First of all, the right hand part of Eq. (166) is a sinusoidal function of $k a$, with amplitude $(1+$ $\left.\alpha^{2}\right)^{1 / 2}$ - see Fig. 25, while its left hand part is a sinusoidal function of $q a$ with amplitude 1.


Fig. 2.25. Graphical solution of the characteristic equation (166) for a fixed value of parameter $\alpha$. The ranges of $k a$ that yield with $|\cos q a|<1$, correspond to the allowed energy bands, while those with $|\cos q a|>1$, to gaps between them.

As a result, within each period $\Delta(k a)=2 \pi$, the characteristic equation does not have a real solution for $q$ inside two intervals of $k a$ - and hence inside two intervals of energy $E=\hbar^{2} k^{2} / 2 m$. (These intervals are exactly the energy gaps mentioned above, while the complementary intervals of $k a$ and $E$, where a real $q$ exists, are the allowed energy bands.) In contrast, parameter $q$ can take any real values, so it is more convenient to plot the eigenenergy $E=\hbar^{2} k^{2} / 2 m$ as the function of $q$ (or, even more
conveniently, $q a$ ) rather than $k a .{ }^{54}$ While doing that, we need to recall that parameter $\alpha$, defined by the last of Eqs. (127), depends on wave vector $k$ as well, so that if we vary $q$ (and hence $k$ ), it is better to characterize the structure by a different, $k$-independent dimensionless parameter, for example

$$
\begin{equation*}
\beta \equiv(k a) \alpha=\frac{m a w}{\hbar^{2}}, \tag{2.197}
\end{equation*}
$$

so that Eq. (166) becomes

$$
\begin{equation*}
\cos q a \equiv \cos k a+\beta \frac{\sin k a}{k a} \tag{2.198}
\end{equation*}
$$

Characteristic equation for system in Fig. 24

Figure 26 shows the plots of $E$ and $k$, following from Eq. (198), for a particular, moderate value of parameter $\beta$. The band structure of the energy spectrum is apparent. Another evident feature is the $2 \pi$-periodicity of the pattern, that we have already predicted from the general Bloch theorem arguments. (Due to this periodicity, the complete band/gap pattern may be studied on just one interval $-\pi \leq q a \leq+$ $\pi$, called the $I^{\text {st }}$ Brillouin zone - the so-called reduced zone picture. For some applications, however, it is more convenient to use the extended zone picture with $-\infty \leq q a \leq+\infty-$ see, e.g., the next section.)


Fig. 2.26. (a) "Real" momentum $k$ of a particle in the periodic delta-functional potential profile shown in Fig. 24, and (b) its energy $E=\hbar^{2} k^{2} / 2 m$ (in units of $E_{0} \equiv \hbar^{2} / 2 m a^{2}$ ), as functions of the quasi-momentum $q$, for a particular value $(\beta=3)$ of the dimensionless potential parameter $\beta \equiv(k a) \alpha=m W a / \hbar^{2}$. Arrows in the lower right corner of panel (b) illustrate the definition of the energy band $\left(\Delta E_{n}\right)$ and energy gap $\left(\Delta_{n}\right)$ widths.

[^508]However, maybe the most surprising fact, clearly visible in Fig. 26, is that there is a infinite number of energy bands, with different energies $E_{n}(q)$ for the same value of $q$. Mathematically, it is evident from Eq. (198) - see also Fig. 25. Indeed, for each value of $q a$ there are two solutions $k a$ to this equation on each period $\Delta(k a)=2 \pi$ - see also panel (a) in Fig. 26. Each of such solutions gives a different value of particle energy $E=\hbar^{2} k^{2} / 2 m$. A continuous set of similar solutions for various $q a$ forms a particular energy band.

Since the band theory is one of the most vital results of quantum mechanics, it is important to understand the physics of these different solutions - and hence of the whole band picture. For that, let us explore analytically two different potential strength limits. An important advantage of this approach is that both analyses may be carried out for an arbitrary periodic potential $U(x)$, rather than for the simplest model shown in Fig. 24.
(i) Tight-binding approximation. This approximation is sound when eigenenergy $E_{n}$ is much lower than the height of the potential barriers separating the potential minima (serving as quantum wells) - see Fig. 27. As should be clear from our discussion in Sec. 6, the wavefunction is mostly localized in the classically allowed regions at points $x_{j}$ of the potential energy minima - see the dashed lines in Fig. 27. Essentially the only role of coupling between these quantum well states (via tunneling through the separating barriers) is to establish certain phase shifts $\Delta \varphi=q a$ between the pairs of adjacent quasi-localized wavefunction "lumps" $u\left(x-x_{j}\right)$ and $u\left(x-x_{j+1}\right)$.


Fig. 2. 27. Tight binding approximation (schematically).

To describe this effect quantitatively, let us first return to the problem of two coupled wells considered in Sec. 6, and recast result (184) as

$$
\begin{equation*}
\Psi_{n}(x, t)=\left[a_{R}(t) \psi_{R}(x)+a_{L}(t) \psi_{L}(x)\right] \exp \left\{-i \frac{E_{n}}{\hbar} t\right\}, \tag{2.199}
\end{equation*}
$$

where functions $a_{R}$ and $a_{L}$ oscillate sinusoidally in time:

$$
\begin{equation*}
a_{R}(t)=\cos \frac{\delta_{n}}{\hbar} t, \quad a_{L}(t)=i \sin \frac{\delta_{n}}{\hbar} t . \tag{2.200}
\end{equation*}
$$

This evolution satisfies the following system of two equations whose structure reminds Eq. (1.59):

$$
\begin{equation*}
i \hbar \dot{a}_{R}=-\delta_{n} a_{L}, \quad i \hbar \dot{a}_{L}=-\delta_{n} a_{R} . \tag{2.201}
\end{equation*}
$$

Later in the course (in Chapter 6) we will prove that such equations are indeed valid, in the tightbinding approximation, for any system of two coupled quantum wells. These equations may be readily generalized to the case of many similar coupled wells. Here, in this case, instead of Eq. (199), we evidently should write

$$
\begin{equation*}
\Psi_{n}(x, t)=\exp \left\{-i \frac{E_{n}}{\hbar} t\right\} \sum_{j} a_{j}(t) u_{n}\left(x-x_{j}\right), \tag{2.202}
\end{equation*}
$$

where $E_{n}$ are the eigenenergies, and $u_{n}$ the eigenfunctions of each isolated well. In the tight binding limit, only the adjacent wells are coupled, so that instead of Eq. (201) we should write an infinite system of similar equations

$$
\begin{equation*}
i \hbar \dot{a}_{j}=-\delta_{n} a_{j-1}-\delta_{n} a_{j+1} \tag{2.203}
\end{equation*}
$$

for each well number $j$, where parameters $\delta_{n}$ describe the coupling between two adjacent quantum wells. Repeating the calculation outlined in the end of Sec. 6 for our new situation, we get the result essentially similar to the last form of Eq. (190):

$$
\begin{equation*}
\delta_{n}=\frac{\hbar^{2}}{m} u_{n}\left(x_{0}\right) \frac{d u_{n}}{d x}\left(a-x_{0}\right), \tag{2.204}
\end{equation*}
$$

Tight binding limit: coupling energy
where $x_{0}$ is the distance between the well bottom and the middle of the tunnel barrier on the right of it see Fig. 27. The only substantial new feature of this expression in comparison with Eq. (190) is that the sign of $\delta_{n}$ alternates with the level number $n: \delta_{1}>0, \delta_{2}<0, \delta_{3}>0$, etc. Indeed, the number of "wiggles" (formally, zeros) of eigenfunctions $u_{n}(x)$ of any potential well increases as $n-$ see, e.g., Fig. $1.7,{ }^{55}$ so that the difference of the exponential tails of the functions, sneaking under the left and right barriers limiting the well also alternates with $n$.

The infinite system of ordinary differential equations (203) allows one to explore a large range of important problems (such as the spread of the wavefunction that was initially localized in one well, etc.), but our main task now is to find its stationary states, i.e. the solutions proportional to $\exp \{-$ $\left.i\left(\varepsilon_{n} / \hbar\right) t\right\}$, where $\varepsilon_{n}$ is a still unknown, $q$-dependent addition to the background energy $E_{n}$ of $n$-th level. In order to satisfy the Bloch theorem (193) as well, such solution should have the form

$$
\begin{equation*}
a_{j}(t)=a \exp \left\{i q x_{j}-i \frac{\varepsilon_{n}}{\hbar} t+\text { const }\right\}, \tag{2.205}
\end{equation*}
$$

where $a$ is a constant. Plugging this solution into Eq. (203) and canceling the common exponent, we get

$$
\begin{equation*}
E=E_{n}+\varepsilon_{n}=E_{n}-\delta_{n}\left(e^{-i q a}+e^{i q a}\right)=E_{n}-2 \delta_{n} \cos q a \tag{2.206}
\end{equation*}
$$

so that in this approximation, the energy band width $\Delta E_{n}$ (see Fig. 26b) equals $4\left|\delta_{n}\right|$.
Relation (206), whose validity is restricted to $\left|\delta_{n}\right| \ll E_{n}$, describes the particular lowest energy bands plotted in Fig. 26b reasonably well. (For larger $\beta$, the agreement would be even better.) So, this calculation explains what the energy bands really are - in the tight binding limit they are best interpreted as isolated well's energy levels $E_{n}$, broadened into bands by the interwell interaction. Also, this result gives a clear proof that the energy band extremes correspond to $q a=2 \pi l$ and $q a=2 \pi(l+1 / 2)$, with integer $l$. Finally, the sign alteration of the coupling coefficient $\delta_{n}(204)$ with number $n$ explains why the energy maxima of one band are aligned, on the $q a$ axis, with energy minima of the adjacent bands.

[^509]Tight binding
limit: energy bands
(ii) Weak-potential limit. Surprisingly, the energy band structure is also compatible with a completely different physical picture that can be developed in the opposite limit. Let energy $E$ be so high that the periodic potential $U(x)$ may be treated as a small perturbation. Naively, we would have the parabolic dispersion relation between particle's energy and momentum. However, if we are plotting energy as a function of $q$ rather than $k$, we need to add $2 \pi l / a$, with arbitrary integer $l$, to the argument. Let us show this by expanding all variables into the spatial Fourier series. For a periodic potential energy $U(x)$ such an expansion is straightforward: ${ }^{56}$

$$
\begin{equation*}
U(x)=\sum_{l^{\prime \prime}} U_{l^{\prime \prime}} \exp \left\{-i \frac{2 \pi x}{a} l^{\prime \prime}\right\}, \tag{2.207}
\end{equation*}
$$

where the summation is over all integers $l$ ", from $-\infty$ to $+\infty$. However, for the wavefunction we should show due respect to the Bloch theorem (193). To understand how to proceed, let us define another function

$$
\begin{equation*}
u(x) \equiv \psi(x) e^{-i q x} \tag{2.208}
\end{equation*}
$$

and study its periodicity:

$$
\begin{equation*}
u(x+a)=\psi(x+a) e^{-i q(x+a)}=\psi(x) e^{-i q x}=u(x) \tag{2.209}
\end{equation*}
$$

We see that the new function is $a$-periodic, and hence we can use Eqs. (208)-(209) to rewrite the Bloch theorem as

$$
\begin{equation*}
\psi(x)=u(x) e^{i q x}, \quad \text { with } u(x+a)=u(x) \tag{2.210}
\end{equation*}
$$

Now it is safe to expand the periodic function $u(x)$ exactly as $U(x)$ :

$$
\begin{equation*}
u(x)=\sum_{l^{\prime}} u_{l^{\prime}} \exp \left\{-i \frac{2 \pi x}{a} l^{\prime}\right\}, \tag{2.211}
\end{equation*}
$$

so that, according to the Bloch theorem,

$$
\begin{equation*}
\psi(x)=e^{i q x} \sum_{l^{\prime}} u_{l^{\prime}} \exp \left\{-i \frac{2 \pi x}{a} l^{\prime}\right\}=\sum_{l^{\prime}} u_{l^{\prime}} \exp \left\{i\left(q-\frac{2 \pi}{a} l^{\prime}\right) x\right\} . \tag{2.212}
\end{equation*}
$$

The only nontrivial part of plugging this expression into the stationary Schrödinger equation (61) is the calculation of the product term, using expansions (207) and (211):

$$
\begin{equation*}
U(x) \psi=\sum_{l, l^{\prime \prime}} U_{l^{\prime \prime}} u_{l^{\prime}} \exp \left\{i\left(q-\frac{2 \pi x}{a}\left(l^{\prime}+l^{\prime \prime}\right)\right)\right\} . \tag{2.213}
\end{equation*}
$$

At fixed $l^{\prime}$, we may change summation over $l^{\prime \prime}$ to that over $l \equiv l^{\prime}+l^{\prime \prime}$ (so that $l^{\prime \prime}=l-l$ '), and write:

$$
\begin{equation*}
U(x) \psi=\sum_{l} \exp \left\{i\left(q-\frac{2 \pi x}{a} l\right)\right\} \sum_{l^{\prime}} u_{l} U_{l-l^{\prime}} \tag{2.214}
\end{equation*}
$$

[^510]Now plugging Eqs. (212) (with index $l$ ' now replaced by $l$ ) and (214) into the stationary Schrödinger equation (61), and requiring the coefficients of each spatial exponent to match, we get an infinite system of linear equations for $u_{l}:{ }^{57}$

$$
\begin{equation*}
\sum_{l^{\prime}} U_{l-l^{\prime}} u_{l^{\prime}}=\left[E-\frac{\hbar^{2}}{2 m}\left(q-\frac{2 \pi}{a} l\right)^{2}\right] u_{l} . \tag{2.215}
\end{equation*}
$$

So far, this system is an equivalent alternative to the initial Schrödinger equation - and, by the way, is very efficient for fast numerical calculations, for virtually any potential strength, though in systems with tight binding it may require taking into account a large number of harmonics $u_{l}$. In the weak potential limit, i.e. if all the Fourier coefficients $U_{n}$ are small,58 we can complete all the calculation analytically. ${ }^{59}$ Indeed, in the so-called $0^{\text {th }}$ approximation we can ignore all $U_{n}$, so that in order to have at least one $u_{l}$ different from 0, Eq. (215) requires that

$$
\begin{equation*}
E \rightarrow E_{l} \equiv \frac{\hbar^{2}}{2 m}\left(q-\frac{2 \pi l}{a}\right)^{2} \tag{2.216}
\end{equation*}
$$

( $u_{l}$ itself should be obtained from the normalization condition). This result means that the dispersion relation $E(q)$ has an infinite number of similar quadratic branches numbered by integer $l-$ see Fig. 28.


Fig. 2.28. 1D band picture in the weak potential case $\left(\Delta_{n} \ll E^{(n)}\right)$. Shading shows the $1^{\text {st }}$ Brillouin zone.

On any branch, the eigenfunction has just one Fourier coefficient, i.e. presents a monochromatic traveling wave

$$
\begin{equation*}
\psi_{l} \rightarrow u_{l} e^{i k x}=u_{l} \exp \left\{i\left(q-\frac{2 \pi l}{a}\right) x\right\} . \tag{2.217}
\end{equation*}
$$

[^511]This fact allows us to rewrite Eq. (215) in a more transparent form

$$
\begin{equation*}
\sum_{l \neq l} U_{l^{\prime}-l} u_{l^{\prime}}=\left(E-E_{l}\right) u_{l}, \tag{2.218}
\end{equation*}
$$

that may be formally solved for $u_{i}$ :

$$
\begin{equation*}
u_{l}=\frac{1}{E-E_{l}} \sum_{l \neq l} U_{l^{\prime}-l} u_{l^{\prime}} . \tag{2.219}
\end{equation*}
$$

If the Fourier coefficients $U_{n}$ are nonvanishing but small, this formula shows that wavefunctions do acquire other Fourier components (besides the main one, with the index corresponding to the branch number), but these additions are all small, besides narrow regions near the points $E_{l}=E_{l}$, where two branches (216) of the dispersion relation $E(q)$, with some specific numbers $l$ and $l^{\prime}$, cross. This happens when

$$
\begin{equation*}
\left(q-\frac{2 \pi}{a} l\right) \approx-\left(q-\frac{2 \pi}{a} l^{\prime}\right), \tag{2.220}
\end{equation*}
$$

i.e. at $q \approx q_{m} \equiv \pi m / a$ (with integer $\left.m \equiv l+l^{\prime}\right)^{60}$ corresponding to
 energy gap positions

$$
\begin{equation*}
\frac{E_{l}-E_{l^{\prime}}}{2} \approx \gamma \widetilde{q}, \quad \text { with }\left.\gamma \equiv \frac{d E_{l}}{d q}\right|_{q=q_{m}}=\frac{\pi \hbar^{2} n}{m a}=\frac{2 a E^{(n)}}{\pi n}, \quad \text { and } \widetilde{q} \equiv q-q_{m} \tag{2.225}
\end{equation*}
$$

while parameters $E_{\text {ave }} \equiv\left(E_{l}+E_{l}\right) / 2=E^{(n)}$ and $U_{n} U_{n}^{*}=\left|U_{n}\right|^{2}$ do not depend on $\widetilde{q}$, i.e. the distance from the central point $q_{m}$. This is why Eq. (224) may be plotted as the famous level anticrossing (also called "avoided crossing", or intended crossing", or "non-crossing") diagram (Fig. 29), with the energy gap width $\Delta_{n}$ equal to $2\left|U_{n}\right|$, i.e. just double the magnitude of the $n$-th Fourier harmonic of the periodic potential $U(x)$. Such anticrossings are also clearly visible in Fig. 28 that shows the results of the exact solution of Eq. (198) for $\beta=0.5 .{ }^{62}$


We will run into the anticrossing diagram again and again in the course, notably at the discussion of spin. Such diagram characterizes any quantum systems with two weakly-interacting eigenstates with close energies. It is also repeatedly met in classical mechanics, for example at the calculation of eigenfrequencies of coupled oscillators. ${ }^{63,64}$ In our current case of the weak potential limit, the diagram describes the weak interaction of two sinusoidal de Broglie waves (216), with oppositely directed wave vectors, $l$ and $-l^{\prime}$, via the $\left(l-l^{\prime}\right)^{\text {th }}$ (i.e. $\left.n^{\text {th }}\right)$ Fourier harmonic of the potential profile $U(x)$. This effect exists also for the classical wave theory, and is known as the Bragg reflection, describing, for example, the 1D case of the wave reflection by a crystal lattice (Fig. 1.5) in the limit of weak interaction between the incident particles and the lattice.

Returning for the last time to our initial result - the band structure for the delta-functional $U(x)$ (Fig. 24), shown in Fig. 26, we may wonder how general it is, taking into account the peculiar properties of the delta-function approximation. A partial answer may be obtained from the band structure for two more realistic and relatively simple periodic functions $U(x)$ : the sinusoidal potential (Fig. 30a) and the rectangular Kronig-Penney potential shown in Fig. 30b.

For the sinusoidal potential (Fig. 30a), with $U(x)=U_{1} \cos (2 \pi x / a)$, the stationary Schrödinger equation (61) takes the form

[^512]\[

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi}{d x^{2}}+U_{1} \cos \frac{2 \pi x}{a} \psi=E \psi \tag{2.226}
\end{equation*}
$$

\]

By the introduction of dimensionless variables

$$
\begin{equation*}
\xi \equiv \frac{\pi x}{a}, \quad \alpha \equiv \frac{E}{E^{(1)}}, \quad 2 \beta \equiv \frac{U_{1}}{E^{(1)}}, \tag{2.227}
\end{equation*}
$$

where $E^{(1)}$ is defined by Eq. (221), Eq. (226) may be reduced to the canonical form of the well-known Mathieu equation ${ }^{65}$

$$
\begin{equation*}
\frac{d^{2} \psi}{d \xi^{2}}+(\alpha-2 \beta \cos 2 \xi) \psi=0 \tag{2.228}
\end{equation*}
$$



(b)

Figure 31 shows the so-called characteristic curves of the Mathieu equation, i.e. the relations between parameters $\alpha$ and $\beta$, corresponding to the energy band edges separating them from the adjacent bands. (Such curves may be readily calculated numerically, for example, using Eqs. (215) with the bandedge values $q a=0$ and $q a=\pi$ ). In such "phase plane" plots, the detailed information about the energy dependence on the quasi-momentum is lost, but we already know from Fig. 26 that the dependence is not too eventful. The most remarkable feature of these plots is the fast (exponential) disappearance of the allowed energy bands at $2 \beta>\alpha$ (in Fig. 31, above the red dashed line), i.e. at $E<U_{1}$. This may be readily explained by our tight-binding approximation result (206): as soon as the eigenenergy drops significantly below the potential maximum $U_{\max }=U_{1}$ (see Fig. 30a), quantum states in the adjacent potential wells are only connected by tunneling through the separating potential barriers, with exponentially small amplitudes $\delta_{n}$ - see Eq. (204).

On the other hand, the characteristic curves below the dashed line, i.e. at $2 \beta<\alpha$, correspond to virtually free motion of the particle with energy $E$ above $U_{\max }=U_{1}$. Naturally, in this region the energy bands rapidly expand while gaps virtually disappear. This could be expected from the weak potential limit analysis (see Fig. 28 and its discussion); however, based on that analysis one could expect that the

[^513]energy gaps $\Delta_{n} \approx 2\left|U_{n}\right|$ would disappear more gradually. The fast decline of the gaps at $U_{1} \rightarrow 0$ (i.e. $\beta$ $\rightarrow 0$ ) in the Mathieu equation is an artifact of the sinusoidal potential $U(x)$, with no Fourier harmonics $U_{n}$ above the first one. (In order to calculate the correct asymptotic behavior $\Delta_{n} \propto \beta^{n}$ at $\beta \rightarrow 0$, one needs to go beyond the first approximation we have used in the weak potential limit analysis.)


Fig. 2.31. Characteristic curves of the Mathieu equation. In application to the band theory, dotted regions correspond to the energy gaps, while regions between them, to energy bands. The red dashed line corresponds to condition $\alpha=2 \beta$, i.e. $E=U_{1}$ $\equiv U_{\max }$, separating the regions of tunneling and over-barrier motion. Figure adapted from http://www.enm.bris.ac.uk/teaching/.

If one wants to study the details of transition between the two limits in the 1 D band theory without the artifacts of the delta-functional model shown in Fig. 24 (with infinite number of harmonics $U_{n}$ independent of $n$ ) and of the Mathieu equation (with all $U_{n}=0$ for $n \neq \pm 1$ ), the standard way is to examine the Kronig-Penney potential shown in Fig. 30b. For this potential, the characteristic equation may be readily derived using our rectangular barrier analysis in Sec. 3. For the case $E<U_{0}$, the result is the following natural generalization of Eq. (166):

$$
\begin{equation*}
\cos q a=\cosh \kappa d \cos k(a-d)+\frac{1}{2}\left(\frac{\kappa}{k}-\frac{k}{\kappa}\right) \sinh \kappa d \sin k(a-d) \tag{2.229}
\end{equation*}
$$

where parameters $k$ and $\kappa$ are defined, as functions of $E$ and $U_{0}$, by Eqs. (62) and (65). In the opposite case $E>U_{0}$, one can use the same formula with the replacement (73). Plots $E(q)$, described by these formulas, ${ }^{66}$ are very similar to those shown in Figs. $26 b$ and 28 above. In order to see some difference, one needs to plot the characteristic curves $U_{0}(E)$. This may be done by taking $q a=0$ and $q a=\pi$ (i.e. $\cos q a= \pm 1$ ) in Eq. (229), and solving the resulting transcendental equation for $U_{0}$ numerically. The curves are generally similar to those shown in Fig. 31, but, in accordance with Eq. (224), exhibit a more gradual decrease of energy gaps:

$$
\begin{equation*}
\Delta_{n} \rightarrow 2\left|U_{n}\right| \propto \frac{U_{0}}{n}, \quad \text { at } E \sim E^{(n)} \gg U_{0} . \tag{2.230}
\end{equation*}
$$

To conclude this section, let me address the effect of periodic potential on the number of eigenstates in 1D systems of large but finite length $l \gg a, k^{-1}$. Surprisingly, the Bloch theorem makes the analysis of this problem elementary, for arbitrary $U(x)$. Indeed, let us assume that $l$ is comprised of

[^514]an integer number of periods $a$, and its ends are described by the similar boundary conditions - both assumptions evidently inconsequential for $l \gg a$ (such as a $1-\mathrm{cm}$-scale crystal with $\sim 10^{8}$ atoms along each direction). Then, according to Eq. (210), the boundary conditions impose, on the quasi-momentum $q$, exactly the same quantization condition as we had for $k$ for a free 1D motion. Hence, instead of Eq. (1.94) we can write

1D density of states summation
rule

$$
\begin{equation*}
d N=\frac{l}{2 \pi} d q \tag{2.231}
\end{equation*}
$$

with the corresponding change of the summation rule:

$$
\begin{equation*}
\sum_{q} f(q) \rightarrow \frac{l}{2 \pi} \int f(q) d k \tag{2.232}
\end{equation*}
$$

Hence, the density of states in 1D $q$-space, $d N / d q=l / 2 \pi$, does not depend on the potential profile at all! Note, however, that the profile does affect the density of states on the energy axis, $d N / d E$. As an extreme example, on the bottom and at the top of each energy band we have $d E / d q \rightarrow 0$, and hence

$$
\begin{equation*}
\frac{d N}{d E}=\frac{d N}{d q} / \frac{d E}{d q}=\frac{l}{2 \pi} / \frac{d E}{d q} \rightarrow \infty \tag{2.233}
\end{equation*}
$$

This divergence (which survives in higher spatial dimensionalities as well) of the state density has important implications for the operation of several electron and optical devices, in particular semiconductor lasers.

### 2.8. Effective mass and the Bloch oscillations

The band structure of the energy spectrum has profound implications not only on the density of states, but also on the dynamics of particles in periodic potentials. In order to see that, let us consider the simplest case: motion of a wave packet consisting of Bloch functions (210), all in the same (say, $n^{\text {th }}$ ) energy band. Similarly to Eq. (27) for the a free particle, we can describe such a packet as

$$
\begin{equation*}
\Psi(x, t)=\int a_{q} u_{q}(x) e^{i[q x-\omega(q) t]} d q \tag{2.234}
\end{equation*}
$$

where the $a$-periodic functions $u(x)$, defined by Eq. (208), are now indexed to emphasize their dependence on the quasi-momentum, and $\omega(q) \equiv E_{n}(q) / \hbar$ is the function of $q$ describing the shape of the corresponding energy band - see, e.g., Fig. 26b or Fig. 28. If the packet is narrow, i.e. the width $\delta q$ of the distribution $a_{q}$ is much smaller than all the characteristic scales of the dispersion relation $\omega(q)$, in particular $\pi / a$, we may simplify Eq. (234) exactly as we have done in Sec. 2 for a free particle, despite the presence of factors $u_{q}(x)$ under the integral. In the linear approximation of the Taylor expansion, we again get Eq. (32), but now with ${ }^{67}$

$$
\begin{equation*}
v_{\mathrm{gr}}=\left.\frac{d \omega}{d q}\right|_{q=q_{0}}, \quad \text { and } v_{\mathrm{ph}}=\left.\frac{\omega}{q}\right|_{q=q_{0}} \tag{2.235}
\end{equation*}
$$

[^515]where $q_{0}$ is the central point of the quasi-momentum distribution. Despite the formal similarity with Eq. (33) for the free particle, this result is much more eventful; for example, as evident from the dispersion relation's topology (see Figs. 26b, 28), the group velocity vanishes not only at $q=0$, but at all values of $q$ that are multiples of $(\pi / a)$, at the bottom and on the top of each energy band. At these points, packet's envelope does not move in either direction - though may keep spreading. ${ }^{68}$

Even more fascinating phenomena take place if a particle in the periodic potential is the subject of an additional external force $F(t)$. (For electrons in a crystal lattice, this may be, for example, the Lorentz force of the applied electric and/or magnetic field.) Let the force be relatively weak, so that product $F a$ (i.e. the scale of energy increment from the additional force per one lattice period) is much smaller than the relevant energy scales the dispersion relation $E(q)$ - see Fig. 26b:

$$
\begin{equation*}
F a \ll \Delta E_{n}, \Delta_{n} . \tag{2.236}
\end{equation*}
$$

This relation allows one to neglect the force-induced interband transitions, so that the wave packet (234) includes the Bloch eigenfunctions belonging to only one (initial) energy band at all times. For the time evolution of its center $q_{0}$, theory yields ${ }^{69}$ an extremely simple equation of motion

$$
\begin{equation*}
\dot{q}_{0}=\frac{1}{\hbar} F(t) . \tag{2.237}
\end{equation*}
$$

Time evolution of quasimomentum

This equation is physically very transparent: it is essentially the $2^{\text {nd }}$ Newton law for the time evolution of the quasi-momentum $\hbar q$ under the effect of the additional force $F(t)$ only, excluding the periodic force $-\partial U(x) / \partial x$ of the background potential $U(x)$. This is very natural, because $\hbar q$ is essentially the particle's momentum averaged over potential's period, and the periodic force effect drops out at such an averaging.

Despite the simplicity of Eq. (237), the results of its solution may be highly nontrivial. First, let us use Eqs. (235) and (237) find the instant group acceleration of the particle (i.e. the acceleration of its wave packet's envelope):

$$
\begin{equation*}
a_{\mathrm{gr}} \equiv \frac{d v_{\mathrm{gr}}}{d t}=\frac{d}{d t} \frac{d \omega\left(q_{0}\right)}{d q_{0}}=\frac{d}{d q_{0}} \frac{d \omega\left(q_{0}\right)}{d q_{0}} \frac{d q_{0}}{d t}=\frac{d^{2} \omega\left(q_{0}\right)}{d q_{0}^{2}} \frac{d q_{0}}{d t}=\left.\frac{1}{\hbar} \frac{d^{2} \omega}{d q^{2}}\right|_{q=q_{0}} F(t) . \tag{2.238}
\end{equation*}
$$

This means that the second derivative of the dispersion relation plays the role of the effective reciprocal mass of the particle:

$$
\begin{equation*}
m_{\mathrm{ef}}=\frac{\hbar}{d^{2} \omega / d q^{2}}=\frac{\hbar^{2}}{d^{2} E / d q^{2}} \tag{2.239}
\end{equation*}
$$

For the particular case of a free particle, described by Eq. (216), this expression is reduced to the original (and constant) mass $m$, but generally the effective mass depends on the wave packet's momentum. According to Eq. (239), at the bottom of any energy band, $m_{\text {ef }}$ is always positive, but depends on the strength of particle's interaction with the periodic potential. In particular, according to Eq. (206), in the tight binding limit, the effective mass is very large:

[^516]\[

$$
\begin{equation*}
\left|m_{\mathrm{ef}}\right|_{q=(\pi / a) n}=\frac{\hbar^{2}}{2 \delta_{n} a^{2}}=m \frac{E^{(1)}}{\pi^{2} \delta_{n}} \gg m . \tag{2.240}
\end{equation*}
$$

\]

On the contrary, in the weak potential limit, the effective mass is close to $m$ at most points of each energy band, but at the edges of the (narrow) bandgaps it is much smaller. Indeed, expanding Eq. (224) in the Taylor series near point $q=q_{m}$, we get

$$
\begin{equation*}
\left.E_{ \pm}\right|_{E \approx E^{(n)}} \approx \pm\left|U_{n}\right| \pm \frac{1}{2\left|U_{n}\right|}\left(\frac{d E_{l}}{d q}\right)_{q=q_{m}}^{2} \quad \widetilde{q}^{2}= \pm\left|U_{n}\right| \pm \frac{\gamma^{2}}{2\left|U_{n}\right|} \widetilde{q}^{2} \tag{2.241}
\end{equation*}
$$

where $\gamma$ and $\widetilde{q}$ are defined by Eq. (225), so that

$$
\begin{equation*}
\left|m_{\mathrm{ef}}\right|_{q=q_{m}}=\left|U_{n}\right| \frac{\hbar^{2}}{\gamma^{2}}=m \frac{\left|U_{n}\right|}{2 E^{(n)}} \ll m . \tag{2.242}
\end{equation*}
$$

The effective mass effects in real solids may be very significant. For example, the charge carriers in the ubiquitous field-effect transistors of silicon integrated circuits have $m_{\mathrm{ef}} \approx 0.19 m_{e}$ in the lowest normally-empty energy band (traditionally called the conduction band), and $m_{\mathrm{ef}} \approx 0.98 m_{e}$ in the lower, normally-filled valence band. In some semiconducting compounds the conduction-band electron mass may be even smaller - down to $0.0145 m_{\mathrm{e}}$ in InSb!

However, the absolute value of the effective mass in not the most surprising effect. The more shocking corollary of Eq. (239) is that on the top of each energy band the effective mass is negative please revisit Figs. 26, 28, and 29 again. This means that the particle (or more strictly its wave packet's envelope) is accelerated in the direction opposite to the force. This is exactly what electronic engineers, working with electrons in semiconductors, call holes, characterizing them by positive mass and positive charge. If the particle does not leave a close vicinity of the energy band's top (say, due to scattering effects), such flip of signs does not lead to an error, because the Lorentz force is proportional to electron's charge $(q=-e)$, so that particle's acceleration $a_{\mathrm{gr}}$ is proportional to ratio ( $q / m_{\mathrm{ef}}$ ). ${ }^{70}$

However, at some phenomena the usual image of a hole as a particle with $q>0$ and $m_{\text {ef }}>0$ is unacceptable. For example, let us form a narrow wave packet at the bottom of the lowest energy band, ${ }^{71}$ and then exert on it a constant force $F>0$ - say, due to a constant external electric field directed along axis $x$. According to Eq. (237), this would lead to a linear growth of $q_{0}$ in time, so that in the quasimomentum space, the packet's center would slide, with constant speed, along the $q$ axis - see Fig. 32a. Close to the energy band bottom, this motion would correspond to a positive effective mass (possibly, somewhat larger than the genuine particle's mass $m$ ), and hence be close to free particle's acceleration. However, as soon as $q_{0}$ has reached the inflection point, where $d^{2} E_{1} / d q^{2}=0$, the effective mass, and hence acceleration (238) change signs to negative, i.e. the packet starts to slow down (in the direct space

[^517]$x$ ) while still moving ahead in the quasi-momentum space. Finally, at the energy band's top the particle stops at certain $x_{\text {max }}$, while continuing to move in the $q$-space.


Fig. 2.32. The Bloch oscillations (red lines) and the Landau-Zener tunneling (blue arrows) within: (a) the time-domain picture, and (b) the energy-domain picture. On panel (b), the tilted gray strips show the allowed energy bands, and the bold red lines, the Wannier-Stark ladder.

Now we have two alternative ways to look at the further time evolution of the wave packet. From the extended zone picture (which is the simplest for this analysis, see Fig. 32a), ${ }^{72}$ we may say that the particle crosses the $1^{\text {st }}$ Brillouin zone boundary and starts going forward in $q$, i.e. down the lowest energy band. According to Eq. (235), this region (up to the next inflection point) corresponds to a negative group velocity. After $q_{0}$ has reached the next minimum of the energy band at $q a=2 \pi$, the whole process repeats again (and again, and again).

These are the famous Bloch oscillations - the effect that was predicted (by the same F. Bloch) as early as in 1929, but evaded experimental observation until the 1980s - see below. Their time period may be readily found from Eq. (237):

$$
\begin{equation*}
\Delta t_{\mathrm{B}}=\frac{\Delta q}{d q / d t}=\frac{2 \pi / a}{F / \hbar}=\frac{2 \pi \hbar}{F a}, \tag{2.243}
\end{equation*}
$$

so that the Bloch oscillation frequency

$$
\begin{equation*}
\omega_{\mathrm{B}} \equiv \frac{2 \pi}{\Delta t_{\mathrm{B}}}=\frac{F a}{\hbar} . \tag{2.244}
\end{equation*}
$$

Bloch oscillations: frequency

The direct-space motion of the wave packet's center $x_{0}(t)$ during the Bloch oscillation process may be analyzed by integrating Eq. (235) over some time interval $\Delta t$ :

[^518]\[

$$
\begin{equation*}
\Delta x_{0}(t)=\int_{0}^{\Delta t} v_{\mathrm{gr}} d t=\int_{0}^{\Delta t} \frac{d \omega\left(q_{0}\right)}{d q_{0}} d t=\int_{0}^{\Delta t} \frac{d \omega\left(q_{0}\right)}{d q_{0} / d t}=\frac{\hbar}{F} \int_{t=0}^{t=\Delta t} d \omega=\frac{\hbar}{F} \Delta \omega\left(q_{0}\right) . \tag{2.245}
\end{equation*}
$$

\]

If interval $\Delta t$ is equal to the Bloch oscillation period $\Delta t_{\mathrm{B}}$ (234), the initial and final moments of $E\left(q_{0}\right)=$ $\hbar \omega\left(q_{0}\right)$ are equal, giving $\Delta x_{0}=0$ : in the end of the period, the wave packet returns to its initial position. However, if we carry this integration only from the smallest to the largest values of $\omega\left(q_{0}\right)$, i.e. the points where the group velocity vanishes, we get the oscillation swing
 spatial swing

$$
\begin{equation*}
\Delta x_{\max }=\frac{\hbar}{F}\left(\omega_{\max }-\omega_{\min }\right)=\frac{\Delta E_{1}}{F} \tag{2.246}
\end{equation*}
$$

This simple result may interpreted using an alternative energy diagram (Fig. 32b) that results from the following arguments. The additional force $F$ may be described not only via the $2^{\text {nd }}$ Newton law version (237), but, alternatively, by its contribution $U_{F}=-F x$ to the total ("Gibbs" ${ }^{73}$ ) potential energy

$$
\begin{equation*}
U_{\Sigma}(x)=U(x)-F x \tag{2.247}
\end{equation*}
$$

of the system. The direct solution of the Schrödinger equation (61) with such potential may be hard to find, but if the force is weak in the sense of Eq. (236), as we are assuming now, one can argue that our quantum-mechanical treatment including the periodic potential $U(x)$ should be still correct, if the second term in Eq. (247) is considered as a constant at the wave packet width scale $\delta x$, but dependent on position $x_{0}$ of the packet's center. In this approximation, the total energy of the wave packet may be found as

$$
\begin{equation*}
E_{\Sigma}=E\left(q_{0}\right)-F x_{0} . \tag{2.248}
\end{equation*}
$$

In a plot of such energy as a function of $x_{0}$ (Fig. 32b), the information on energy dependence on $q_{0}$ is lost, but we already know it is rather uneventful, and well characterized by the position of band-gap edges on the energy axis. ${ }^{74}$ In this representation, the Bloch oscillations of a relatively wide $(\delta x \gg a)$ wave packet should keep the full energy $E_{\Sigma}$ constant, i.e. follow a horizontal line in Fig. 32b, limited by the classical turning points corresponding to the bottom and the top of the allowed energy band. The distance $\Delta x_{\text {max }}$ between these point is evidently given by Eq. (246).

Besides this second look at the oscillation swing result, the total energy diagram shown in Fig. 32b enables one more remarkable result. Let a wave packet be so narrow in the momentum space ( $\delta q \rightarrow$ 0 ) that $1 / q \gg \Delta x_{\max }$; then the horizontal line segment in Fig. 32b presents the spatial extension of the eigenfunction of the Schrödinger equation with potential (247). But this equation is evidently invariant with respect to the following simultaneous translation in coordinate and energy:

$$
\begin{equation*}
x \rightarrow x+a, \quad E \rightarrow E-F a \tag{2.249}
\end{equation*}
$$

WannierStark ladder

This means that it is satisfied with an infinite set of similar solutions, each corresponding to one of the horizontal red lines shown in Fig. 32b. This is the famous Wannier-Stark ladder, with the step height

$$
\begin{equation*}
\Delta E_{S}=F a \tag{2.250}
\end{equation*}
$$

[^519]The importance of this alternative representation of the Bloch oscillations is due to the following fact. In most experimental realizations, the power of radiation at frequency (244), that may be extracted from the oscillations by their electromagnetic coupling to an external detector, is very low, so that their direct detection presents a hard problem. ${ }^{75}$ However, let us apply to a Bloch oscillator an additional rf field at frequency $\omega \sim \omega_{\mathrm{B}}$. As these frequencies are brought close together, the external signal should synchronize ("phase lock") Bloch oscillations, ${ }^{76}$ resulting in certain observable changes - for example, a resonant absorption of the external radiation. Now let us notice that Eqs. (244) and (250) yield the following remarkable relation:

$$
\begin{equation*}
\Delta E_{S}=\hbar \omega_{\mathrm{B}} . \tag{2.251}
\end{equation*}
$$

This means that the resonant phenomena at $\omega \approx \omega_{\mathrm{B}}$ allow for an alternative (but equivalent) interpretation - as the result of rf-induced transitions ${ }^{77}$ between the steps of the Wannier-Stark ladder! (Such occasions when two very different languages may be used for the interpretation of the same phenomenon is one of the most beautiful features of physics.)

This effect has been used for the first experimental confirmation of the Bloch oscillation theory. For this purpose, the natural periodic structures, solid state crystals, are inconvenient due to their very small period $a \sim 10^{-10} \mathrm{~m}$. Indeed, according to Eq. (244), such structures require very high forces $F$ (and hence high electric fields $\varepsilon=F / e$ ) to bring $\omega_{\mathrm{B}}$ to an experimentally convenient range. This problem has been overcome by fabricating artificial periodic structures (superlattices) of certain semiconductor compounds, such as $\mathrm{Ga}_{1-x} \mathrm{Al}_{x} \mathrm{As}$ with various degrees $x$ of gallium to aluminum atom replacement, whose layers may be grown over each other epitaxially, i.e., without very few crystal structure violations. These superlattices, with periods $a \sim 10 \mathrm{~nm}$, has allowed a clear observation of resonant effects at $\omega \approx \omega_{\mathrm{B}}$, and hence the measurement of the Bloch oscillation frequency, in particular its proportionality to the applied dc electric field, predicted by Eq. (244). ${ }^{78}$

Very soon after this observation, the Bloch oscillations have been observed in small Josephson junctions. ${ }^{79}$ Since this experiment involved two important conceptual issues, let me discuss it in a little bit more detail. As was discussed in Sec. 2.3, the Josephson junction dynamics may be reasonably well described by two simple equations (54) and (55). They may be combined to calculate the work of an external voltage source at Josephson phase change between arbitrary initial ( $\varphi_{\text {ini }}$ ) and final ( $\varphi_{\text {fin }}$ ) values, as the integral of its power $I V$ over the time interval $\Delta t$ of the change:

$$
\begin{equation*}
\text { work }=\int_{\Delta t} I V d t=\int_{\Delta t}\left(I_{c} \sin \varphi\right)\left(\frac{\hbar}{2 e} \frac{d \varphi}{d t}\right) d t=\frac{\hbar I_{c}}{2 e} \int_{\varphi_{\mathrm{ini}}}^{\varphi_{\mathrm{fin}}} \sin \varphi d \varphi=-\frac{\hbar I_{c}}{2 e}\left(\cos \varphi_{\mathrm{fin}}-\cos \varphi_{\mathrm{ini}}\right) . \tag{2.252}
\end{equation*}
$$

We see that the work depends only on the initial and final values of $\varphi$ (but not on the law phase evolution in time $)$, i.e. may be presented as the difference $U\left(\varphi_{\text {fin }}\right)-U\left(\varphi_{\text {ini }}\right)$, where function

[^520]Josephson
coupling energy

$$
\begin{equation*}
U(\varphi)=-E_{\mathrm{J}} \cos \varphi+\mathrm{const}, \quad \text { with } E_{\mathrm{J}} \equiv \frac{\hbar I_{C}}{2 e} \tag{2.250}
\end{equation*}
$$

may be interpreted as the potential energy of the junction (if we consider the Josephson phase as a generalized coordinate). This energy apart, the Josephson junction, as a system of two close, nearly isolated (super)conductors, has a certain capacitance $C$ and the associated electrostatic energy $E_{C}=$ $C V^{2} / 2$. Using Eq. (54) again, we may present it as

$$
\begin{equation*}
E_{C}=\frac{C}{2} V^{2}=C\left(\frac{\hbar}{2 e}\right)^{2}\left(\frac{d \varphi}{d t}\right)^{2} . \tag{2.251}
\end{equation*}
$$

This means that from the point of view at phase $\varphi$ as a generalized coordinate, $E_{C}$ should be considered the kinetic energy of the system, whose dependence on the generalized velocity $d \varphi / d t$ is similar to that of a 1D mechanical particle, with an effective mass ${ }^{81}$

$$
\begin{equation*}
m_{\mathrm{J}}=C\left(\frac{\hbar}{2 e}\right)^{2} \tag{2.252}
\end{equation*}
$$

Hence the total energy of the junction, $E_{C}+U(\varphi)$, is formally similar to that of a 1 D non-relativistic particle in the sinusoidal potential with the $\varphi$-axis period $a_{\mathrm{J}}=2 \pi$.

However, before using the results of the 1D band theory to this system, we have to resolve one paradox (that was the subject of a lively discussion just about 30 years ago). When we develop the band theory, we imply that its translation by period $a$ is (in principle) measurable, i.e. particle positions $x$ and $(x+a)$ are distinguishable - otherwise Eq. (193) with $q \neq 0$ would not have much sense. For a mechanical particle this assumption is very plausible, but less so for a Josephson junction. Indeed, for example, if we change $\varphi$ by $a_{\mathrm{J}}=2 \pi$ via changing the phase of one of superconductors, say $\varphi_{1}$ (Fig. 3) by $2 \pi$, then its wavefunction becomes $|\psi| \exp \left\{i\left(\varphi_{1}+2 \pi\right)\right\}=|\psi| \exp \left\{i \varphi_{1}\right\}$, and it is not immediately clear whether these two states may be distinguished. In order to resolve this contradiction, it is sufficient to have a look at Eq. (54). It shows that if $\varphi$ changes in time by $2 \pi$ (say, by a fast ramp-up), voltage $V$ across the junction exhibits a pulse with "area"

$$
\begin{equation*}
\int V(t) d t=\frac{\hbar}{2 e} \int \frac{d \varphi}{d t} d t=\frac{\hbar}{2 e} \int d \varphi=\frac{\hbar}{2 e} 2 \pi=\frac{h}{2 e} \approx 2 \times 10^{-15} \mathrm{~V} \cdot \mathrm{~s} . \tag{2.253}
\end{equation*}
$$

Such single-flux-quantum (SFQ) pulses ${ }^{82}$ not only may be measured experimentally, but even have been used for signaling and ultrafast (sub-THz) computation, to the best of my knowledge still keeping the absolute records for the highest speed and smallest energy consumption at computation. ${ }^{83}$

Hence, the $2 \pi$-shifts of phase $\varphi$ are measurable, and in the absence of dissipation the Josephson junction dynamics is indeed similar to that of a 1D particle in a periodic (sinusoidal) potential, and its energy spectrum forms energy bands and gaps described by the Mathieu equation - see Fig. 31. Experimentally, the easiest way to verify this picture is to measure the corresponding Bloch oscillations

[^521]induced by an external current $I_{\mathrm{ex}}(t)$. In order to find the frequency of these oscillations, it is sufficient to replace Eq. (237), which expresses the $2^{\text {nd }}$ Newton law averaged over period a of potential $U(x)$, with the charge balance equation
\[

$$
\begin{equation*}
\frac{d Q}{d t}=I_{\mathrm{ex}}(t) \tag{2.254}
\end{equation*}
$$

\]

where $Q$ is the "quasi-charge" ${ }^{84}$, i.e. the electric charge of the capacitor averaged over the period $2 \pi$ of the periodic potential $U(\varphi)$. (Notice that at such averaging, current (55) is averaged out from the equation, so that is affects the phenomena "only" via its contribution to the energy band structure.)

Since the Josephson-junction analog of the genuine wave number $k=m(d x / d t) / \hbar$ of a particle is

$$
\begin{equation*}
k_{\mathrm{J}}=\frac{m_{\mathrm{J}}}{\hbar} \frac{d \varphi}{d t}=\frac{m_{\mathrm{J}}}{\hbar} \frac{2 e}{\hbar} V=\frac{C V}{2 e}, \tag{2.255}
\end{equation*}
$$

and $C V$ is the genuine charge on the capacitor, the analog of $q$ (the quasi-momentum divided by $\hbar$ ) may be obtained just by the replacement of that product with quasi-charge $Q$ :

$$
\begin{equation*}
q_{\mathrm{J}}=\frac{Q}{2 e} . \tag{2.256}
\end{equation*}
$$

Comparing this expression with Eq. (254), we see that $q_{\mathrm{J}}$ obeys the following equation of motion:

$$
\begin{equation*}
\frac{d q_{\mathrm{J}}}{d t}=\frac{I_{\mathrm{ex}}(t)}{2 e} \tag{2.257}
\end{equation*}
$$

so that the role of force $F$ is now played by $F_{\mathrm{J}}=\hbar I / 2 e$. Hence if $I_{\mathrm{ex}}(t)=$ const $=\bar{I}$, we can use Eq. (244) with that replacement, and also $a \rightarrow a_{\mathrm{J}}=2 \pi$, to get

$$
\begin{equation*}
f_{\mathrm{B}} \equiv \frac{\omega_{\mathrm{B}}}{2 \pi}=\frac{1}{2 \pi} \frac{F_{\mathrm{J}} a_{\mathrm{J}}}{\hbar}=\frac{\bar{I}}{2 e} . \tag{2.258}
\end{equation*}
$$

This very simple result has the following physical sense. ${ }^{85}$ In the quantum operation mode, the junction is recharged by the external current, following Eq. (256), until its electric charge reaches $e$ (i.e. $q_{\mathrm{J}} a_{\mathrm{J}}=(Q / 2 e) 2 \pi$ reaches $\pi$-see Fig. 32a); then one Cooper pair passes through the junction changing its charge to $e-(2 e)=-e$, with the same charging energy (251) - the process analogous to crossing the border of the $1^{\text {st }}$ Brillouin zone; then the process repeats again and again. It is remarkable that Eq. (258), describing the frequency of such a quantum property of the Josephson phase $\varphi$ as its Bloch oscillations, does not include the Planck constant, while Eq. (56), describing the classical motion of $\varphi$, does. ${ }^{86}$

[^522]In this context, one may wonder which of these two types of oscillations would a dc-biased Josephson junction generate. For the dissipation-free junction, the answer is: the Bloch oscillations (258) with frequency proportional to dc current. However, any practical junction has some energy losses that may be (approximately) described by a certain Ohmic conductance $G$ connected in parallel to the junction. Very luckily for Dr. Josephson and his Nobel Prize, it is much easier to fabricate and test junctions with $G \gg 1 / R_{Q}$, where $R_{Q}$ is the so-called quantum unit of resistance

$$
\begin{equation*}
R_{Q} \equiv \frac{\pi \hbar}{2 e^{2}} \approx 6.45 \mathrm{k} \Omega \tag{2.259}
\end{equation*}
$$

the fundamental constant that jumps out at analysis of several other effects as well - see, e.g., Sec. 3.2. As will be discussed in Chapter 7, such high energy losses provide what is called dephasing - the suppression of the quantum coherence between different quantum states of the system - in our current case, between the wavefunctions $u(\varphi-2 \pi j)$ localized at different minima of the periodic potential $U(\varphi)$, and thus make the dynamics of the Josephson phase $\varphi$ virtually classical, obeying equations (54) and (55). As we have seen in Sec. 2, dc biasing of such a junction leads to Josephson oscillations with frequency (56) proportional to the applied dc voltage.

### 2.9. Landau-Zener tunneling

All the Bloch oscillation discussion in the last section was based on the premise that the particle stays within one (say, the lowest) energy band. However, just a single look at Fig. 32 shows that this assumption becomes unrealistic if the energy gap separating this band from the next one becomes very small, $\Delta_{1} \rightarrow 0$. Indeed, in the weak potential approximation, that is adequate in this limit, at $\left|U_{1}\right| \rightarrow 0$, the two dispersion curve branches (216) cross without any interaction, so that if our particle (the wave packet) is driven to approach that point, it should continue to move up in energy - see the dashed blue arrow in Fig. 32a. Similarly, in the "energy-domain" presentation shown in Fig. 32b, it is intuitively clear that at $\Delta_{1} \rightarrow 0$, the particle residing at one of the steps of the Wannier-Stark ladder should able to somehow overcome the vanishing spatial gap $\Delta x_{0}=\Delta_{1} / F$ and to leak into the next band - see the horizontal dashed blue arrow on that panel.

This process, called the Landau-Zener (or "interband", or "band-to-band") tunneling ${ }^{87}$ is indeed possible. In order to analyze it, let us first take $F=0$, and consider what happens if a quantum particle described by an $x$-long (i.e. $E$-narrow) wave packet is incident from the free space upon a periodic structure of a large but finite length $l \gg a$. If packet's energy $E$ is within one of the energy bands, it may evidently propagate through the structure (though may be partly reflected from its front end). The corresponding quasi-momentum may be found by solving the dispersion relation for $q$; for example, in the weak-potential limit, Eq. (224), which is valid near the gap, yields

$$
\begin{equation*}
q=q_{m}+\widetilde{q}, \quad \widetilde{q}= \pm \frac{1}{\gamma}\left[\widetilde{E}^{2}-\left|U_{n}\right|^{2}\right]^{1 / 2}, \quad \text { where } \widetilde{E} \equiv E_{ \pm}-E^{(n)} \tag{2.260}
\end{equation*}
$$

and $\gamma$ is given by the second of Eqs. (225).

[^523]Now, if energy $E$ corresponds to one of the energy gaps $\Delta_{n}$, the propagation is impossible, so that the packet is completely reflected back. However, our analysis of the potential step problem in Sec. 3 implies that the wavefunction would still have an exponential tail protruding into the periodic structure and decaying on some length $\delta$ - see Eq. (67). Indeed, a review of the calculation leading to Eq. (260) shows that they remain valid within the gap as well, if the quasi-momentum is understood as a purely imaginary number:

$$
\begin{equation*}
\widetilde{q} \rightarrow \pm i \kappa, \quad \text { where } \kappa \equiv \frac{1}{\gamma}\left[\left.U_{n}\right|^{2}-\widetilde{E}^{2}\right]^{1 / 2}, \quad \text { for } \widetilde{E}^{2} \leq\left|U_{n}\right|^{2} . \tag{2.261}
\end{equation*}
$$

With such contribution, the Bloch solution (193b) indeed describes an exponential decay of the wavefunction at length $\delta=1 / \kappa$.

Now returning to the effects of weak force $F$ in the energy-domain approach, presented by Eq. (248) and illustrated in Fig. 32b, we may recast Eq. (261) as

$$
\begin{equation*}
\kappa \rightarrow \kappa(x)=\frac{1}{\gamma}\left[\left.U_{n}\right|^{2}-(F \tilde{x})^{2}\right]^{1 / 2}, \tag{2.262}
\end{equation*}
$$

where $\tilde{x}$ is particle's (i.e. wave packet center's) deviation from the mid-gap point. Thus the gap has created a potential barrier of a finite width $\Delta x_{0}=2\left|U_{n}\right| / F$, through which the wave packet may tunnel with a finite probability. As we already know, in the WKB approximation (in our case requiring $\kappa \Delta x_{0}$ $\gg 1$ ) this probability is just the tunnel barrier's transparency $T$, which may be calculated from Eq. (117):

$$
\begin{equation*}
-\ln T=2 \int_{\kappa(x)^{2}>0} \kappa(x) d x=\frac{2}{\gamma} \int_{-x_{c}}^{x_{c}}\left[\left|U_{n}\right|^{2}-(F \widetilde{x})^{2}\right]^{1 / 2} d \widetilde{x}=\frac{2\left|U_{n}\right|}{\gamma} 2 x_{c} \int_{0}^{1}\left(1-\xi^{2}\right)^{1 / 2} d \xi \tag{2.263}
\end{equation*}
$$

where $\pm x_{c} \equiv \pm \Delta x_{0} / 2= \pm\left|U_{n}\right| / F$ are the classical turning points. Working out this simple integral (which may be viewed upon as the quarter of the unit circle's area, and hence equal to $\pi / 4$ ), we get

$$
\begin{equation*}
T=\exp \left\{-\frac{\pi\left|U_{n}\right|^{2}}{\gamma F}\right\} . \tag{2.264}
\end{equation*}
$$

This famous result was obtained by Landau and Zener in a more complex way, whose advantage is a constructive proof that Eq. (264) is valid for arbitrary relation between $\gamma F$ and $\left|U_{n}\right|^{2}$, i.e. arbitrary $T$, while our simple derivation was limited to the WKB approximation, i.e. to $T \ll 1.88$

Returning to Eq. (225) and (237), we can rewrite the product $\gamma F$ participating in Eq. (264) as

$$
\begin{equation*}
\gamma F=\frac{1}{2}\left|\frac{d\left(E_{l}-E_{l^{\prime}}\right)}{d q_{0}}\right|_{E_{l}=E_{l}=E_{n}} \hbar \frac{d q_{0}}{d t}=\frac{\hbar}{2}\left|\frac{d\left(E_{l}-E_{l^{\prime}}\right)}{d t}\right|_{E_{l}=E_{l}=E_{n}}=\frac{\hbar u}{2}, \tag{2.265}
\end{equation*}
$$

where $u$ has the meaning of the "speed" of the energy level crossing in the absence of the gap. Hence, Eq. (264) may be presented in a form

[^524]\[

$$
\begin{equation*}
T=\exp \left\{-\frac{2 \pi\left|U_{n}\right|^{2}}{\hbar u}\right\} \tag{2.266}
\end{equation*}
$$

\]

that is more physically transparent. ${ }^{89}$ Indeed, the fraction $2\left|U_{n}\right| / u=\Delta_{n} u$ gives the time scale $\Delta t$ of energy's crossing the gap region, and according to the Fourier transform, its reciprocal, $\omega_{\max } \sim 1 / \Delta t$ gives the upper cutoff of frequencies involved in the Bloch oscillation process. Hence Eq. (266) means that

$$
\begin{equation*}
-\ln T \approx \frac{\Delta_{n}}{\hbar \omega_{\max }} \tag{2.267}
\end{equation*}
$$

This formula allows us to interpret the Landau-Zener tunneling as for system's excitation across the energy gap $\Delta_{\mathrm{n}}$, by the maximum energy quantum $\hbar \omega_{\max }$ available from the Bloch oscillation process.

The interband tunneling is an important ingredient of several physical phenomena and even some practical devices, for example the tunneling (or "Esaki") diodes. This simple device is just a junction of two semiconductor electrodes, one of them is so strongly $n$-doped by electron donors that the additional electrons form a degenerate Fermi gas at the bottom of the conduction band. Similarly, the opposite electrode is $p$-doped so strongly that the Fermi level of electrons in the valence band is lowered below the band edge (Fig. 33).


Eig. 2.33. Tunneling diode: (a) the band edge diagram of the device at zero bias; (b) the same diagram at modest positive bias $\mathrm{eV} \sim \Delta / 2$, and (c) the $I-V$ curve (schematically). Dashed lines show the Fermi level positions.

At thermal equilibrium, and in the absence of external voltage bias, the Fermi levels self-align, ${ }^{90}$ leading to the build-up of the contact potential difference $\phi / e$, with $\phi$ somewhat larger than the energy bandgap $\Delta$ - see Fig. 33a. This potential difference creates an internal electric field that tilts the energy bands (just as the external field did in Fig. 32b), and leads to the formation of the so-called deletion layer in which the Fermi level located is within the energy gap and hence there are no charge carriers ready to move. In usual $p-n$ junctions, this layer is broad and prevents any current at applied voltages $V$ lower than $\sim \Delta / e$. In contrast, in a tunneling diode the depletion layer is so thin (below $\sim 10 \mathrm{~nm}$ ) that the

[^525]interband tunneling is possible and provides a substantial Ohmic current at small applied voltages - see Fig. 33c.

However, at substantial positive bias, $e V \sim \Delta / 2$, the conduction band become aligned with the middle of the gap in the $p$-doped electrode, and electrons cannot tunnel there. Similarly, these are no electrons in the $n$-doped semiconductor to tunnel into the available states just above the Fermi level in the $p$-doped electrode - see Fig. 33b. As a result, current drops significantly, to grow again only when $e V$ exceeds $\sim \Delta$ and allows the electron motion through the within each energy band. Thus the tunnel junction's $I-V$ curve has a part with negative differential resistance $(d V / d I<0)$. This effect may be used for the amplification of analog signals, including self-excitation of electrical oscillators (i.e. rf signal generation), ${ }^{91}$ and signal swing restoration in digital electronics.

### 2.10. Harmonic oscillator: A brute force approach

To complete our review of 1D systems, we have to consider the famous harmonic oscillator, i.e. a 1 D particle moving in the quadratic-parabolic potential (111). This is just a smooth quantum well providing "soft" confinement, whose discrete spectrum we have already found in the WKB approximation - see Eq. (114). Let us try to solve the same problem exactly - not because there is anything conceptually interesting in it (there is not :-), but because of its enormous importance for applications. For that, let us write the stationary Schrödinger equation for potential (111):

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2} \psi}{d x^{2}}+\frac{m \omega_{0}^{2}}{2} x^{2} \psi=E \psi \tag{2.268}
\end{equation*}
$$

From the solution of Exercise Problem 1.5, the reader already knows ${ }^{92}$ one of the eigenfunctions of this equation,

$$
\begin{equation*}
\psi_{0}=C_{0} \exp \left\{-\frac{m \omega_{0} x^{2}}{2 \hbar}\right\} \tag{2.269}
\end{equation*}
$$

and the corresponding eigenenergy

$$
\begin{equation*}
E_{0}=\frac{\hbar \omega_{0}}{2} \tag{2.270}
\end{equation*}
$$

Expression (269) shows that the characteristic scale of wavefunction's spatial spread ${ }^{93}$ is equal to

$$
\begin{equation*}
x_{0} \equiv\left(\frac{\hbar}{m \omega_{0}}\right)^{1 / 2} \tag{2.271}
\end{equation*}
$$

Due to the importance of this scale, let us give its crude estimates for several typical systems:

[^526](i) Electrons in solids and fluids: $m \approx 10^{-30} \mathrm{~kg}, \omega_{0} \sim 10^{15} \mathrm{~s}^{-1}$, giving $x_{0} \sim 0.3 \mathrm{~nm}$, comparable with inter-atomic distances $a$. As a result, classical mechanics is not valid at all for the analysis of their motion.
(ii) Atoms in solids: $m \approx 10^{-24}-10^{-26} \mathrm{~kg}, \omega_{0} \sim 10^{13} \mathrm{~s}^{-1}$, giving $x_{0} \sim 0.01-0.1 \mathrm{~nm}$, i.e. from $\sim$ a few percent to a few tens percent of $a$. Because of that, methods based classical mechanics (e.g., molecular dynamics) are approximately valid for the analysis of atomic motion, though may miss some fine effects of motion of lighter atoms - e.g., quantum tunneling of hydrogen atoms through energy barriers of the potential profile created by its neighbors.
(iii) Probe masses in modern gravity-wave detectors (Advanced LIGO, VIRGO, KAGRA, etc.): ${ }^{94} m \sim 10^{2} \mathrm{~kg}, \omega_{0} \sim 10^{2} \mathrm{~s}^{-1}$, giving $x_{0} \sim 10^{-19} \mathrm{~m}$. After several decades of development, the sensitivity of these instruments is still limited by various noise sources at the level of the order of $10^{-18} \mathrm{~m} .{ }^{95}$ Thus the prospects of observing quantum-mechanical effects in such installations do not look very realistic.

Returning to the Schrödinger equation (268), let us recast it into a dimensionless form by introducing dimensionless variable $\xi \equiv x / x_{0}$. This gives

$$
\begin{equation*}
-\frac{d^{2} \psi}{d \xi^{2}}+\xi^{2} \psi=\varepsilon \psi \tag{2.272}
\end{equation*}
$$

where $\varepsilon \equiv 2 E / \hbar \omega_{0}=E / E_{0}$. In this notation, the ground state wavefunction is proportional to $\exp \left\{-\xi^{2} / 2\right\}$, so that let us look for the solutions to Eq. (272) in the form

$$
\begin{equation*}
\psi=C \exp \left\{-\frac{\xi^{2}}{2}\right\} H(\xi) \tag{2.273}
\end{equation*}
$$

where $H(\xi)$ is a new function. With this substitution, Eq. (272) yields

$$
\begin{equation*}
\frac{d^{2} H}{d \xi^{2}}-2 \xi \frac{d H}{d \xi}+(\varepsilon-1) H=0 \tag{2.274}
\end{equation*}
$$

It is evident that $H=$ const and $\varepsilon=1$ is one of its solutions, describing the eigenstate (269) with energy (270), but what are the other eigenstates and eigenvalues? This equation has been studied in detail in the mid-1800s by C. Hermite who has shown that all eigenvalues are given by equation

$$
\begin{equation*}
\varepsilon_{n}-1=2 n, \quad \text { with } \quad n=0,1,2, \ldots, \tag{2.275}
\end{equation*}
$$

so that our WKB result (114) is indeed exact for any $n$, and Eqs. (269) and (270) describe the groundstate of the oscillator. The eigenfunction corresponding to eigenvalue $\varepsilon_{n}$ is a polynomial (now called the Hermite polynomial) of degree $n$, that may be most conveniently calculated using the following explicit formula:

Hermite polynomials

$$
\begin{equation*}
H_{n}=(-1)^{n} \exp \left\{\xi^{2}\right\} \frac{d^{n}}{d \xi^{n}} \exp \left\{-\xi^{2}\right\} . \tag{2.276}
\end{equation*}
$$

[^527]It is easy to use this formula to calculate several lowest-degree polynomials - see Fig. 34a:

$$
\begin{equation*}
H_{0}=1, \quad H_{1}=2 \xi, \quad H_{2}=4 \xi^{2}-2, \quad H_{3}=8 \xi^{3}-12 \xi, \quad H_{4}=16 \xi^{4}-48 \xi^{2}+12, \ldots \tag{2.277}
\end{equation*}
$$


(a)

Fig. 2.34. (a) A few lowest Hermite polynomials and (b) the corresponding eigenenergies (dashed lines) and eigenfunctions (solid lines) of the harmonic oscillator. The black dashed line shows the potential profile $U(x)$, drawn on the same scale as energies $E_{n}$, so that the line crossings with the energy levels correspond to the classical turning points.

The most important properties of the polynomials are as follows:
(i) their "parity" (symmetry-antisymmetry) alternates with number $n$,
(ii) $H_{n}(\xi)$ crosses the $\xi$-axis exactly $n$ times (has $n$ zeros), and
(iii) the polynomials are mutually orthonormal in the following sense:

$$
\begin{equation*}
\int_{-\infty}^{+\infty} H_{n}(\xi) H_{n^{\prime}}(\xi) \exp \left\{-\xi^{2}\right\} d \xi=\pi^{1 / 2} 2^{n} n!\delta_{n, n^{\prime}} \tag{2.278}
\end{equation*}
$$

Using Eq. (273) to translate this result to functions $\psi_{n}(x)$, we get the following orthonormal eigenfunctions of the harmonic oscillator (Fig.34b): ${ }^{96}$

$$
\begin{equation*}
\psi_{n}(x)=\frac{1}{\left(2^{n} n!\right)^{1 / 2} \pi^{1 / 4} x_{0}^{1 / 2}} \exp \left\{-\frac{x^{2}}{2 x_{0}^{2}}\right\} H_{n}\left(\frac{x}{x_{0}}\right) \tag{2.279}
\end{equation*}
$$

Besides its own importance, this is a typical example of eigenstates of particle confined in a softwall quantum well. It is very instructive to compare them with eigenstates of a the rectangular quantum well, with its ultimately-hard walls - see Eq. (1.76) and Fig. 1.7. Let us list their similar features:
(i) Wavefunctions oscillate in the classically-allowed regions with $E_{n}>U(x)$, while dropping exponentially beyond the boundaries of that region.
(ii) Each step up the energy level ladder increases the number of the oscillation halfwaves (and hence the number of its zeros), by one. ${ }^{97}$

Here are the major features specific for the soft confinement:
(i) The spatial spread of the wavefunction grows with $n$, following the gradual increase of the classically allowed region.
(ii) Correspondingly, $E_{n}$ exhibits a slower growth than the $E_{n} \propto n^{2}$ law given by Eq. (1.77), because of the gradual reduction of confinement, which moderates the growth of kinetic energy.

Unfortunately, the brute-force approach to the harmonic oscillator problem, discussed above, is not too appealing intellectually. First, the proof of Eq. (276) is rather longish. More importantly, it is hard to use Eq. (279) for calculation of the so-called matrix elements of the system - as we will see in Chapter 4, virtually the only numbers important for applications. Finally, it is also almost evident that there should be some straightforward math leading to any formula as simple as Eq. (114) for $E_{n}$. Indeed, there is a much more efficient, operator-based approach to this problem; it will be described in Sec. 5.4.

### 2.11. Exercise problems

2.1. The initial wave packet of a free 1D particle is described by Eq. (2.20) of the lecture notes:

$$
\Psi(x, 0)=\int a_{k} e^{i k x} d k
$$

(i) Obtain a compact expression for the expectation value $\langle p\rangle$ of particle's momentum. Does $\langle p\rangle$ depend on time?
(ii) Calculate $\langle p\rangle$ for the case when function $\left|a_{k}\right|^{2}$ is symmetric with respect to some value $k_{0}$.
2.2. Calculate the function $a_{k}$, defined by Eq. (2.20), for the wave packet with a rectangular envelope:

[^528]\[

\Psi(x, 0)=\left\{$$
\begin{array}{cc}
C \exp \left\{i k_{0} x\right\}, & \text { for }-a / 2 \leq x \leq+a / 2 \\
0, & \text { otherwise }
\end{array}
$$\right.
\]

Analyze the result in the limit $k_{0} a \rightarrow \infty$.
2.3. Prove Eq. (49) for the 1D propagator of a free quantum particle, starting from Eq. (48).
2.4. Express the 1D propagator, defined by Eq. (44), via eigenfunctions and eigenenergies of a particle moving in an arbitrary stationary potential $U(x)$. (For the notation simplicity, assume that the energy spectrum of the system is discrete.)
2.5. Calculate the change of the wavefunction of a 1 D particle, resulting from a short pulse of an external force, which may be approximated by the delta-function: ${ }^{98}$

$$
F(t)=P \delta(t)
$$

2.6. Analyze the effect of phase locking of Josephson oscillations on the dc current flowing through the junction, assuming that external microwave source applies a fixed sinusoidal ac voltage,

$$
V(t)-\bar{V}=A \cos \omega t
$$

to a junction with sinusoidal current-phase relation (55), using Eq. (54) for time evolution of phase $\varphi$.
2.7. Calculate the transmission coefficient $T$ as a function of particle's energy $E$ for the rectangular potential barrier,

$$
U(x)=\left\{\begin{array}{cc}
0, & \text { for } x<-d / 2 \\
U_{0}, & \text { for }-d / 2<x<+d / 2 \\
0, & \text { for } d / 2<x
\end{array}\right.
$$

for the case $E>U_{0}$. Analyze and interpret the result, taking into account that $U_{0}$ may be either positive or negative. (In the last case, we are speaking about particle's passage over a rectangular potential well of finite depth.)
2.8. Looking at the lower (red) line in Fig. 1.7, it seems plausible that the 1 D ground-state function $X(x) \propto \sin (\pi x / a)$ of the simple quantum well (1.69) may be well approximated by an inverted parabola:

$$
X_{\text {trial }}(x)=C x(a-x),
$$

where $C$ is the normalization constant, and $a \equiv a_{x}$ for brevity. Explore how good this approximation is. ${ }^{99}$
2.9. Spell out the stationary wavefunctions of a harmonic oscillator in the WKB approximation, and use them to calculate the expectation values $\left\langle x^{2}\right\rangle$ and $\left\langle x^{4}\right\rangle$ for arbitrary state number $n$.

[^529]2.10. ${ }^{*}$ A 1D particle of mass $m$ is placed into the following triangular quantum well: ${ }^{100}$
\[

U(x)=\left\{$$
\begin{array}{ll}
+\infty, & \text { for } x<0, \\
F x, & \text { for } x>0,
\end{array}
$$ with F>0 .\right.
\]

(i) Calculate its energy spectrum using the WKB approximation.
(ii) Estimate the ground state energy using the variational method.
(iii) Calculate the three lowest energy levels, and also for the $10^{\text {th }}$ level, with at least $0.1 \%$ accuracy, from the exact solution of the problem.
(iv) Compare and discuss the results.

## Hints:

- In Task (ii), try to incorporate a certain parameter $\lambda$ into your trial wavefunction, and then use its adjustment to minimize the expectation value of system's Hamiltonian (mentioned in Chapter 1):

$$
\langle H\rangle_{\text {trial }} \equiv \int_{-\infty}^{+\infty} \psi_{\text {trial }}^{*} \hat{H} \psi_{\text {trial }} d x,
$$

where the trial function is assumed to be properly normalized. The variational method is based on the easily provable ${ }^{101}$ fact that this expectation value cannot be less than the genuine $E_{g}$, coinciding with it only if the trial function exactly coincides with the genuine wavefunction $\psi_{g}$ of the ground state. Hence, the lower $\langle H\rangle_{\text {trial }}$ you reach, the better is your result.

- The values of the first zeros of the Airy function, necessary for Task (iii), may be found in many math handbooks, for example, in Table 10.13 of the collection edited by Abramowitz and Stegun - see MA Sec. 16(i).
2.11. For a 1D particle of mass $m$ placed into a potential well with the following profile,

$$
U(x)=a x^{2 s}, \quad \text { with } a>0 \text { and } s>0,
$$

(i) calculate its energy spectrum using the WKB approximation, and
(ii) estimate the ground state energy using the variational method.

Compare the ground state energy results for parameter $s$ equal to $1,2,3$, and 100 .
2.12. Prove Eq. (117) for the case $T_{\mathrm{WKB}} \ll 1$, using the connection formulas (104).
2.13. Use the WKB approximation to express the expectation value of the kinetic energy of a 1 D particle, confined in a soft potential well, in its $n^{\text {th }}$ stationary state, via the derivative $d E_{n} / d n$, for $n \gg 1$.
2.14.* Use the WKB approximation to calculate the transparency $T$ as a function of particle energy $E$, for the following triangular potential barrier:

$$
U(x)=\left\{\begin{array}{cc}
0, & \text { for } x<0 \\
U_{0}-F x, & \text { for } x>0,
\end{array}\right.
$$

[^530]with $F, U_{0}>0$.
Hint: Be careful treating the sharp potential step at $x=0$.
2.15.* Prove that the symmetry of the scattering matrix elements describing an arbitrary timeindependent scatterer allows its representation in the form (136a), with the additional restriction (136b).
2.16. Prove the universal relations between elements of the transfer matrix T of a stationary (but otherwise arbitrary) 1D scatterer, which were mentioned in Sec. 5.
2.17. For a deep and narrow 1 D quantum well, modeled by a delta-function,
\[

$$
\begin{equation*}
U(x)=-w \delta(x), \quad \text { with } w>0, \tag{*}
\end{equation*}
$$

\]

find the localized eigenfunction(s) $\psi_{n}$ (with $\left|\psi_{n}(x)\right| \rightarrow 0$ at $|x| \rightarrow \infty$ ), and the corresponding value(s) $E_{n}$.
2.18. A 1D particle was localized in the delta-functional well, with $U(x)=-w \delta(x)$, such as the one analyzed in the previous problem. Then (say, at $t=0$ ) the well's bottom is suddenly lifted, so that the particle becomes free to move. Calculate the probability density, $w(k)$ to find the particle in a state with wave number $k$ at $t>0$, and the final total energy of the system.
2.19. Calculate the lifetime of the metastable localized state of a 1D particle in the potential

$$
U(x)=-w \delta(x)-F x, \quad \text { with } w>0
$$

using the WKB approximation. Formulate the condition of validity of the result.
2.20. Analyze the localized eigenfunction(s) and the characteristic equation(s) for eigenenergies of a 1D particle in the following two-well potential

$$
U(x)=-w\left[\delta\left(x-\frac{a}{2}\right)+\delta\left(x+\frac{a}{2}\right)\right], \quad \text { with } w>0
$$

Explore asymptotic behaviors of the eigenenergies in the limits of very strong and very weak potential, and find the number of localized states as a function of distance $a$.
2.21. ${ }^{*}$ Consider a symmetric system of two quantum wells of the type shown in Fig. 23, but with $U(0)=U( \pm \infty)=0-$ see Fig. on the right. What is the sign of well interaction force due to a quantum particle of mass $m$, shared by them, for the cases when the particle is in:
(i) a symmetric eigenstate, with $\psi_{s}(-x)=\psi_{s}(x)$ ?
(ii) an asymmetric eigenstate, with $\psi_{a}(-x)=-\psi_{a}(x)$ ?

Use a different approach to confirm your result for the particular case of delta-functional wells, considered in the previous problem.

2.22. Derive and analyze the characteristic equation for eigenvalues for a particle in a rectangular well of a finite depth:

$$
U(x)=\left\{\begin{array}{cl}
-U_{0}, & \text { for }|x| \leq a / 2 \\
0, & \text { otherwise }
\end{array}\right.
$$

In particular, calculate the number of localized states as a function of well's width $a$, and explore the limit $U_{0} \ll \hbar^{2} / 2 m a^{2}$.
2.23. Calculate energy $E$ of the localized state in a quantum well of an arbitrary shape $U(x)$, provided that its width $a$ is finite, and the average depth is very small:

$$
|\bar{U}| \ll \frac{\hbar^{2}}{2 m a^{2}}, \quad \text { where } \bar{U} \equiv \frac{1}{a} \int_{\text {well }} U(x) d x
$$

2.24.* A particle of mass $m$ is moving in a field with the following potential:

$$
U(x)=U_{0}(x)+w \delta(x)
$$

where $U_{0}(x)$ describes a smooth, symmetric function with $U_{0}(0)=0$, growing monotonically at $x \rightarrow \pm \infty$.
(i) Use the WKB approximation to derive the characteristic equation for the energy spectrum;
(ii) semi-quantitatively describe the spectrum structure evolution at the increase of $|\boldsymbol{w}|$, for both signs of this parameter, and make the results more specific for the quadratic potential

$$
U_{0}(x)=\frac{m}{2} \omega_{0}^{2} x^{2}
$$

2.25. Prove Eq. (191), starting from Eq. (190).
2.26. For the problem explored in the beginning of Sec. 7, i.e. 1D particle's motion in a deltafunctional periodic potential shown in Fig. 24,

$$
U(x)=w \sum_{j=-\infty}^{+\infty} \delta(x-j a), \quad \text { with } w>0
$$

(where $j$ are integers), write explicit expressions for its eigenfunctions:
(i) at the bottom, and
(ii) at the top
of the lowest energy band. Sketch both eigenfunctions.
2.27.* A 1D particle of mass $m$ moves in an infinite periodic system of very narrow and deep quantum wells that may be described by delta-functions:

$$
U(x)=w \sum_{j=-\infty}^{+\infty} \delta(x-j a), \quad \text { with } w<0
$$

(i) Sketch the energy band structure of the system for relatively small and relatively large values of the quantum well's "area" $|\mathcal{W}|$, and
(ii) calculate explicitly the ground state energy of the system in the limits of very small and very large $|\boldsymbol{\psi}|$.
2.28.* For the system discussed in the previous problem, write explicit expressions for the eigenfunctions of the system, corresponding to:
(i) the bottom points of the lowest energy band, and
(ii) the top points of that band, and
(iii) the lowest points of each higher energy band, and sketch the functions.
2.29.* The 1D "crystal", analyzed in the last two problems, now extends along only to $x>0$, while bordering a flat potential step at $x=0:{ }^{102}$

$$
U(x)= \begin{cases}w \sum_{j=1}^{+\infty} \delta(x-j a), & \text { with } w<0, \\ U_{0}>0, & \text { for } x>0 \\ x<0\end{cases}
$$

Prove that the system can have a set of so-called Tamm states, localized near the "surface" $x=0$, and calculate their energies in the limit when $U_{0}$ is very large but finite. (Quantify this condition.)
2.30. Calculate the whole transfer matrix of the rectangular tunnel barrier, specified by Eq. (76), for particle energies both below and above $U_{0}$.
2.31. Use results of the previous problem to calculate the transfer matrix of one period of the periodic Kronig-Penney potential shown in Fig. 30b (reproduced in Fig. on the right).

2.32. Using results of the previous problem, derive the characteristic equations for particle's motion in the periodic Kronig-Penney potential, for both $E<U_{0}$ and $E>U_{0}$. Try to bring the equations to a form similar to that obtained in Sec. 5 for the delta-functional barriers - see Eq. (166). Use the equations to formulate the conditions of applicability of the tight-binding and weak-potential approximations, in terms of parameters $U_{0}, d$, and $a$ of the potential profile, and particle's mass $m$ and energy $E$.
2.33.* For the Kronig-Penney potential, use the tight binding approximation to calculate the widths of the allowed energy bands. Compare the results with those of the previous problem (in the corresponding limit).

[^531]2.34.* For the same Kronig-Penney potential, use the weak potential limit formulas to calculate the energy gap widths. Again, compare the results with those of Problem 30, in the corresponding limit.
2.35. 1D periodic chains of atoms may exhibit what is called the so-called Peierls instability, leading to the Peierls transition to phase in which atoms are slightly displaced by $\Delta x_{j}=(-1)^{j} \Delta x$, with $\Delta x$ $\ll a$. These displacements lead to the alternation of coupling amplitudes $\delta_{n}$ (see Eq. (204)) between some values $\delta_{n}^{+}$and $\delta_{n}^{-}$. Use the tight-binding approximation to calculate the resulting change of the $n^{\text {th }}$ energy band, and discuss the result.
2.36. Assuming the quantum effects to be small, calculate the lower part of the energy spectrum of the following system: a small bead of mass $m$, free to move without friction along a ring of radius $R$ that is rotated about its vertical diameter with a constant angular velocity $\omega$ - see Fig. on the right. ${ }^{103}$ Formulate a quantitative condition of validity of your results.

2.37. A 1D harmonic oscillator (with mass $m$ and frequency $\omega_{0}$ ) had been in its ground state; then an additional force $F$ was suddenly applied (and retained constant in time). Find the probability of the oscillator staying in its ground state.
2.38. A 1D particle of mass $m$ has been placed into a quadratic potential well (111),
$$
U(x)=\frac{m \omega_{0}^{2}}{2} x^{2}
$$
and allowed to relax into the ground state. harmonic oscillator had been in its ground state. At $t=0$, the well starts to be moved with velocity $v$, without changing its profile, so that at $t \geq 0$ the above formula for $U$ is valid with the replacement $x \rightarrow x$ ' $\equiv x-v t$. Calculate the probability for the system to still be in the ground state at $t>0$.
2.39. A 1 D particle is placed into the following potential well:
\[

U(x)= $$
\begin{cases}+\infty, & \text { for } x<0 \\ m \omega_{0}^{2} x^{2} / 2, & \text { for } x \geq 0\end{cases}
$$
\]

(i) Find its eigenstates and eigenenergies.
(ii) This system had been let to relax into its ground state, and then the potential wall at $x<0$ was rapidly removed, so that the system was instantly turned into the usual harmonic oscillator (with the same $m$ and $\omega_{0}$ ). Find the probability for the oscillator to be in its ground state.
2.40. Prove the following formula for the propagator of the 1 D harmonic oscillator:

[^532]$$
G\left(x, t ; x_{0}, t_{0}\right)=\left(\frac{m \omega_{0}}{2 \pi i \hbar \sin \left[\omega_{0}\left(t-t_{0}\right)\right]}\right)^{1 / 2} \exp \left\{\frac{i m \omega_{0}}{2 \hbar \sin \left[\omega_{0}\left(t-t_{0}\right)\right]}\left[\left(x^{2}+x_{0}^{2}\right) \cos \left[\omega_{0}\left(t-t_{0}\right)\right]-2 x x_{0}\right]\right\} .
$$

Discuss the relation between this formula and the propagator of a free 1D particle.
2.41. Use the variational method to estimate the ground state energy $E_{g}$ of the following confined 1D systems:
(i) a harmonic oscillator, with $U(x)=m \omega_{0}^{2} x^{2} / 2$, and
(ii) a particle in the following potential well: $U(x)=-U_{0} \exp \left\{-\alpha^{2} x^{2}\right\}$, and $U_{0}>0$.

In the latter case, get explicit results in the limits of small and large $U_{0}$, and give their interpretation.
2.42.* Use the WKB approximation to calculate the lifetime of the metastable ground state of a 1D particle of mass $m$ in the "pocket" of the potential profile

$$
U(x)=\frac{m \omega_{0}^{2}}{2} x^{2}-\alpha x^{3}
$$

Contemplate the significance of this problem.
2.43. In the context of the Sturm oscillation theorem mentioned in Sec. 10, prove that the number of zeros of stationary wavefunctions of a particle, confined in an arbitrary potential well, always increases with energy.

Hint: You may like to use the suitably modified Eq. (189).

## Chapter 3. Higher Dimensionality Effects

The coverage of multi-dimensional problems of wave mechanics in this course is minimal: it is limited to a few phenomena (such as the AB effect and Landau levels) that cannot take place in one dimension due to topological reasons, and a few key 3D problems (such as the Born approximation in scattering theory and the Bohr atom) whose solutions are necessary for numerous applications.

### 3.1. Quantum interference and the AB effect

In the past two chapters, we have already discussed some effects of the de Broglie wave interference. For example, standing waves inside a quantum well, or even on the top of a tunnel barrier, may be considered as a result of the incident and reflected waves. However, there are some remarkable new effects made possible by the spatial separation of such traveling waves, and such separation requires a higher (either 2D or 3D) dimensionality. A good example of such separation is provided by the Young-type experiment (Fig. 1) in which particles are passed through two narrow holes (or slits) is an otherwise opaque partition.


If the particles emitted by the source do not interact (which is always true if the emission rate is sufficiently low), the average rate of particle counting by the detector is proportional to the probability density $w(\mathbf{r}, t)=\Psi(\mathbf{r}, t) \Psi^{*}(\mathbf{r}, t)$ to find a single particle at the detector's location $\mathbf{r}$, where $\Psi(\mathbf{r}, t)$ is the solution of the single-particle Schrödinger equation (1.25). Let us describe this experiment for the case when the particles may be represented by monochromatic waves of energy $E$ (e.g., very $\mathbf{r}$-long wave packets), so that the wavefunction may be taken in the form given by Eqs. (1.56) and (1.61): $\Psi(\mathbf{r}, t)=$ $\psi(\mathbf{r}) \exp \{-i E t / \hbar\}$. In this case, in the free-space parts of the system, $\psi(\mathbf{r})$ satisfies the stationary Schrödinger equation (1.60) with Hamiltonian (1.27a):

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi=E \psi . \tag{3.1a}
\end{equation*}
$$

With the standard definition $k \equiv(2 m E)^{1 / 2} / \hbar$, it may be rewritten as the 3D Helmholtz equation

$$
\begin{equation*}
\nabla^{2} \psi+k^{2} \psi=0 \tag{3.1b}
\end{equation*}
$$

- an evident 3D generalization of Eqs. (1.75) or (2.81).

The opaque parts of the partition may be well described as classically forbidden regions, so if their size scale $a$ is much larger than the wavefunction penetration depth $\delta(2.67)$, we can use on their surface $S$ the same boundary conditions as for the quantum barrier of infinite height:

$$
\begin{equation*}
\left.\psi\right|_{S}=0 \tag{3.2}
\end{equation*}
$$

Equations (1) and (2) formulate the standard boundary problem of the theory of propagation of scalar waves of any nature. For an arbitrary geometry, such problem does not have a simple analytical solution. However, for a conceptual discussion of interference we use certain natural assumptions that will allow us to find its particular, approximate solution.

First, let us discuss wave emission, into free space, by a small-size source located at the origin. Naturally, the emitted wave should be spherically-symmetric: $\psi(\mathbf{r})=\psi(r)$. Using the well-known expression for the Laplace operator in spherical coordinates, ${ }^{1}$ we then reduce Eq. (1) to an ordinary differential equation

$$
\begin{equation*}
\frac{1}{r^{2}} \frac{d}{d r}\left(r^{2} \frac{d \psi}{d r}\right)+k^{2} \psi=0 \tag{3.3}
\end{equation*}
$$

Let us introduce a new function, $f(r)=r \psi(r)$. Plugging the reciprocal relation $\psi=f / r$ into Eq. (3), we see that it is reduced to the 1 D wave equation,

$$
\begin{equation*}
\frac{d^{2} f}{d r^{2}}+k^{2} f=0 \tag{3.4}
\end{equation*}
$$

whose solutions were discussed in detail in Sec. 2.2. For a fixed $k$, the general solution of Eq. (4) is

$$
\begin{equation*}
f=f_{+} e^{i k r}+f_{-} e^{-i k r} \tag{3.5}
\end{equation*}
$$

so that the full wavefunction

$$
\begin{equation*}
\psi(\mathbf{r})=\frac{f_{+}}{r} e^{i k r}+\frac{f_{-}}{r} e^{-i k r} \text {, i.e. } \Psi(\mathbf{r}, t)=\frac{f_{+}}{r} e^{i(k r-\omega t)}+\frac{f_{-}}{r} e^{-i(k r+\omega t)}, \quad \text { with } \omega \equiv \frac{E}{\hbar}=\frac{\hbar k^{2}}{2 m} . \tag{3.6}
\end{equation*}
$$

If the source is located at point $\mathbf{r}^{\prime} \neq 0$, the obvious generalization of Eq. (6)

$$
\begin{equation*}
\Psi(\mathbf{r}, t)=\frac{f_{+}}{R} e^{i(k R-\omega t)}+\frac{f_{-}}{R} e^{-i(k R+\omega t)}, \quad \text { with } R \equiv|\mathbf{R}|, \quad \mathbf{R} \equiv \mathbf{r}-\mathbf{r}^{\prime} \tag{3.7}
\end{equation*}
$$

The first term of this solution describes a spherically-symmetric wave propagating from the source outward, while the second one, a wave converging onto the source point $\mathbf{r}$ ' from large distances. Though the latter solution is possible at some very special circumstances (say, when the outgoing wave is reflected back from a spherical shell), for our problem, only the outgoing waves are relevant, so that we may keep only the first term (proportional to $f_{+}$) in Eq. (7). Note that factor $R$ is the denominator (that was absent in 1D geometry) has a simple physical sense: it provides the independence of the full probability current $I=4 \pi R^{2} j(R)$, with $j(R) \propto k \Psi \Psi^{*} \propto 1 / R^{2}$, of the distance $R$ between the observation point and the source.

[^533]Now let us assume that the partition's geometry is not too complicated - for example, it is planar as shown in Fig. 1, and consider the region of the particle detector location far behind the partition (at $z$ $\gg 1 / k$ ), and at a relatively small angle to it: $|x| \ll z$. Then it should be physically clear that the spherical waves (7) emitted by each point inside the slit cannot be perturbed too much by the opaque parts of the partition, and their only role is the restriction of the set of such emitting points by the area of the slits. Hence, an approximate solution of the boundary problem is given by the following Huygens principle: the wave behind the partition looks as if it was the sum of contributions (7) of point sources located in the slits, with each source's strength $f_{+}$proportional to the amplitude of the wave arriving at this pseudo-source from the real source - see Fig. 1. This principle finds its confirmation in strict wave theory, which shows ${ }^{2}$ that with our assumptions, the solution of the boundary problem (1)-(2) may be presented as the following Kirchhoff integral:

Kirchhoff integral

$$
\begin{equation*}
\psi(\mathbf{r})=c \int_{\text {slits }} \frac{\psi\left(\mathbf{r}^{\prime}\right)}{R} e^{i k R} d^{2} r^{\prime}, \quad \text { with } c=\frac{k}{2 \pi i} . \tag{3.8}
\end{equation*}
$$

If the source is also far from the partition, its wave front is almost parallel to the slit plane, and the slits are not too broad, we can take $\psi\left(\mathbf{r}^{\prime}\right)$ constant $\left(\psi_{1,2}\right)$ at each slit, so that Eq. (8) is reduced to

$$
\begin{equation*}
\psi(\mathbf{r})=a_{1}^{\prime \prime} \exp \left\{i k l_{1}\right\}+a_{2}^{\prime \prime} \exp \left\{i k l_{2}^{\prime \prime}\right\}, \quad \text { with } a_{1,2}^{\prime \prime}=\frac{c A_{1,2}}{l_{1,2}^{\prime \prime}} \psi_{1,2}, \tag{3.9}
\end{equation*}
$$

where $A_{1,2}$ are the slit areas. The wavefunctions on the slits be calculated approximately ${ }^{3}$ by applying the same Eq. (7) to the space before the slits: $\psi_{1,2} \approx\left(f_{+} / l^{\prime}{ }_{1,2}\right) \exp \left\{i k l_{1,2}\right\}$. As a result, Eq. (9) may be rewritten as

Wave-
function superposition

Quantum interference: the pattern and phase shift

$$
\begin{equation*}
\psi(\mathbf{r})=a_{1} \exp \left\{i k l_{1}\right\}+a_{2} \exp \left\{i k l_{2}\right\}, \quad \text { with } l_{1,2} \equiv l_{1,2}^{\prime}+l_{1,2}^{\prime \prime}, \quad a_{1,2} \equiv \frac{c f_{+} A_{1,2}}{l_{1,2}^{\prime} l_{1,2}^{\prime \prime}} \tag{3.10}
\end{equation*}
$$

(As Fig. 1 shows, each of $l_{1,2}$ is the length of the full classical path of the particle from the source, through the corresponding slit, and further to the observation point $\mathbf{r}-$ see Fig. 1).

According to Eq. (10), the resulting rate of particle counting is proportional to

$$
\begin{equation*}
w(\mathbf{r})=\psi(\mathbf{r}) \psi^{*}(\mathbf{r})=\left|a_{1}\right|^{2}+\left|a_{2}\right|^{2}+2\left|a_{1} a_{2}\right| \cos \varphi_{12} \tag{3.11}
\end{equation*}
$$

where

$$
\begin{equation*}
\varphi_{12} \equiv k\left(l_{2}-l_{1}\right) \tag{3.12}
\end{equation*}
$$

is the difference of the total wave phase accumulations along each of two alternative trajectories. The last expression may be evidently generalized as

[^534]\[

$$
\begin{equation*}
\varphi_{12}=\oint_{C} \mathbf{k} \cdot d \mathbf{r} \tag{3.13}
\end{equation*}
$$

\]

with integration along the virtually closed contour $C$ (see the dashed line in Fig. 1), i.e. from point 1, in the positive (i.e. counterclockwise) direction to point 2. (From our experience with the 1D WKB approximation we may expect such generalization to be valid even if $k$ changes, sufficiently slowly, along the paths.)

Our result (11) shows that the counting rate oscillates as a function of the difference ( $l_{2}-l_{1}$ ) that in turn changes with detector's position, giving the famous interference pattern, with the amplitude proportional to the product $\left|a_{1} a_{2}\right|$, and hence vanishing if any of the slits is closed. For a wave theory, this is a well-known result, ${ }^{4}$ but for particle physics, is was (and still is :-) rather shocking. Indeed, our analysis pertains to a very low particle emission/detection rate, so that there is no other way to interpret it rather than resulting from particle's interference with itself, or rather the interference of its wavefunction parts passing through each of two slits.

Let us now discuss a very interesting effect of magnetic field on the quantum interference. In order to make the discussion simpler, let us consider an alternative version of the two-slit experiment, in which each of alternative path is fixed to a narrow channel using a partial confinement - see Fig. 2. (In this arrangement, moving the particle detector without changing channels' geometry, and hence local values of $k$ may be more problematic in experimental practice, so let us think about its position $\mathbf{r}$ fixed.)


In this case, because of the effect of the walls providing the path confinement, we cannot use expressions (10) for amplitudes $a_{1,2}$. However, from the discussions in Sec. 1.6 and Sec. 2.2, it should be clear that the first of expressions (10) remains valid, though may be with a value of $k$ specific for each channel.

The benefit of this geometry is that we can now apply magnetic field $\mathcal{B}$, perpendicular to the plane of particle motion, that would pierce contour $C$, but would not touch the particle propagation channels. In classical physics, magnetic field's effect on a particle with electric charge $q$ is described by the Lorentz force ${ }^{5}$

$$
\begin{equation*}
\mathbf{F}_{\mathbb{B}}=q \mathbf{v} \times \mathbf{B}, \tag{3.14}
\end{equation*}
$$

[^535]where $B$ is the field value at the point of its particle's location, so that for the experiment shown in Fig. $2, \mathbf{F}_{\mathcal{B}}=0$, and the field would not affect the particle motion at all. In quantum mechanics, this is not so, and the field does affect the probability density $w$, even if $B=0$ in all points where the wavefunction $\psi(\mathbf{r})$ is not equal to zero.

In order to describe this surprising effect, let us first develop a general framework for account of effects of electromagnetic fields on a quantum particle, which will also give us some important byproduct results. In order to do that, we need to calculate the Hamiltonian operator of a charged particle in the field. For an electrostatic field, this hardly present any problem. Indeed, from classical electrodynamics we know that such field may be presented as a gradient of its electrostatic potential $\phi$,

$$
\begin{equation*}
\varepsilon=-\nabla \phi(\mathbf{r}) \tag{3.15}
\end{equation*}
$$

so that the force exerted by the field on a particle with electric charge $q$,

$$
\begin{equation*}
\mathbf{F}_{\mathcal{E}}=q \mathcal{E}, \tag{3.16}
\end{equation*}
$$

may be described by adding the potential energy of the field,

$$
\begin{equation*}
U(\mathbf{r})=q \phi(\mathbf{r}) \tag{3.17}
\end{equation*}
$$

to other (possible) components of the full potential energy of the particle. As we have already discussed, such a function of coordinates may be included to the Hamiltonian operator just by adding it to the kinetic energy operator (1.27).

However, magnetic field's effect is peculiar: since its Lorentz force (14) cannot do any work on the particle:

$$
\begin{equation*}
d W_{\mathcal{B}} \equiv \mathbf{F}_{\mathcal{B}} \cdot d r=\mathbf{F}_{\mathcal{B}} \cdot \mathbf{v} d t=q(\mathbf{v} \times \mathcal{B}) \cdot \mathbf{v} d t=0 \tag{3.18}
\end{equation*}
$$

the field cannot be presented by any potential energy, so it may not be immediately clear how to account for it in the Hamiltonian. Help comes from the analytical-mechanics approach to classical electrodynamics: ${ }^{6}$ in the non-relativistic limit, the Hamiltonian function of a particle in electromagnetic field looks superficially like that in electrostatic field only:

$$
\begin{equation*}
H=\frac{m v^{2}}{2}+U=\frac{p^{2}}{2 m}+q \phi \tag{3.19}
\end{equation*}
$$

however, the momentum $\mathbf{p} \equiv m \mathbf{v}$ that participates in this expression is now the difference

$$
\begin{equation*}
\mathbf{p}=\mathbf{P}-q \mathbf{A} . \tag{3.20}
\end{equation*}
$$

Here $\mathbf{A}$ is the vector-potential, defined by the well-known relations for the electric and magnetic field: ${ }^{7}$

$$
\begin{equation*}
\varepsilon=-\nabla \phi-\frac{\partial \mathbf{A}}{\partial t}, \quad B=\nabla \times \mathbf{A} \tag{3.21}
\end{equation*}
$$

while $\mathbf{P}$ is the canonical momentum whose Cartesian components may be calculated (in classics) from the Lagrangian function, ${ }^{8}$ using the standard formula of analytical mechanics,

[^536]\[

$$
\begin{equation*}
P_{j} \equiv \frac{\partial L}{\partial v_{j}} . \tag{3.22}
\end{equation*}
$$

\]

To emphasize the difference between the two momenta, $\mathbf{p}=m \mathbf{v}$ is frequently called the kinematic momentum (or " $m \mathbf{v}$-momentum"). The distinction between $\mathbf{p}$ and $\mathbf{P}=\mathbf{p}+q \mathbf{A}$ becomes even more clear if we notice that vector-potential is not gauge-invariant: according to the second of Eqs. (21), at the so-called gauge transformation

$$
\begin{equation*}
\mathbf{A} \rightarrow \mathbf{A}+\nabla \chi \tag{3.23}
\end{equation*}
$$

with an arbitrary single-valued scalar gauge function $\chi=\chi(\mathbf{r}, t)$, the magnetic field does not change. Moreover, according to the first of Eqs. (21), if we make the simultaneous replacement

$$
\begin{equation*}
\phi \rightarrow \phi-\frac{\partial \chi}{\partial t} \tag{3.24}
\end{equation*}
$$

the gauge transformation does not affect the electric field either. With that, the gauge function does not change the classical particle's equation of motion, and hence the velocity $\mathbf{v}$ and momentum $\mathbf{p}$. Hence, the kinematic momentum is gauge-invariant, while $\mathbf{P}$ is not, because it changes by $q \nabla \chi$.

Now the standard way of transfer to quantum mechanics is to treat the canonical rather than kinematic momentum according to correspondence postulate discussed in Sec. 1.2. This means that in the coordinate representation, the operator of this variable is given by Eq. (1.26): ${ }^{9}$

$$
\begin{equation*}
\hat{\mathbf{P}}=-i \hbar \nabla \tag{3.25}
\end{equation*}
$$

Hence the Hamiltonian operator corresponding to the classical function (19) is

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m}(-i \hbar \nabla-q \mathbf{A})^{2}+q \phi=-\frac{\hbar^{2}}{2 m}\left(\nabla-\frac{i q}{\hbar} \mathbf{A}\right)^{2}+q \phi \tag{3.26}
\end{equation*}
$$

so that the Schrödinger equation of a particle moving in electromagnetic field (but otherwise free) is

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left(\nabla-\frac{i q}{\hbar} \mathbf{A}\right)^{2} \psi+q \phi \psi=E \psi \tag{3.27}
\end{equation*}
$$

We may now repeat all the calculations of Sec. 1.4 for the case $\mathbf{A} \neq 0$, and readily get the following generalized expression for the probability current density:

$$
\begin{equation*}
\mathbf{j}=\frac{\hbar}{2 i m}\left[\psi^{*}\left(\nabla-\frac{i q}{\hbar} \mathbf{A}\right) \psi-\text { c.c }\right]=\frac{1}{2 m}\left[\psi^{*} \hat{\mathbf{p}} \psi-\text { c.c }\right]=\frac{\hbar}{m}|\psi|^{2}\left(\nabla \varphi-\frac{q}{\hbar} \mathbf{A}\right) . \tag{3.28}
\end{equation*}
$$

$$
L=\frac{m v^{2}}{2}+q \mathbf{v} \cdot \mathbf{A}-q \phi
$$

- see EM Sec. 9.7. Note that this function includes $\mathbf{A}$ within a term that cannot be interpreted as either the purely kinetic energy (as the first term) or the purely potential energy (as the last term with the minus sign).
${ }^{9}$ The validity of this choice is clear from the fact that if the kinetic momentum was described by this differential operator, the Hamiltonian operator corresponding to the classical Hamiltonian function (19) would not include the magnetic field at all, and hence solutions of the corresponding Schrödinger equation could not satisfy the correspondence principle.

We see that the current density is gauge-invariant (as required for any observable) only if the wavefunction's phase $\varphi$ changes as

$$
\begin{equation*}
\varphi \rightarrow \varphi+\frac{q}{\hbar} \chi . \tag{3.29}
\end{equation*}
$$

This may be a point of concern: since the quantum interference is described by the spatial dependence of phase $\varphi$, can the observed interference pattern depend on the gauge function choice (which would not make sense)? Fortunately, this is not true, because the spatial phase difference between two interfering paths, participating in Eq. (11), is gauge-transformed as

$$
\begin{equation*}
\varphi_{12} \rightarrow \varphi_{12}+\frac{q}{\hbar}\left(\chi_{2}-\chi_{1}\right) . \tag{3.30}
\end{equation*}
$$

But $\chi$ has to be a single-valued function of coordinates, hence in the limit when points 1 and 2 coincide, $\chi_{1}=\chi_{2}$, so that $\Delta \varphi$ (and hence the interference pattern) is gauge-invariant.

However, the difference $\varphi$ may be affected by the magnetic field, even if it is localized outside the channels in which the particle propagates. Indeed, in this case the field cannot not affect particle's velocity and current density $\mathbf{j}$ :

$$
\begin{equation*}
\left.\mathbf{j}(\mathbf{r})\right|_{\mathfrak{B} \neq 0}=\left.\mathbf{j}(\mathbf{r})\right|_{\mathfrak{B}=0}, \tag{3.31}
\end{equation*}
$$

so that the last form of Eq. (28) yields

$$
\begin{equation*}
\left.\nabla \varphi(\mathbf{r})\right|_{\mathcal{B} \neq 0}=\left.\nabla \varphi(\mathbf{r})\right|_{\mathcal{B}=0}+\frac{q}{\hbar} \mathbf{A} . \tag{3.32}
\end{equation*}
$$

Integrating this equation along contour $C$ (Fig. 2), for the phase difference between points 1 and 2 we get

$$
\begin{equation*}
\left.\varphi_{12}\right|_{\mathcal{B} \neq 0}=\left.\varphi_{12}\right|_{\mathcal{B}=0}+\frac{q}{\hbar} \oint_{C} \mathbf{A} \cdot d \mathbf{r}, \tag{3.33}
\end{equation*}
$$

where the integral should be taken along the same virtually closed contour $C$ as before (in Fig. 2, from point 1 , counterclockwise along the dashed line to point 2 ). But from the classical electrodynamics we know $^{10}$ that as points 1 and 2 are overlapped, i.e. contour $C$ becomes closed, the last integral is just the magnetic flux $\Phi \equiv \int \mathcal{B}_{n} d^{2} r$ through any smooth surface limited by contour $C$, so that Eq. (33) may be presented as

$$
\begin{equation*}
\left.\varphi_{12}\right|_{\mathcal{B} \neq 0}=\left.\varphi_{12}\right|_{\mathcal{B}=0}+\frac{q}{\hbar} \Phi \tag{3.34a}
\end{equation*}
$$

In terms of the interference pattern, this means a shift of interference fringes, proportional to the magnetic flux (Fig. 3). This phenomenon is usually called the "Aharonov-Bohm" (or just the $A B$ ) effect. ${ }^{11}$ For particles with a single elementary charge, $q= \pm e$, this result is frequently presented as

[^537]\[

$$
\begin{equation*}
\left.\varphi_{12}\right|_{\mathcal{B} \neq 0}=\left.\varphi_{12}\right|_{\mathcal{B}=0} \pm 2 \pi \frac{\Phi}{\Phi_{0}{ }^{\prime}}, \tag{3.34b}
\end{equation*}
$$

\]

where the fundamental constant $\Phi_{0}{ }^{\prime} \equiv 2 \pi \hbar / e=h / e \approx 4.14 \times 10^{-15} \mathrm{~Wb}$ has the meaning of flux necessary to change $\varphi_{12}$ by $2 \pi$, i.e. shift the interference pattern (11) by one period, and is called the normal magnetic flux quantum, because of the reasons we will soon discuss.

(b)

Fig. 3.3. Typical results of a two-paths interference experiment by A. Tonomura et al., Phys. Rev. Lett. 56, 792 (1986), showing the AB effect for electrons well shielded from the applied magnetic field. In this particular experimental geometry, the AB effect produces a relative shift of the interference patterns inside and outside the dark ring. (a) $\Phi=\Phi_{0}{ }^{\prime} / 2$, (b) $\Phi=\Phi_{0}{ }^{\prime}$. © 1986 APS.

The AB effect may be "almost explained" classically, in terms of Faraday's electromagnetic induction. Indeed, a change $\Delta \Phi$ of magnetic flux in time causes a vortex-like electric field $\Delta \mathcal{\varepsilon}$ around it. That field is not restricted to the magnetic field's location, i.e. may reach particle's trajectories. The field's magnitude ( or rather of its integral along contour $C$ ) may be readily calculated by integration of the first of Eqs. (21):

$$
\begin{equation*}
\Delta V \equiv \oint_{C} \Delta \boldsymbol{\varepsilon} \cdot d \mathbf{r}=-\frac{d \Phi}{d t}, \tag{3.35}
\end{equation*}
$$

I hope that in this expression the reader readily recognizes the integral ("undergraduate") form of Faraday's induction law. Now let us assume that the variable separation described in Sec. 1.5 may be applied to the end points 1 and 2 of particle's alternative trajectories as two independent systems, ${ }^{12}$ and that the magnetic flux' change by certain amount $\Delta \Phi$ does not change the spatial parts $\psi_{j}$ of wavefunctions of these systems. Then change (35) leads to the change of potential energy difference $\Delta U$ $=q \Delta V$ between the two points, and repeating the arguments that were used in Sec. 2.3 at the discussion of the Josephson effect, we may rewrite Eq. (2.53) as

$$
\begin{equation*}
\frac{d \varphi_{12}}{d t}=-\frac{\Delta U}{\hbar}=-\frac{q}{\hbar} \Delta V=\frac{q}{\hbar} \frac{d \Phi}{d t} . \tag{3.36}
\end{equation*}
$$

Integrating this relation over the time of magnetic field's change, we get
experimental observation by R. Chambers in 1960 and several other groups soon after that. Later, the experiments were improved, using ferromagnetic cores and/or superconducting shielding to provide better separation between the electron trajectories and the applied magnetic field,- see in the work whose results are shown in Fig. 3.
${ }^{12}$ This assumption may seem a bit of a stretch, but the resulting relation (37) may be indeed proven for a rather realistic model, though that would take more time and space that I can afford.

$$
\begin{equation*}
\Delta \varphi_{12}=\frac{q}{\hbar} \Delta \Phi \tag{3.37}
\end{equation*}
$$

- superficially, the same result as given by Eq. (34).

However, this interpretation of the AB effect is limited. Indeed, it requires the particle to be in the system (on the way from the source to the detector) during the flux change, i.e. when the induced electric field $\varepsilon$ may affect its dynamics. On the contrary, Eq. (34) predicts that the interference pattern would shift even if the field change has been made when the there is no particle in the system, and hence field $\varepsilon$ could not be felt by it. Experiment confirms the latter conclusion. Hence, there is something in the space where a particle propagates (i.e., outside of the magnetic field region), which transfers information about even the static magnetic field to the particle. The standard interpretation of this surprising fact is as follows: the vector-potential $\mathbf{A}$ is not just a convenient mathematical tool, but a physical reality (just as its electric counterpart $\phi$ ), despite the large freedom of choice we have in prescribing specific spatial and temporal dependences of these potentials without affecting any observable - see Eqs. (23)-(24).

Let me briefly discuss the very interesting form the AB effect takes in superconductivity. In this case, our results require two changes. The first one is simple: since superconductivity may be interpreted as the Bose-Einstein condensate of Cooper pairs with electric charge $q=2 e, \Phi_{0}$ ' has to be replaced by the so-called superconducting flux quantum ${ }^{13}$

$$
\begin{equation*}
\Phi_{0} \equiv \frac{\pi \hbar}{e} \approx 2.07 \times 10^{-15} \mathrm{~Wb}=2.07 \times 10^{-7} \mathrm{Gs} \cdot \mathrm{~cm}^{2} \tag{3.38}
\end{equation*}
$$

Second, since the pairs are Bose particles and are all condensed in the same quantum state, described by the same wavefunction, the total electric current density, proportional to the probability current density $j$, may be extremely large - in real superconducting materials, up to $\sim 10^{12} \mathrm{~A} / \mathrm{m}^{2}$. In these conditions, one cannot neglect the contribution of that current into the magnetic field and hence its flux $\Phi$, which (according to the Lenz rule of the Faraday induction law) tries to compensate changes in external flux. In order to see possible results of this contribution, let us consider a closed superconducting loop (Fig. 4).


Fig. 3.4. Flux quantization in a superconducting loop.

Due to the Meissner effect (which is just another version of the flux self-compensation), current and magnetic field penetrate inside the superconductor by only a small distance (called the London

[^538]penetration depth) $\delta_{\mathrm{L}} \sim 10^{-7} \mathrm{~m} .{ }^{14}$ If the loop is made of a superconducting wire that is considerably thicker than $\delta_{\mathrm{L}}$, we can draw a contour deep inside the wire, at that the current density is negligible. According to Eq. (28), everywhere at the contour,
\[

$$
\begin{equation*}
\nabla \varphi-\frac{q}{\hbar} \mathbf{A}=0 . \tag{3.39}
\end{equation*}
$$

\]

Integrating this equation along the contour as before (from point 1 to the virtually coinciding point 2 ), we need to have the phase difference $\varphi_{12}=2 \pi n$, because the wavefunction $\psi \propto \exp \{i \varphi\}$ in the initial and final points 1 and 2 should be "essentially" the same, i.e. produce the same observables. As a result, we get

$$
\begin{equation*}
\Phi=\oint_{C} \mathbf{A} \cdot d \mathbf{r}=\frac{2 \pi \hbar}{q} n=\frac{\pi \hbar}{e} n=n \Phi_{0} . \tag{3.40}
\end{equation*}
$$

This is the famous flux quantization effect, ${ }^{15}$ which justifies the term "magnetic flux quantum" for the constant $\Phi_{0}$ given by Eq. (38).

Here I have to mention in passing very interesting effects of "partial flux quantization", that arise when a superconductor loop is closed by a Josephson junction, forming the so-called Superconductor QUantum Interference Device - "SQUID". Such devices are used, in particular, for supersensitive magnetometry and ultrafast, low-power computing. ${ }^{16}$

### 3.2. Landau levels and quantum Hall effect

In the last section, we have used the Schrödinger equation (27) for analysis of static magnetic field effects in "almost-1D", circular geometries shown in Figs. 1, 2, and 4. However, this equation describes very interesting effects in higher dimensions as well, especially in the 2D case. Let us consider a uniform 2D quantum well (say, parallel to the $[x, y]$ plane), with strong confinement in the perpendicular direction $z$. According to the discussion in Sec. 1.6, energy-relaxed particles will always reside in the lowest energy subband, with constant quantization energy $\left(E_{z}\right)_{1}$. Adding this shift to well's flat floor $U(x, y)=$ const, and taking the resulting constant energy as the reference, for the 2D motion of the particle in the well, we reduce Eq. (27) to the similar equation, but with the Laplace operator acting only in directions $x$ and $y$ :

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left(\mathbf{n}_{x} \frac{\partial}{\partial x}+\mathbf{n}_{y} \frac{\partial}{\partial y}-i \frac{q}{\hbar} \mathbf{A}\right)^{2} \psi=E \psi \tag{3.41}
\end{equation*}
$$

Let us find its solutions for the simplest case when the applied static magnetic field is uniform and perpendicular to the plane:

$$
\begin{equation*}
B=B \mathbf{n}_{z} . \tag{3.42}
\end{equation*}
$$

[^539]According to the second of Eqs. (21), this imposes the following restriction on the choice of vectorpotential:

$$
\begin{equation*}
\mathcal{B}=\frac{\partial A_{y}}{\partial x}-\frac{\partial A_{x}}{\partial y}, \tag{3.43}
\end{equation*}
$$

but the gauge transformations still give us a lot of freedom in its choice. The "natural" axiallysymmetric form, $\mathbf{A}=\mathbf{n}_{\varphi} \rho B / 2$, where $\rho=\left(x^{2}+y^{2}\right)^{1 / 2}$ is the distance from some $z$-axis, leads to a cumbersome math. In 1930, L. Landau realized that the energy spectrum of Eq. (41) may be obtained by making a very simple choice

$$
\begin{equation*}
A_{x}=0, \quad A_{y}=\mathcal{B}\left(x-x_{0}\right), \tag{3.44}
\end{equation*}
$$

(with arbitrary $x_{0}$ ), which evidently satisfies Eq. (43), though it ignores the physical equivalence of the $x$ and $y$ directions. Now, expanding the eigenfunction into the Fourier integral in direction $y$ :

$$
\begin{equation*}
\psi(x, y)=\int X_{k}(x) e^{i k\left(y-y_{0}\right)} d k \tag{3.45}
\end{equation*}
$$

we see that for each component of this integral, Eq. (41) yields a specific equation

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left[\mathbf{n}_{x} \frac{d}{d x}+i \mathbf{n}_{y}\left(k-\frac{q}{\hbar} \mathcal{B}\left(x-x_{0}\right)\right)\right]^{2} X_{k}=E X_{k} . \tag{3.46}
\end{equation*}
$$

Since the vectors inside the square brackets are mutually perpendicular, its square has no crossterms, so that Eq. (46) may be rewritten as

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m} \frac{d^{2}}{d x^{2}} X_{k}+\frac{\hbar^{2}}{2 m}\left[\frac{q}{\hbar} B\left(x-x_{0}{ }^{\prime}\right)\right]^{2} X_{k}=E X_{k}, \quad \text { where } x_{0}{ }^{\prime} \equiv x_{0}+\frac{\hbar k}{q B} . \tag{3.47}
\end{equation*}
$$

But this 1D Schrödinger equation is identical to Eq. (2.268) for the 1D harmonic oscillator, but with the center at point $x_{0}$ ', and frequency $\omega_{0}$ equal to

$$
\begin{equation*}
\omega_{c}=\frac{|q| \mathcal{B}}{m} . \tag{3.48}
\end{equation*}
$$

In this expression, it is easy to recognize the classical cyclotron frequency of particle's motion in the magnetic field. (It may be readily obtained using the $2^{\text {nd }}$ Newton law for a circular orbit of radius $r$,

$$
\begin{equation*}
m \frac{v^{2}}{r}=F_{\mathcal{B}}=q v \mathcal{B}, \tag{3.49}
\end{equation*}
$$

and noting that the resulting ratio $v / r=q B / m$ is just the radius-independent angular velocity $\omega_{c}$ of particle's rotation.) Hence, the energy spectrum for each Fourier component of integral (45) is the same:

$$
\begin{equation*}
E_{n}=\hbar \omega_{c}\left(n+\frac{1}{2}\right) \tag{3.50}
\end{equation*}
$$

and does not depend on either $x_{0}$, or $y_{0}$, or $k$.
This is an example of a highly degenerate system: for each eigenvalue $E_{n}$, there are many different eigenfunctions that differ by the positions $\left\{x_{0}, y_{0}\right\}$ of their center on axis $x$, and the rate $k$ of
their phase change along axis $y$. They may be used to assemble a large variety of linear combinations, including 2D wave packets whose centers move along classical circular orbits with some radius $r$ determined by initial conditions. Note, however, that such radius cannot be smaller than the so-called Landau radius,

$$
\begin{equation*}
r_{\mathrm{L}} \equiv\left(\frac{\hbar}{q B}\right)^{1 / 2} \tag{3.51}
\end{equation*}
$$

which characterizes the minimum radius of the wave packet itself, and results from Eq. (2.271) after replacement (48). This radius is remarkably independent on particle's mass, and may be interpreted in the following way: the scale $B A_{\text {min }}$ of the applied magnetic field's flux through the effective area $A_{\text {min }}=$ $2 \pi r_{\mathrm{L}}{ }^{2}$ of the smallest wave packet is just one normal flux quantum $\Phi_{0}{ }^{\prime}=2 \pi \hbar / q$.

A detailed analysis of such wave packets (for which we would not have time in this course) shows that magnetic field does not change the average density $d N_{2} / d E$ of different 2 D states on the energy scale, but just "assembles" them on the Landau levels (see Fig. 5a), so that the number of states on each Landau area (per unit area) is

$$
\begin{equation*}
n_{L} \equiv \frac{N_{2}}{A}=\left.\frac{1}{A} \frac{d N_{2}}{d E}\right|_{\mathcal{B} \neq 0} \Delta E=\left.\frac{1}{A} \frac{d N_{2}}{d E}\right|_{\mathcal{B}=0} \Delta E=\frac{m}{2 \pi \hbar^{2}} \hbar \omega_{c}=\frac{q \mathcal{B}}{2 \pi \hbar}=\frac{q \mathcal{B}}{h} . \tag{3.52}
\end{equation*}
$$

This expression may again be interpreted in terms of magnetic flux quanta: $n_{\mathrm{L}} \Phi_{0}{ }^{\prime}=\mathcal{B}$, i.e. there is one particular state on each Landau level per each flux quantum.


Fig. 3.5. (a) "Condensation" of 2D states on Landau levels, and (b) filling the levels by external electrons at the quantum Hall effect.

The most famous application of the Landau levels concept is the explanation of the quantum Hall effect ${ }^{17}$. Generally, the Hall effect ${ }^{18}$ is observed in the geometry sketched in Fig. 6, where electric current $I$ is passed through a thin rectangular conducting sample (frequently called the Hall bar) placed into a magnetic field $\mathcal{B}$ perpendicular to the sample plane. The classical analysis of the effect is based on the notion of the Lorentz force (14). This force the deviates charge carriers (say, electrons) from their straight motion from one external electrode to another, bending them to the isolated edges of the bar (in Fig. 6, parallel to axis $x$ ). Here the carriers accumulate, generating a gradually increasing electric field $\varepsilon$, until its force (16) exactly balances the Lorentz force (14):

[^540]\[

$$
\begin{equation*}
q \varepsilon_{y}=q v_{x} \mathcal{B}, \tag{3.53}
\end{equation*}
$$

\]

where $v_{x}$ is the drift velocity of the electrons along the bar (Fig. 6), providing the sustained balance condition $\varepsilon_{y} / v_{x}=\mathcal{B}_{z}$ at each point of the 2 D sample.


Fig. 3.6. Hall bar geometry. Darker rectangles show external (3D) electrodes.

With $n_{2}$ carriers per unit area, in a sample of width $W$, this condition yields the following classical expression for the so-called Hall resistance $R_{H}$ :

Classical Hall
effect

$$
\begin{equation*}
R_{H} \equiv \frac{V_{y}}{I_{x}}=\frac{\varepsilon_{y} W}{q n_{2} v_{x} W}=\frac{B}{q n_{2}} . \tag{3.54}
\end{equation*}
$$

This formula is broadly used in practice for the measurement of the carrier density $n_{2}$, and (in semiconductors) the carrier type - negative electrons or positive holes.

However, in experiments with high-quality (low-defect) 2D quantum wells at very low, subkelvin temperatures ${ }^{19}$ and high magnetic fields, the linear growth of $R_{H}$ with $\mathcal{B}$, described by Eq. (54), is interrupted by virtually horizontal plateaus (Fig. 7) with constant values

$$
\begin{equation*}
R_{H}=\frac{1}{i} R_{K}, \tag{3.55}
\end{equation*}
$$

where $i$ (only in this context, following tradition!) is an integer, and value

$$
\begin{equation*}
R_{K} \approx 25.812807557 \mathrm{k} \Omega \tag{3.56}
\end{equation*}
$$

is reproduced with extremely high accuracy $\left(\sim 10^{-9}\right)$ from experiment to experiment and from sample to sample. Such stability is a very rare exception in solid state physics were most results are noticeably dependent on the particular material and particular sample under study.

Let us apply the Landau level picture. The 2D sample is typically in a weak contact with 3D electrodes whose conductivity electrons form a Fermi sea with certain Fermi energy $E_{F}$, so that at low temperatures all states with $E<E_{F}$ are filled with electrons - see Fig. 5b. As $\mathcal{B}$ is increased, spacing $\hbar \omega_{c}$ between the Landau levels increases, so that fewer and fewer of these levels are below $E_{F}$ and are filled, and within broad ranges of field variation, the number $i$ of filled levels is constant. (In Fig. 5b, $i=$ 2.) So, plugging $n_{2}=i n_{L}$ and $q= \pm e$ into Eq. (54), we get

$$
\begin{equation*}
R_{H}=\frac{1}{i} \frac{B}{q n_{L}}=\frac{1}{i} \frac{2 \pi \hbar}{e^{2}}=\frac{1}{i} \frac{h}{e^{2}}, \tag{3.57}
\end{equation*}
$$

[^541]i.e. exactly the experimental result (55), with
\[

$$
\begin{equation*}
R_{K}=\frac{h}{e^{2}} \equiv 4 \frac{\pi \hbar}{2 e^{2}} . \tag{3.58}
\end{equation*}
$$

\]

This constant, exactly 4 times the quantum unit of resistance $R_{Q}$ given by Eq. (2.259), is in an excellent agreement with experimental value (56), and is sometimes called the Klitzing constant.


Fig. 3.7. Typical record of the quantum Hall effect. The lower trace (with sharp peaks) shows the longitudinal component, $V_{x} / I_{x}$, of the resistance tensor. (Adapted from www.prequark.org/Prequark.htm.)

However, this oversimplified explanation of the quantum Hall effect does not take into account several important factors, including:
(i) the role of nonuniformity of the quantum well bottom potential $U(x, y)$, and of the localized states this nonuniformity produces, and the surprisingly small effect of these factors on the extraordinary accuracy of Eq. (55); ${ }^{20}$ and
(ii) the mutual Coulomb interaction of the electrons, in high-quality samples leading to the formation of $R_{H}$ plateaus with not only integer, but also fractional values of $i\left(1 / 3,2 / 5,3 / 7\right.$, etc.). ${ }^{21}$

Unfortunately, a thorough discussion of these interesting features is well beyond the framework of this course. ${ }^{22}$

### 3.3. Scattering and diffraction

The second class of quantum effects that become more rich in multi-dimensional space is typically referred to as either diffraction or scattering - depending on the context. (Diffraction is essentially the interference, but of waves emitted by several many coherent sources.) Just as in the two -

[^542]slits in the Young-type experiment (Fig. 1), these sources are most frequently the elementary re-emitters of some initial wave from a single source. More generally, such re-emitting is called scattering; this term is also applied to particles - even if their quantum properties may be ignored. ${ }^{23}$

Figure 8 shows the general scattering situation. Most commonly, the detector of scattered particles (in the quantum case, read de Broglie waves) is located at a large distance $r \gg a$ from the scatterer. ${ }^{24}$ In this case, the main observable independent of $r$ is the flux (number of particles per unit time) of particles scattered in a certain direction, i.e. their flux per unit solid angle. Since such flux is proportional to the incident flux of particles per unit area, the ability of the scatterer to re-emit in a particular direction may be characterized by the ratio of these two fluxes. This ratio has the dimensionality of area per unit angle, and is called the differential cross-section of the scatterer:


Full
cross-
section

$$
\begin{equation*}
\frac{d \sigma}{d \Omega} \equiv \frac{\text { flux of scatterd particles per unit solid angle }}{\text { flux of incident particles per unit area }} . \tag{3.58}
\end{equation*}
$$



Such name and notation stem from the fact that the integral of $d \sigma / d \Omega$ over all scattering angles,

$$
\begin{equation*}
\sigma \equiv \oint \frac{d \sigma}{d \Omega} d \Omega=\frac{\text { total flux of scattered particles }}{\text { incident flux per per unit area }} \tag{3.59}
\end{equation*}
$$

(also with the dimensionality of area), has a simple interpretation as the full cross-section of scattering. For the simplest case when a macroscopic solid object scatters all classical particles hitting its surface, but does not affect the particles flying by it, $\sigma$ is just the geometrical cross-section of the object, as visible from the direction of incoming particles.

In classical mechanics, ${ }^{25}$ we first calculate the particle scattering angle as a function of the impact parameter $b$, and then average the result over all values of $b$, considered random. In this sense the calculations in wave mechanics are simpler, because a parallel beam of incident particles of fixed energy $E$ may be fairly presented by a plane de Broglie wave

$$
\begin{equation*}
\psi_{0}=a_{0} e^{i \mathbf{k}_{0} \cdot \mathbf{r}}, \tag{3.60}
\end{equation*}
$$

[^543]with the free-space wave number $k_{0}=(2 m E)^{1 / 2} / \hbar$ and constant probability current density (1.49):
\[

$$
\begin{equation*}
\mathbf{j}_{0}=\left|a_{0}\right|^{2} \frac{\hbar}{m} \mathbf{k}_{0} . \tag{3.61}
\end{equation*}
$$

\]

This current density is exactly the flux of incident particles per unit area that is used in the denominator of definition (58), so the "only" remaining thing to do is to calculate the numerator of that fraction.

To do this, let us write the Schrödinger equation for the scattering problem (now in the whole space including the scatterer) in the form

$$
\begin{equation*}
\left(E-\hat{H}_{0}\right) \psi=U(\mathbf{r}) \psi \tag{3.62}
\end{equation*}
$$

where

$$
\begin{equation*}
\hat{H}_{0} \equiv-\frac{\hbar^{2}}{2 m} \nabla^{2}, \quad \text { and } \quad E=\frac{\hbar^{2} k_{0}^{2}}{2 m}=\frac{\hbar^{2} k^{2}}{2 m} . \tag{3.63}
\end{equation*}
$$

the potential energy $U(\mathbf{r})$ describes the effect of scatterer. Looking for the solution of Eq. (62) in the natural form

$$
\begin{equation*}
\psi=\psi_{0}+\psi_{s}, \tag{3.64}
\end{equation*}
$$

where $\psi_{0}$ is the incident wave (60), and $\psi_{\mathrm{s}}$ has the sense of the scattered wave, and taking into account that former wave satisfies the free-space equation

$$
\begin{equation*}
\hat{H}_{0} \psi_{0}=E \psi_{0} \tag{3.65}
\end{equation*}
$$

we may reduce Eq. (62) to

$$
\begin{equation*}
\left(E-\hat{H}_{0}\right) \psi_{s}=U(\mathbf{r})\left(\psi_{0}+\psi_{s}\right) \tag{3.66}
\end{equation*}
$$

The most straightforward (and common) simplification of this problem is possible if the scattering potential $U(\mathbf{r})$ is in some sense weak. (We will derive the exact condition of this smallness below.) Then since at $U(\mathbf{r})=0$ the scattering wave $\psi_{s}$ disappears, we may expect that at small but nonvanishing $U(\mathbf{r})$, the main part of $\psi_{s}$ is proportional to its scale $U_{0}$. Then all terms in Eq. (66) are proportional to $U_{0}$, besides the product $U \psi_{s}$, which is proportional to $U_{0}{ }^{2}$. Hence, in the first approximation in $U_{0}$, that term may be ignored, and Eq. (66) reduces to the famous equation of the Born approximation: ${ }^{26}$

$$
\begin{equation*}
\left(E-\hat{H}_{0}\right) \psi_{s}=U(\mathbf{r}) \psi_{0} \tag{3.67a}
\end{equation*}
$$

[^544]This simplification changes the situation drastically, because the linear superposition principle allows finding an explicit solution of this equation (in the form of an integral) for an arbitrary function $U(\mathbf{r})$. Indeed, after rewriting Eq. (67a) as

[^545]\[

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) \psi_{s}=\frac{2 m}{\hbar^{2}} U(\mathbf{r}) \psi_{0}(\mathbf{r}) \tag{3.67b}
\end{equation*}
$$

\]

we may notice that $\psi_{s}$ is just a response of a linear system to a certain "excitation" (represented by the right-hand part) that is fixed, i.e. does not depend on the solution. Hence we can present $\psi_{s}$ as a sum of responses to elementary excitations from elementary volumes $d^{3} r^{\prime}$ :

$$
\begin{equation*}
\psi_{s}(\mathbf{r})=\frac{2 m}{\hbar^{2}} \int U\left(\mathbf{r}^{\prime}\right) \psi_{0}\left(\mathbf{r}^{\prime}\right) G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) d^{3} r^{\prime} \tag{3.68}
\end{equation*}
$$

Spatial Green's function

Here $G(\mathbf{r}, \mathbf{r}$ ') is the spatial Green's function, defined as such an elementary response of the free-space Schrödinger equation to a point excitation, i.e. the solution of the following equation ${ }^{27}$

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) G=\delta\left(\mathbf{r}-\mathbf{r}^{\prime}\right) \tag{3.69}
\end{equation*}
$$

But we already know the physically-relevant spherically-symmetric solution of this equation - see Eq. (7) and its discussion:

$$
\begin{equation*}
G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=\frac{f_{+}}{R} e^{i k R} \tag{3.70}
\end{equation*}
$$

so that we need just to calculate the coefficient $f_{+}$for Eq. (67). This can be done in several ways, for example by noticing that at $r \ll k^{-1}$, the second term in Eq. (70) is negligible, and it is reduced to the well-known Poisson equation with delta-functional right-hand part, which describes, for example, the electrostatic potential generated by a point electric charge. Either recalling the Coulomb law, or applying the Gauss theorem, ${ }^{28}$ we readily get the asymptote

$$
\begin{equation*}
G \rightarrow-\frac{1}{4 \pi R}, \quad \text { at } k r \ll 1, \tag{3.71}
\end{equation*}
$$

which is compatible with Eq. (70) only if $f_{+}=-1 / 4 \pi$, i.e. if

Green's function for free space

$$
\begin{equation*}
G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)=-\frac{1}{4 \pi R} e^{i k R} \tag{3.72}
\end{equation*}
$$

Plugging this result into Eq. (68), we get the final solution of Eq. (67):

$$
\begin{equation*}
\psi_{s}(\mathbf{r})=-\frac{m}{2 \pi \hbar^{2}} \int U\left(\mathbf{r}^{\prime}\right) \frac{\psi_{0}\left(\mathbf{r}^{\prime}\right)}{R} e^{i k R} d^{3} r^{\prime} \tag{3.73}
\end{equation*}
$$

Note that if function $U(\mathbf{r})$ is smooth, the singularity in the denominator is integrable (i.e. not dangerous); indeed, the contribution of a sphere of radius $R \rightarrow 0$, with the center in point $\mathbf{r}^{\prime}=0$, scales as

$$
\begin{equation*}
\int_{R<R} \frac{d^{3} R}{R}=4 \pi \int_{0}^{R} \frac{R^{2} d R}{R}=4 \pi \int_{0}^{R} R d R=2 \pi R^{2} \rightarrow 0 \tag{3.74}
\end{equation*}
$$

[^546]Actually, Eq. (73) gives us more than we wanted: it evaluates the scattered wave at any point, including those within of the scattering object, while our goal was to find the wave far from the scatterer - please revisit Fig. 8 if you need. However, before going to that limit, we can use the general formula to find the quantitative criterion of the Born approximation's validity. Indeed, let us estimate the magnitude of the right hand part of this equation, for a scatterer of linear size $\sim a$, and the potential magnitude scale $U_{0}$, in two limits:
(i) If $k a \ll 1$, then inside the scatterer (i.e., at distances $r^{\prime} \sim a$ ), both $\psi_{0} \sim \exp \{i k r\}$ and the second exponent under the integral change slowly, so that a crude estimate of the solution is

$$
\begin{equation*}
\left|\psi_{s}\right| \sim \frac{m}{2 \pi \hbar^{2}} U_{0}\left|\psi_{0}\right| a^{2} . \tag{3.75}
\end{equation*}
$$

(ii) In the opposite limit $k a \gg 1$, the integration along one of the dimensions (that of the wave propagation) is cut out on distances of the order of the de Broglie wavelength $k^{-1}$, so that the integral is correspondingly smaller:

$$
\begin{equation*}
\left|\psi_{\mathrm{s}}\right| \sim \frac{m}{2 \pi \hbar^{2}} U_{0}\left|\psi_{0}\right| \frac{a^{2}}{k a} \tag{3.76}
\end{equation*}
$$

Since the reduction of Eq. (66) to Eq. (67) requires $\left|\psi_{s}\right| \ll\left|\psi_{0}\right|$ everywhere within the scatterer, we may now formulate the conditions of this requirement as

$$
\begin{equation*}
U_{0} \ll \frac{\hbar^{2}}{m a^{2}} \max [k a, 1] . \tag{3.77}
\end{equation*}
$$

In the first factor of the right-hand part, we may readily recognize the scale of the kinetic (quantumconfinement) energy $E_{a}$ of the particle inside a quantum well of size $\sim a$, so that the Born approximation is valid essentially if the potential energy of particle's interaction with the scatterer is smaller than $E_{a}$. Note, however, that estimates (75) and (76) are not valid in special situations when the effects of scattering accumulate in some direction. This is frequently the case for small scattering angles in extended objects (when $k a \gg 1$ but $k a \theta<1$ ), and especially in 1D (or quasi-1D) scatterers oriented along the incident particle beam.

Now let us proceed to large distances $r \gg r^{\prime} \sim a$, and simplify Eq. (73) using an approximation similar to the dipole expansion in electrodynamics. ${ }^{29}$ In denominator's $R$, we can merely ignore $r$ ' in comparison with $r$, but the exponent requires more care, because even if $r^{\prime} \sim a \ll r$, the product $k r^{\prime} \sim k a$ may still be larger than 1. In the first approximation in $r^{\prime}$, we can take (Fig. 9a):


Fig. 3.9. (a) Dipole expansion in the Born approximation and (b) definitions of vector $\mathbf{q}$ and angles $\chi$ and $\theta$.

[^547]\[

$$
\begin{equation*}
R \equiv\left|\mathbf{r}-\mathbf{r}^{\prime}\right| \approx r-\mathbf{n}_{r} \cdot \mathbf{r}^{\prime}, \tag{3.78}
\end{equation*}
$$

\]

and since the directions of vectors $\mathbf{k}$ and $\mathbf{r}$ coincide, i.e. $\mathbf{k}=k \mathbf{n}_{r}$,

$$
\begin{equation*}
k R \approx k r-\mathbf{k} \cdot \mathbf{r}^{\prime}, \quad \text { and } e^{i k R} \approx e^{i k r} e^{-i \mathbf{k} \cdot \mathbf{r}^{\prime}} \tag{3.79}
\end{equation*}
$$

With this replacement, and the incident wave in form (60), the Born approximation yields

$$
\begin{equation*}
\psi_{s}(\mathbf{r})=-\frac{m}{2 \pi \hbar^{2}} \frac{a_{0}}{r} e^{i k r} \int U\left(\mathbf{r}^{\prime}\right) e^{-i\left(\mathbf{k}-\mathbf{k}_{0}\right) \cdot \mathbf{r}^{\prime}} d^{3} r^{\prime} \tag{3.80}
\end{equation*}
$$

This relation may be presented in a general form ${ }^{30}$

Scattering function

$$
\begin{equation*}
\psi_{s}=a_{0} \frac{f\left(\mathbf{k}, \mathbf{k}_{0}\right)}{r} e^{i k r} \tag{3.81}
\end{equation*}
$$

where $f\left(\mathbf{k}, \mathbf{k}_{0}\right)$ is called the scattering function. ${ }^{31}$ Its physical sense becomes clear from the calculation of the corresponding probability current density $\mathbf{j}_{s}$. For that, generally we need to use Eq. (1.47) with the gradient operator having all spherical-coordinate components. ${ }^{32}$ However, at $k r \gg 1$ the main contribution to $\nabla \psi_{s}$, proportional to $k \gg 1 / r$, is provided by the term $\exp \{i k r\}$ which changes fast in the common direction of vectors $\mathbf{r}$ and $\mathbf{k}$, so that

$$
\begin{equation*}
\nabla \psi_{s} \approx \mathbf{n}_{r} \frac{\partial}{\partial r} \psi_{s} \approx \mathbf{k} \psi_{s}, \quad \text { at } k r \gg 1 \tag{3.82}
\end{equation*}
$$

so that Eq. (1.47) yields

$$
\begin{equation*}
\mathbf{j}_{s}(\theta) \approx \frac{\hbar}{m}\left|a_{0}\right|^{2} \frac{\left|f\left(\mathbf{k}, \mathbf{k}_{0}\right)\right|^{2}}{r^{2}} \mathbf{k} \tag{3.83}
\end{equation*}
$$

Since this vector is parallel to $\mathbf{k}$ and hence to $\mathbf{r}$, the flux in the numerator of Eq. (58), i.e. the probability current per unit solid angle, is just $r^{2} j_{s}$. Hence, the differential cross-section is simply

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\frac{j_{s} r^{2}}{j_{0}}=\left|f\left(\mathbf{k}, \mathbf{k}_{0}\right)\right|^{2}, \tag{3.84}
\end{equation*}
$$

and the total cross-section is

$$
\begin{equation*}
\sigma=\oint\left|f\left(\mathbf{k}, \mathbf{k}_{0}\right)\right|^{2} d \Omega \tag{3.85}
\end{equation*}
$$

so that the scattering function $f\left(\mathbf{k}, \mathbf{k}_{0}\right)$ gives us everything we need (and in fact more, because the function also contains information about the phase of the scattered wave).

[^548]According to Eq. (80), in the Born approximation the scattering function may be presented as the Born integral

$$
\begin{equation*}
f\left(\mathbf{k}, \mathbf{k}_{0}\right)=-\frac{m}{2 \pi \hbar^{2}} \int U(\mathbf{r}) e^{-i \mathbf{q} \cdot \mathbf{r}^{3}} d^{3} r \tag{3.86}
\end{equation*}
$$

where for the notation simplicity I have replaced $\mathbf{r}$ ' with $\mathbf{r}$, and also introduced the scattering vector

$$
\begin{equation*}
\mathbf{q} \equiv \mathbf{k}-\mathbf{k}_{0} \tag{3.87}
\end{equation*}
$$

with length $q=2 k \sin (\theta / 2)$, where $\theta$ is the scattering angle between vectors $\mathbf{k}$ and $\mathbf{k}_{0}-$ see Fig. 9 b . For the differential cross-section, Eq. (86) yields

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\left(\frac{m}{2 \pi \hbar^{2}}\right)^{2}\left|\int U(\mathbf{r}) e^{-i \mathbf{q} \cdot \mathbf{r}} d^{3} r\right|^{2} \tag{3.88}
\end{equation*}
$$

and the total cross-section may be now readily calculated from the first of Eqs. (59). ${ }^{33}$
This is the main result of this section; it may be further simplified for spherically-symmetric scatterers, with

$$
\begin{equation*}
U(\mathbf{r})=U(r) \tag{3.89}
\end{equation*}
$$

Here, it is convenient to present the exponent in the Born integral as $\exp \{-i q r \cos \chi\}$, where $\chi$ is the angle between vectors $\mathbf{k}$ (i.e. the direction $\mathbf{n}_{r}$ toward the detector) and $\mathbf{q}$ (rather than the incident wave vector $\mathbf{k}_{0}!$ ) - see Fig. 9b. Now, for fixed $\mathbf{q}$, we can take this vector's direction as the polar axis of a spherical coordinate system, and reduce Eq. (86) to a 1D integral:

$$
\begin{align*}
f\left(\mathbf{k}, \mathbf{k}_{0}\right) & =-\frac{m}{2 \pi \hbar^{2}} \int r^{2} d r U(r) \int_{0}^{2 \pi} d \varphi \int_{0}^{\pi} \sin \chi d \chi \exp \{-i q r \cos \chi\}  \tag{3.90}\\
& =-\frac{m}{2 \pi \hbar^{2}} \int r^{2} d r U(r) 2 \pi \frac{2 \sin q r}{q r}=-\frac{2 m}{\hbar^{2} q} \int U(r) \sin (q r) r d r .
\end{align*}
$$

As a simple example, let us use the Born approximation to analyze scattering on the following spherically-symmetric potential:

$$
\begin{equation*}
U(\mathbf{r})=U_{0} \exp \left\{-\frac{r^{2}}{2 a^{2}}\right\} \tag{3.91}
\end{equation*}
$$

In this particular case, it is better to avoid the temptation to exploit the spherical symmetry by using Eq. (90), and instead use the generic Eq. (88), because it falls apart into a product of three similar Cartesian factors:

$$
\begin{equation*}
f\left(\mathbf{k}, \mathbf{k}_{0}\right)=-\frac{m U_{0}}{2 \pi \hbar^{2}} I_{x} I_{y} I_{z} \tag{3.92}
\end{equation*}
$$

with

[^549]\[

$$
\begin{equation*}
I_{x}=\int_{-\infty}^{+\infty} \exp \left\{-\left(\frac{x^{2}}{2 a^{2}}+i q_{x} x\right)\right\} d x \tag{3.93}
\end{equation*}
$$

\]

and similar integrals for $I_{y}$ and $I_{z}$. From Chapter 2, we already know that Gaussian integrals like $I_{x}$ may be readily worked out by complementing the exponent to the full square, in our current case giving

$$
\begin{equation*}
I_{x}=(2 \pi)^{1 / 2} a \exp \left\{-\frac{q_{x}^{2} a^{2}}{2}\right\}, \quad \text { etc. } \tag{3.94}
\end{equation*}
$$

so that, finally,

$$
\begin{equation*}
\frac{d \sigma}{d \Omega}=\left|f\left(\mathbf{k}, \mathbf{k}_{0}\right)\right|^{2}=\left(\frac{m U_{0}}{2 \pi \hbar^{2}} I_{x} I_{y} I_{z}\right)^{2}=2 \pi a^{2}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2} e^{-q^{2} a^{2}} . \tag{3.95}
\end{equation*}
$$

Now, the total cross-section $\sigma$ is an integral of $d \sigma / d \Omega$ over all directions of vector $\mathbf{k}$. Since in our case the scattering intensity does not depend on the azimuthal angle $\varphi$, the integration is reduced to that over the scattering angle $\theta$ (Fig. 9b):

$$
\begin{align*}
& \sigma \equiv \oint \frac{d \sigma}{d \Omega} d \Omega=2 \pi \int_{0}^{\pi} \frac{d \sigma}{d \Omega} \sin \theta d \theta=4 \pi^{2} a^{2}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2} \int_{0}^{\pi} \sin \theta d \theta \exp \left\{-\left(2 k \sin \frac{\theta}{2}\right)^{2} a^{2}\right\}  \tag{3.96}\\
& =4 \pi^{2} a^{2}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2} \int_{\theta=0}^{\theta=\pi} \exp \left\{-2 k^{2} a^{2}(1-\cos \theta)\right\} d(1-\cos \theta)=\frac{2 \pi^{2}}{k^{2}}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2}\left[1-e^{-4 k^{2} a^{2}}\right]
\end{align*}
$$

Let us analyze these formulas. In the low-energy limit, $k a \ll 1$ (and hence $q a \ll 1$ for any scattering angle), the scattered wave is virtually isotropic: $d \sigma / d \Omega \approx$ const - a very typical feature of scattering by small objects, in any approximation. Notice that in this limit, the Born expression for $\sigma$,

$$
\begin{equation*}
\sigma \approx 8 \pi^{2} a^{2}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2} \tag{3.97}
\end{equation*}
$$

is only valid if $\sigma$ is much smaller than the scale $a^{2}$ of the physical cross-section of the scatterer.
In the opposite, high-energy limit $k a \gg 1$, the scattering is dominated by small angles $\theta \approx q / k \sim$ $1 / k a \sim \lambda / a$ :

$$
\begin{equation*}
\frac{d \sigma}{d \Omega} \approx 2 \pi a^{2}\left(\frac{m U_{0} a^{2}}{\hbar^{2}}\right)^{2} \exp \left\{-(k a \theta)^{2}\right\} \tag{3.98}
\end{equation*}
$$

This is, again, very typical for diffraction. Notice, however, that due to the smooth character of the Gaussian potential (91), the diffraction pattern exhibits no oscillations; such oscillations of $d \sigma / d \Omega$ as function of angle naturally appear for potentials with sharp borders - see, e.g., Problems 2 and 3.

The Born approximation, while being very simple and used more often than any other scattering theory, is not without substantial shortcomings, as is clear from the following example. It is not too difficult to prove the following general optical theorem, valid for an arbitrary scatterer:

$$
\begin{equation*}
\operatorname{Im} f\left(\mathbf{k}_{0}, \mathbf{k}_{0}\right)=\frac{k}{4 \pi} \sigma \tag{3.99}
\end{equation*}
$$

However, Eq. (86) shows that in the Born approximation, function $f$ is purely real at $q=0$ (i.e. $\mathbf{k}=\mathbf{k}_{0}$ ), and hence cannot satisfy the optical theorem. Even more evidently, it cannot describe such a simple effect as a dark shadow $(\psi \approx 0)$ cast by an opaque object (say, with $U_{0} \gg E$ ).

There are several ways to improve the Born approximation, while still holding the general idea of approximate treatment of $U$.
(i) Instead of the main assumption $\psi_{s} \propto U_{0}$, we can use a complete perturbation series:

$$
\begin{equation*}
\psi_{s}=\psi_{1}+\psi_{2}+\ldots \tag{3.100}
\end{equation*}
$$

with $\psi_{n} \propto U_{0}{ }^{n}$, and find successive approximations $\psi_{n}$ one by one. In the $1^{\text {st }}$ approximation we of course return to the Born formula, but already the $2^{\text {nd }}$ approximation yields

$$
\begin{equation*}
\operatorname{Im} f_{2}\left(\mathbf{k}_{0}, \mathbf{k}_{0}\right)=\frac{k}{4 \pi} \sigma_{1}, \tag{3.101}
\end{equation*}
$$

where $\sigma_{1}$ is the full cross-section calculated in the 1st approximation, so that the optical theorem (99) is "almost" satisfied. ${ }^{34}$
(ii) As was mentioned above, the Born approximation does not work very well for small-angle scattering by extended objects. This deficiency may be corrected by the so-called eikonal approximation (from Greek word $\varepsilon 1 \kappa 0 v$, meaning "icon") that replaces the plane wave exponent $\exp \left\{i k_{0} x\right\}$ representation of the incident wave by a WKB-like exponent, though still in the first nonvanishing approximation in $U \rightarrow 0$ :

$$
\begin{equation*}
\exp \left\{i k_{0} x\right\} \rightarrow \exp \left\{i \int_{0}^{x} k\left(x^{\prime}\right) d x^{\prime}\right\}=\exp \left\{i \int_{0}^{x} \frac{\left\{2 m\left[E-U\left(x^{\prime}\right)\right]\right\}^{1 / 2}}{\hbar} d x^{\prime}\right\} \approx \exp \left\{i\left[k_{0} x-\frac{m}{\hbar^{2} k_{0}} \int_{0}^{x} U\left(x^{\prime}\right) d x^{\prime}\right]\right\} . \tag{3.102}
\end{equation*}
$$

This approximation's results satisfy the optical theorem (99) already in the $1^{\text {st }}$ approximation in $U$.

### 3.4. Energy bands in higher dimensions

In Sec. 2.5, we have discussed the 1 D band theory for potential profiles $U(x)$ that obey the periodicity condition (2.192). For what follows, let us notice that that condition may be rewritten as

$$
\begin{equation*}
U(x+X)=U(x), \tag{3.103}
\end{equation*}
$$

[^550]where $X=\tau a$, with $\tau$ being an arbitrary integer. One can say that the set of points $X$ forms a periodic $l D$ lattice in the direct ( $x$-) space. We have also seen that each Bloch state (i.e., each eigenstate of the Schrödinger equation for such periodic potential) is characterized by the quasi-momentum $\hbar q$ and its energy does not change if $q$ is changed by a multiple of $2 \pi / a$. Hence if we form, in the reciprocal ( $k$-) space, a 1D lattice of points $Q=l b$, with $b=2 \pi / a$ and integer $l$, any pair of points from these two mutually reciprocal lattices satisfies the following rule:
\[

$$
\begin{equation*}
\exp \{i Q X\}=\exp \left\{i l \frac{2 \pi}{a} \tau a\right\}=e^{2 \pi i \tau l}=1 \tag{3.104}
\end{equation*}
$$

\]

In this form, the results of Sec. 2.5 may be readily extended to $d$-dimensional periodic potentials whose translational symmetry obeys the following generalization of Eq. (103):

$$
\begin{equation*}
U(\mathbf{r}+\mathbf{R})=U(\mathbf{r}) \tag{3.105}
\end{equation*}
$$

where points $\mathbf{R}$, which may be numbered by $d$ integers $\tau_{j}$, form the so-called Bravais lattice ${ }^{35}$ of points

$$
\begin{equation*}
\mathbf{R}=\sum_{j=1}^{d} \tau_{j} \mathbf{a}_{j} \tag{3.106}
\end{equation*}
$$

with $d$ primitive vectors $\mathbf{a}_{j}$. The simplest example of a 3D Bravais lattice are given by the simple cubic lattice (Fig. 10a), which may be described by the system of mutually perpendicular primitive vectors $\mathbf{a}_{j}$ of equal length. However, not in any lattice these vectors are perpendicular; for example Figs. 10b and 10c show possible sets of the primitive vectors describing the face-centered cubic lattice (fcc) and bodycentered cubic lattice (bcc). In 3D, the science of crystallography, based on the group theory, distinguishes, by their symmetry properties, 14 Bravais lattices grouped into 7 different lattice systems. ${ }^{36}$
(a)

(b)


Fig. 3.10. The simplest (and most common) 3D Bravais lattices: (a) simple cubic, (b) face-centered cubic (fcc), and (c) body-centered cubic (bcc), and possible choices of their primitive vector sets (blue arrows).

Note, however, not all highly symmetric sets of points form Bravais lattices. As probably the most striking example, nodes of the very simple 2D honeycomb lattice (Fig. 11a) cannot be described by

[^551]a Bravais lattice - while the 2D hexagonal lattice, shown in Fig. 11b, can. The most prominent 3D case of such a lattice is the diamond structure (Fig. 11c), which describes, in particular, atoms of world's most important crystal - silicon. ${ }^{37}$ In cases like these, the band theory is much facilitated by the fact that the Bravais lattices using some point assemblies (called primitive unit cells) may describe these point systems. For example, Fig. 11a shows the possible choice of primitive vectors for the honeycomb structure, ${ }^{38}$ with the primitive unit cell formed by any two adjacent points of the original lattice (say, within the dashed ellipses in Fig. 11a). Similarly, the diamond lattice may be described as the fcc Bravais lattice with two-point primitive unit cell. ${ }^{39}$

Now we are ready for the following generalization of the 1D Bloch theorem, given by Eqs. (2.193) and (2.210), to higher dimensions. Any eigenfunction of the Schrödinger equation describing particle's motion in the periodic potential (105) may be presented either as
or as

$$
\begin{equation*}
\psi(\mathbf{r}+\mathbf{R})=\psi(\mathbf{r}) e^{i \mathbf{q} \cdot \mathbf{R}} \tag{3.107}
\end{equation*}
$$

$$
\begin{equation*}
\psi(\mathbf{r})=u(\mathbf{r}) e^{i \mathbf{q} \cdot \mathbf{r}}, \quad \text { with } u(\mathbf{r}+\mathbf{R})=u(\mathbf{r}) \tag{3.108}
\end{equation*}
$$

where the quasi-momentum $\hbar \mathbf{q}$ is again a constant of motion, but now is a vector.

(c)


Two forms of the 3D Bloch theorem

Fig. 3.11. Some important periodic structures that require two-point primitive cells for their Bravais lattice presentation: (a) 2D honeycomb lattice and their primitive vectors and (c) 3D diamond lattice. For a contrast, panel (b) shows the 2D hexagonal structure which forms a Bravais lattice with a single-point primitive cell.

The key notion of the band theory is the reciprocal lattice in the wavevector space, formed as

$$
\begin{equation*}
\mathbf{Q}=\sum_{j=1}^{d} l_{j} \mathbf{b}_{j} \tag{3.109}
\end{equation*}
$$

Reciprocal lattice in q-space

[^552]with integer $l_{j}$, and vectors $\mathbf{b}_{j}$ selected in such way that the following generalization of Eq. (104) is valid for any pair of points of the direct and reciprocal lattices:
\[

$$
\begin{equation*}
e^{i \mathbf{Q} \cdot \mathbf{R}}=1 \tag{3.110}
\end{equation*}
$$

\]

The importance of lattice $\mathbf{Q}$ is immediately clear from the first formulation of the Bloch theorem, given by Eq. (107): if we add to $\mathbf{q}$ any vector $\mathbf{Q}$ of the reciprocal lattice, the wavefunction does not change. This means that all information about the system is contained in just one elementary cell of the reciprocal space $\mathbf{q}$. Its most frequent choice, called the $l^{s t}$ Brillouin zone, is the set of all points $\mathbf{q}$ that are closer to the origin than to any other point of lattice $\mathbf{Q}$.

It is easy to see that primitive vectors $\mathbf{b}_{\mathbf{j}}$ of the reciprocal 3D lattice ${ }^{40}$ may be constructed from those of the initial, direct lattice as

Primitive vectors of the reciprocal lattice

$$
\begin{equation*}
\mathbf{b}_{1}=2 \pi \frac{\mathbf{a}_{2} \times \mathbf{a}_{3}}{\mathbf{a}_{1} \cdot\left(\mathbf{a}_{2} \times \mathbf{a}_{3}\right)}, \quad \mathbf{b}_{2}=2 \pi \frac{\mathbf{a}_{3} \times \mathbf{a}_{1}}{\mathbf{a}_{1} \cdot\left(\mathbf{a}_{2} \times \mathbf{a}_{3}\right)}, \quad \mathbf{b}_{3}=2 \pi \frac{\mathbf{a}_{1} \times \mathbf{a}_{2}}{\mathbf{a}_{1} \cdot\left(\mathbf{a}_{2} \times \mathbf{a}_{3}\right)} . \tag{3.111}
\end{equation*}
$$

Indeed, from the "operand rotation rule" of the vector algebra ${ }^{41}$ it is evident that $\mathbf{a}_{j} \cdot \mathbf{b}_{j}$ ' $=2 \pi \delta_{j j}$. Hence, the exponent in the left-hand part of Eq. (110) is reduced to

$$
\begin{equation*}
e^{i \mathbf{Q} \cdot \mathbf{R}}=\exp \left\{2 \pi i\left(l_{1} \tau_{1}+l_{2} \tau_{2}+l_{3} \tau_{3}\right)\right\} \tag{3.112}
\end{equation*}
$$

Since all $l_{j}$ and $\tau_{j}$ are integers, the expression in the parentheses is also an integer, so the exponent indeed equals 1 , thus satisfying the definition of the reciprocal lattice given by Eq. (110).

As the simplest example, let us return to the simple cubic lattice of period $a$ (Fig. 10a), oriented in space so that

$$
\begin{equation*}
\mathbf{a}_{1}=a \mathbf{n}_{x}, \quad \mathbf{a}_{2}=a \mathbf{n}_{y}, \quad \mathbf{a}_{3}=a \mathbf{n}_{z} \tag{3.113}
\end{equation*}
$$

According to Eq. (111), its reciprocal lattice is (of course) also cubic:

$$
\begin{equation*}
\mathbf{Q}=\frac{2 \pi}{a}\left(l_{x} \mathbf{n}_{x}+l_{y} \mathbf{n}_{y}+l_{z} \mathbf{n}_{z}\right), \tag{3.114}
\end{equation*}
$$

so that the $1^{\text {st }}$ Brillouin zone is a cube with side $b=2 \pi / a$. Almost similarly simple calculations show that the reciprocal lattice of fcc is bcc, and vice versa. Figure 12 shows the resulting $1^{\text {st }}$ Brillouin zone of the fcc lattice.

The notion of the reciprocal lattice ${ }^{42}$ makes the multi-dimensional band theory not much more complex than that in 1 D , especially for numerical calculations, at least for the single-point Bravais lattices. Indeed, repeating all the steps that have led to Eq. (2.218), but now with a $d$-dimensional Fourier expansion of functions $U(\mathbf{r})$ and $u_{l}(\mathbf{r})$, we readily get its generalization:

$$
\begin{equation*}
\sum_{\mathbf{I}^{\prime} \neq 1} U_{\mathbf{1}^{\prime}-1} u_{\mathbf{I}^{\prime}}=\left(E-E_{\mathbf{1}}\right) u_{\mathbf{1}} \tag{3.115}
\end{equation*}
$$

[^553]where $\mathbf{l}$ is now a $d$-dimensional vector of integer indices $l_{j}$. The summation in Eq. (115) should be carried over all (essential) components of this vector (i.e. over all relevant nodes of the reciprocal lattice), so writing a corresponding computer code requires a bit more care than in 1 D ; however, this is just a homogeneous system of linear equations, and numerous routines of finding its eigenvalues $E$ are readily available from both public sources and commercial software packages. ${ }^{43}$


Fig. 3.12. $1^{\text {st }}$ Brillouin zone of the fcc lattice, and the traditional notation of its main directions. Adapted from http://en.wikipedia.org/wiki/Band structure.

What is indeed more complex than in 1D is the presentation (and hence the comprehension :-), of the calculation results and experimental data. Typically, the presentation is limited to plotting the Bloch state eigenenergy as a function of components of vector $q$ along certain special directions the reciprocal space of quasi-momentum (see, e.g., the lines shown in Fig. 12), typically plotted on single panel. Figure 12 shows perhaps the most famous (and certainly the most practically important) of such plots, the band structure of silicon. The dashed horizontal lines mark the "indirect" gap of width 1.12 eV between the "valence" and "conduction" energy bands, which is the playground of virtually all siliconbased electronics.


Fig. 3.13. Band structure of silicon, along the special directions shown in Fig. 12. (Adapted from http://www.tf.uni-kiel.de/matwis/amat/semi en/.)

[^554]In order to understand the reason of this band structure presentation complexity, let us see how we would start to develop the weak-potential approximation for the simplest case of a 2 D square lattice (which is a subset of the cubic lattice, with $\tau_{3}=0$ ). Its $1^{\text {st }}$ Brillouin zone is of course also a square, of area $(2 \pi / a)^{2}$. Let us draw the lines of constant energy of a free particle $(U=0)$ in this zone. Repeating the arguments of Sec. 2.7 (see especially Fig. 2.28 and its discussion), we should conclude that Eq. (2.216) should now be generalized as follows,

$$
\begin{equation*}
E=E_{\mathbf{1}}=\frac{\hbar^{2} k^{2}}{2 m}=\frac{\hbar^{2}}{2 m}\left[\left(q_{x}-\frac{2 \pi l_{x}}{a}\right)^{2}+\left(q_{y}-\frac{2 \pi l_{y}}{a}\right)^{2}\right] \tag{3.116}
\end{equation*}
$$

with all possible integers $l_{x}$ and $l_{y}$. Considering the result only within the $1^{\text {st }}$ Brillouin zone, we see that as energy $E$ grows, the lines of equal energy evolve as shown in Fig. 14. Just like in 1D, the weakpotential effects are only important at the Brillouin zone boundaries, and may be crudely considered as the appearance of narrow energy gaps, but one can see that the band structure in $\mathbf{q}$-space is complex enough even without these effects.

(c)

Fig. 3.14. Lines of constant energy $E$ of a free particle, within the $1^{\text {st }}$ Brillouin zone of a square Bravais lattice, for: (a) $E / E_{1} \approx 0.95$, (b) $E / E_{1}$ $\approx 1.05$; and (c) $E / E_{1} \approx 2.05$, where $E_{1} \equiv \pi^{2} \hbar^{2} / 2 m a^{2}$.

The tight-binding approximation is usually easier to follow. For example, for the same square 2D lattice, we may repeat the arguments that have led us to Eq. (2.203), to write ${ }^{44}$

$$
\begin{equation*}
i \hbar \frac{d a_{0,0}}{d t}=-\delta_{n}\left(a_{-1,0}+a_{+1,0}+a_{0,+1}+a_{0,-1}\right) \tag{3.117}
\end{equation*}
$$

where indices correspond to the deviations of integers $\tau_{x}$ and $\tau_{y}$ from an arbitrarily selected minimum of the potential energy - and hence wavefunction's "hump" quasi-localized at this minimum. Now, looking for the stationary solution of these equations, that corresponds to the Bloch theorem (107), instead of Eq. (2.206) we get

$$
\begin{equation*}
E=E_{n}+\varepsilon_{n}=E_{n}-\delta_{n}\left(e^{i q_{x} a}+e^{-i q_{x} a}+e^{i q_{y} a}+e^{-i q_{y} a}\right)=E_{n}-2 \delta_{n}\left(\cos q_{x} a+\cos q_{y} a\right) . \tag{3.118}
\end{equation*}
$$

Figure 15 shows this result, within the $1^{\text {st }}$ Brillouin zone, in two forms: as the color-coded lines of equal energy and as a 3D plot (also enhanced by color).

[^555]

Fig. 3.15. Allowed band energy $\varepsilon_{n}=E-E_{n}$ for a square 2D lattice, in the tight-binding approximation.

It is evident that the plots of this function along different lines on the $\mathbf{q}$-plane, for example along one of axes (say, $q_{x}$ ) and along a diagonal of the $1^{\text {st }}$ Brillouin zone (say, $q_{x}=q_{y}$ ) give different curves, qualitatively similar to those of silicon (Fig. 13). The latter structure is complicated by the fact that the primitive cell of their Bravais lattices contains more than 2 atoms - see Fig. 11c and its discussion. In this case, even the tight-binding picture becomes more complex. Indeed, even if the atoms in the different positions of the primitive unit cell are similar (as they are, for example, in both graphene and silicon), and hence the potential well shape near those points and the corresponding local wavefunctions $u(\mathbf{r})$ are similar as well, the Bloch theorem (which only pertains to Bravais lattices!) does not forbid them to have different complex amplitudes $a(t)$ whose time evolution should be described by a specific differential equation.

For example, in order to describe the honeycomb lattice shown in Fig. 11a, we have to prescribe different amplitudes to the "top" and "bottom" points of its primitive cell - say, $\alpha$ and $\beta$, correspondingly. Since each of these points is surrounded (and hence weakly interacts) with 3 neighbors of the opposite type, instead of Eq. (117) we have to write two equations

$$
\begin{equation*}
i \hbar \frac{d \alpha}{d t}=-\delta_{n} \sum_{j=1}^{3} \beta_{j}, \quad i \hbar \frac{d \beta}{d t}=-\delta_{n} \sum_{j^{\prime}=1}^{3} \alpha_{j^{\prime}} \tag{3.119}
\end{equation*}
$$

where each summation is over 3 next-neighbor points. (I am using different summation indices just to emphasize that these directions are different for the "top" and "bottom" points of the primitive cell - see Fig. 11a.) Now using the Bloch theorem (107) in the form similar to Eq. (2.205), we get two coupled systems of linear algebraic equations:

$$
\begin{equation*}
\left(E-E_{n}\right) \alpha=-\delta_{n} \beta \sum_{j=1}^{3} e^{i \mathbf{q} \cdot \mathbf{r}_{j}}, \quad\left(E-E_{n}\right) \beta=-\delta_{n} \alpha \sum_{j^{\prime}=1}^{3} e^{i \mathbf{q} \cdot \mathbf{r}_{j^{\prime}}^{\prime}}, \tag{3.120}
\end{equation*}
$$

where $\mathbf{r}_{j}$ and $\mathbf{r}^{\prime}{ }_{j}$, are the next-neighbor positions, as seen from the top and bottom points, respectively. Writing the condition of consistency of this system, we get two equal and opposite values for energy correction for each value of $\mathbf{q}$ :

$$
\begin{equation*}
E_{ \pm}=E_{n} \pm \delta_{n} \Sigma^{1 / 2}, \quad \text { where } \Sigma \equiv \sum_{j, j^{\prime}=1}^{3} e^{i \mathbf{q} \cdot\left(\mathbf{r}_{j}+\mathbf{r}_{j^{\prime}}^{\prime}\right)} \tag{3.121}
\end{equation*}
$$

According to Eq. (120), these two energy bands correspond to the phase shifts (on the top of the regular Bloch shift $\mathbf{q} \cdot \Delta \mathbf{r}$ ) of either 0 or $\pi$ between the adjacent quasi-localized wavefunctions $u(\mathbf{r})$.

The most interesting corollary of such energy symmetry, augmented by the honeycomb lattice symmetry, is that for certain values $\mathbf{q}_{\mathrm{D}}$ of vector $\mathbf{q}$ (that turn out to be in each of 6 corners of the honeycomb-shaped $1^{\text {st }}$ Brillouin zone), the double sum $\Sigma$ vanishes, i.e. the two band surfaces $E_{ \pm}(\mathbf{q})$ touch each other. As a result, in vicinities of these Dirac points ${ }^{45}$ the dispersion relation is linear:

$$
\begin{equation*}
\left.E_{ \pm}\right|_{\mathbf{q} \approx \mathbf{q}_{\mathrm{D}}} \approx E_{n} \pm \hbar v_{n}|\widetilde{\mathbf{q}}|, \quad \text { where } \widetilde{\mathbf{q}} \equiv \mathbf{q}-\mathbf{q}_{\mathrm{D}} \tag{3.122}
\end{equation*}
$$

with $v_{n} \propto \delta_{n}$ being a constant with the dimension of velocity (for graphene, close to $10^{6} \mathrm{~m} / \mathrm{s}$ ). Such a linear dispersion relation ensures several interesting transport properties of graphene. For their discussion, I have to refer the reader to special literature. ${ }^{46}$

### 3.5. Axially-symmetric systems

I cannot conclude this chapter (and hence our review of wave mechanics) without addressing the issue of eigenstates and eigenvalues at full confinement in multi-dimensional potentials $U(\mathbf{r})$. For an arbitrary potential, the stationary Schrödinger equation does not have an analytical solution, but a substantial symmetry of function $U(\mathbf{r})$ may make such solution possible. This pertains, in particular, to the axial symmetry in 2D problems and the spherical symmetry in 3D problems, which are typical for several important situations (or their reasonable models), especially in atomic and nuclear physics.

In rare cases such symmetry may be exploited by the separation of variables in Cartesian coordinates. The most famous example is the $d$-dimensional harmonic oscillator, i.e. a particle moving inside the potential

$$
\begin{equation*}
U=\frac{m \omega_{0}^{2}}{2} \sum_{j=1}^{d} r_{j}^{2} . \tag{3.123}
\end{equation*}
$$

Separating the variables exactly as we did for the rectangular quantum well (see Sec. 1.5), for each degree of freedom we get the Schrödinger equation (2.268) of a 1D oscillator, whose eigenfunctions are given by Eq. (2.278), and the energy spectrum is described by Eq. (2.114). As a result, the total energy spectrum may be indexed by a vector $\mathbf{n}=\left\{n_{1}, n_{2}, \ldots, n_{d}\right\}$ of $d$ independent integers (quantum numbers):

$$
\begin{equation*}
E_{\mathbf{n}}=\hbar \omega_{0}\left(\sum_{j=1}^{d} n_{j}+\frac{d}{2}\right), \tag{3.124}
\end{equation*}
$$

[^556]all of them ranging from 0 to $\infty$. Note that every energy level of this system, with the only exception of the ground state,
\[

$$
\begin{equation*}
\psi_{g}=\prod_{j=1}^{d} \psi_{0}\left(r_{j}\right)=\frac{1}{\pi^{d / 4} x_{0}^{d / 2}} \exp \left\{-\frac{1}{2 x_{0}^{2}} \sum_{j=1}^{d} r_{j}^{2}\right\}, \tag{3.125}
\end{equation*}
$$

\]

is degenerate: several different wavefunctions, each with its own different set of quantum numbers $n_{j}$, but the same value of their sum, have the same energy.

However, the harmonic oscillator problem is an exception: for other central- and sphericallysymmetric problems the solution is made easier by using more appropriate coordinates. Let us start with the simplest axially-symmetric problem: the so-called planar rigid rotator (or "rotor"), i.e. a particle constrained (confined) to move along a plane, round circle of radius $R$ (Fig. 15). ${ }^{47}$


Fig. 3.16. Planar rigid rotator.

The planar rotator has just one degree of freedom, say the displacement arc $l=R \varphi$. So, its classical energy (and Hamiltonian function) is $H=p_{l}^{2} / 2 m, p_{l} \equiv m v=m(d l / d t)$. This function is similar to that of a free 1D particle (with the replacement $x \rightarrow l$ ), and hence rotator's quantum properties may be described by a similar Hamiltonian operator:

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}, \quad \text { with } \quad \hat{p}=-i \hbar \frac{\partial}{\partial l} \tag{3.126}
\end{equation*}
$$

and its eigenfunctions have a similar structure:

$$
\begin{equation*}
\psi=C e^{i k l} \tag{3.127}
\end{equation*}
$$

The "only" new feature is that in the rotator, all observables should be $2 \pi R$-periodic functions of $l$, and hence, as we have already discussed in the context of the magnetic flux quantization (see Fig. 4 and its discussion), as the particle makes one turn about the center, its wavefunction's phase $k l$ may only change by $2 \pi n$, with an arbitrary integer $n$ (from $-\infty$ to $+\infty$ ),:

$$
\begin{equation*}
\psi_{n}(l+2 \pi R)=\psi_{n}(l) e^{2 \pi i n} . \tag{3.128}
\end{equation*}
$$

With eigenfunctions (127), this immediately gives condition gives $k 2 \pi R=2 \pi n$. Thus, wavenumber $k$ can take only quantized values $k_{n}=n / R$, so that the eigenfunctions should be indexed by $n$ :

$$
\begin{equation*}
\psi_{n}=C_{n} \exp \left\{i n \frac{l}{R}\right\} \tag{3.129}
\end{equation*}
$$

[^557]and the energy spectrum is discrete:
\[

$$
\begin{equation*}
E_{n}=\frac{p_{n}^{2}}{2 m}=\frac{\hbar^{2} k_{n}^{2}}{2 m}=\frac{\hbar^{2} n^{2}}{2 m R^{2}} . \tag{3.130}
\end{equation*}
$$

\]

So, while the free translation motion of a quantum particle is continuous, in the sense that its momentum has a continuous spectrum, its rotation is quantized - the most important fact, which has so many implications (including the existence of atoms, molecules, and hence us humans, and hence science including this course :-).

This simple model allows an exact analysis of external magnetic field effects on a quantumconfined motion of an electrically charged particle. Indeed, if this field is uniform and directed perpendicular to rotator's plane, it does not violate the axial symmetry of the system. According to Eq. (26), in this case we have to generalize Eq. (126) as

$$
\hat{H}=\frac{1}{2 m}\left(-i \hbar \mathbf{n}_{\varphi} \frac{\partial}{\partial l}-q \mathbf{A}\right)^{2} .
$$

Here, in contrast to the gauge choice (44), which was so instrumental in the Landau level problem, it is now clearly beneficial to take the vector-potential in a manifestly axially-symmetric form $\mathbf{A}=A(\rho) \mathbf{n}_{\varphi}$, where $\rho \equiv\{x, y\}$ is the 2D radius-vector. Using the well-known expression for curl in cylindrical coordinates, ${ }^{48}$ we can readily check that the requirement $\nabla \times \mathbf{A}=\mathcal{B}_{z}$, with $\mathcal{B}=$ const, is satisfied by the following function:

$$
\begin{equation*}
\mathbf{A}=\mathbf{n}_{\varphi} \frac{B \rho}{2} . \tag{3.132}
\end{equation*}
$$

For the planar rotator, $\rho=R=$ const, so that the stationary Schrödinger equation becomes

$$
\begin{equation*}
\frac{1}{2 m}\left(-i \hbar \frac{\partial}{\partial l}-q \frac{B R}{2}\right)^{2} \psi_{n}=E_{n} \psi_{n} . \tag{3.133}
\end{equation*}
$$

A little bit surprisingly, this equation is still satisfied with the sine-wave eigenfunctions (127). Moreover, since the periodicity condition (128) is also unaffected by the applied magnetic field, we return to field-independent eigenfunctions (129). However, the field does affect the system's energy:

$$
\begin{equation*}
E_{n}=\frac{1}{2 m}\left(\frac{\hbar n}{R}-q \frac{B R}{2}\right)^{2}=\frac{\hbar^{2}}{2 m R^{2}}\left(n-\frac{\Phi}{\Phi_{0}^{\prime}}\right)^{2} \tag{3.134}
\end{equation*}
$$

where $\Phi \equiv \pi R^{2} \mathcal{B}$ is the magnetic flux through the area limited by the particle's trajectory, and $\Phi_{0}{ }^{\prime} \equiv$ $2 \pi \hbar / q$ is the "normal" magnetic flux quantum we have already met in the AB effect context - see Eq. (34) and its discussion. The field also changes the electric current of the particle in $n$-th state:

$$
\begin{equation*}
I_{n}=q \frac{\hbar}{2 i m}\left[\psi_{n}^{*}\left(\frac{\partial}{\partial l}-\frac{i q R \mathcal{B}}{2 \hbar}\right) \psi_{n}-\text { c.c. }\right]=q \frac{\hbar}{m R}\left|C_{n}\right|^{2}\left(n-\frac{\Phi}{\Phi_{0}{ }^{\prime}}\right) . \tag{3.135}
\end{equation*}
$$

Normalizing wavefunction (129) to have $W_{n}=1$, we get $\left|C_{n}\right|^{2}=1 / 2 \pi R$, so that Eq. (135) becomes

[^558]\[

$$
\begin{equation*}
I_{n}=I_{0}\left(n-\frac{\Phi}{\Phi_{0}^{\prime}}\right), \quad \text { with } I_{0} \equiv \frac{\hbar q}{2 \pi m R^{2}} \tag{3.136}
\end{equation*}
$$

\]

Functions $E_{n}(\Phi)$ and $I_{n}(\Phi)$ are shown in Fig. 17. Note that since $\Phi_{0}{ }^{\prime} \propto 1 / q$, for any sign of the particle's charge, $d I_{n} / d \Phi<0$. It is easy to check that this means that the current is diamagnetic, ${ }^{49}$ i.e. corresponds to the Lenz rule of the Faraday's electromagnetic induction: the field-induced current flows in such direction that its own magnetic field tries to compensate the external magnetic flux applied to the loop.


Fig. 3.17. Effect of magnetic field on a charged planar rotator. Dashed lines show possible inelastic transitions between metastable and ground states, due to weak interaction with environment, as the magnetic field is being increased.

This result may be interpreted as a different implementation of the AB effect. ${ }^{50}$ In contrast to the two-slit interference experiment that was discussed in Sec. 1, in the situation shown in Fig. 17 the particle is not absorbed by the detector, but travels around the ring continuously. As a result, its wavefunction is rigid: due to the boundary condition (128), the topological quantum number $n$ is discrete, and magnetic field cannot change the wavefunction gradually. In this sense, the system is similar to a superconducting loop - see Fig. 4 and its discussion. The difference between these systems is two-fold:
(i) For a single charged particle, in a macroscopic systems with practicable values of $q, R$, and $m$, the current scale $I_{0}$ is very small. For example, for $m=m_{e}, q=-e$, and $R=1 \mu \mathrm{~m}$, Eq. (136) yields $I_{0} \approx 3$ pA. ${ }^{51}$ The contribution $L I \sim \mu_{0} R I_{0} \sim 10^{-24} \mathrm{~Wb}$ of the current so small into the net magnetic flux is

[^559]negligible in comparison with $\Phi_{0}{ }^{\prime} \sim 10^{-15} \mathrm{~Wb}$, so that the quantization of $n$ does not lead to the magnetic flux quantization.
(ii) As soon as the magnetic field raises the eigenstate energy $E_{n}$ above that of another eigenstate $E_{n}$, the former state becomes metastable, and weak interactions of the system with its environment (which are neglected in our simple model) may induce a quantum transition of the system to the lowerenergy state, thus reducing the diamagnetic current's magnitude - see the dashed lines in Fig. 17. The flux quantization in superconductors is much more robust to such perturbations. ${ }^{52}$

Now let us return, for one more time, to Eq. (129), and see what do they give for one more observable, particle's angular momentum

$$
\begin{equation*}
\mathbf{L} \equiv \mathbf{r} \times \mathbf{p} \tag{3.137}
\end{equation*}
$$

In our current problem, vector $\mathbf{L}$ has just one component perpendicular to the rotator plane,

$$
\begin{equation*}
L_{z}=R p . \tag{3.138}
\end{equation*}
$$

In classical mechanics, $L_{z}$ of the rotator should be conserved (due to the absence of external torque), but can take arbitrary values. In quantum mechanics the situation changes: with $p=\hbar k$, our result $k_{n}=n / R$ may be rewritten as

$$
\begin{equation*}
L_{z}=\left(L_{z}\right)_{n}=R \hbar k_{n}=\hbar n \tag{3.139}
\end{equation*}
$$

Thus, the angular momentum is quantized: it may be only a multiple of the Planck constant $\hbar-$ confirming Bohr's guess - see Eq. (1.10). As we will see in Chapter 5, this result is very general (though may be modified by spin effects) and that wavefunctions (129) may be interpreted as eigenfunctions of the angular momentum operator.

In order to implement the planar rotator in our 3D world, we needed to provide rigid confinement of the particle both in the motion plane, and along radius $\rho$. Let us proceed to the more general problem when only the former confinement is strict, i.e. to a 2 D particle moving in an arbitrary centrally-symmetric potential

$$
\begin{equation*}
U(\boldsymbol{p})=U(\rho) \tag{3.140}
\end{equation*}
$$

Using the well-known expression for the 2D Laplace operator in polar coordinates, ${ }^{53}$ we may present the 2D stationary Schrödinger equation in the form

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left[\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2}}{\partial \varphi^{2}}\right] \psi+U(\rho) \psi=E \psi . \tag{3.141}
\end{equation*}
$$

Separating the radial and angular variables as ${ }^{54}$
dephasing effects of electron scattering by phonons and other electrons, the effect's observation requires submicron samples and millikelvin temperatures.
${ }^{52}$ Interrupting a superconducting ring with a weak link (Josephson junction), i.e. forming a SQUID, we may get the switching behavior similar to that shown with dashed arrows in Fig. 17 - see, e.g., EM Sec. 6.3.
${ }^{53}$ See, e.g., MA Eq. (10.3) with $\partial / \partial z=0$.
${ }^{54}$ At this stage, I do not want to mark the particular solution (eigenfunction) $\psi$ and corresponding eigenenergy $E$ by any index, because we already may suspect that in a 2 D problem the role of this index will be played by two integers - two quantum numbers.

$$
\begin{equation*}
\psi=R(\rho) F(\varphi), \tag{3.142}
\end{equation*}
$$

we get，after the division by $\psi$ and multiplication by $\rho^{2}$ ，the following equation：

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left[\frac{\rho}{R} \frac{d}{d \rho}\left(\rho \frac{d R}{d \rho}\right)+\frac{1}{F} \frac{d^{2} F}{d \varphi^{2}}\right]+\rho^{2} U(\rho)=\rho^{2} E . \tag{3.143}
\end{equation*}
$$

It is clear that the fraction $\left(d^{2} F / d \varphi^{2}\right) / F$ should be a constant（because all other terms of the equation may be only functions of $\rho$ alone），so that we get for function $F(\varphi)$ an ordinary differential equation，

$$
\begin{equation*}
\frac{d^{2} F}{d \varphi^{2}}+v^{2} F=0, \tag{3.144}
\end{equation*}
$$

where $v^{2}$ is the variable separation constant．The fundamental solution of Eq．（144）is evidently $F \propto$ $\exp \{ \pm i v \varphi\}$ ．Now requiring，as we did for the planar rotator，the $2 \pi$ periodicity of any observable，i．e．

$$
\begin{equation*}
F(\varphi+2 \pi)=F(\varphi) e^{2 \pi i n} \tag{3.145}
\end{equation*}
$$

so that constant $v$ has to be integer（say，$n$ ），and we can write：${ }^{55}$

$$
\begin{equation*}
F_{n}=C_{n} e^{i n \varphi}, \tag{3.146}
\end{equation*}
$$

Plugging the resulting relation $\left(d^{2} F / d \varphi^{2}\right) / F=-n^{2}$ into Eq．（143），we may rewrite is as

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m}\left[\frac{1}{\rho 尺} \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right)-\frac{n^{2}}{\rho^{2}}\right]+U(\rho)=E . \tag{3.147}
\end{equation*}
$$

The physical interpretation of this equation is that the full energy is a sum，

$$
\begin{equation*}
E=E_{\rho}+E_{\varphi}, \tag{3.148}
\end{equation*}
$$

of the radial－motion part

$$
\begin{equation*}
E_{\rho}=-\frac{\hbar^{2}}{2 m} \frac{1}{\rho} \frac{d}{d \rho}\left(\rho \frac{d 尺}{d \rho}\right)+U(\rho) \tag{3.149}
\end{equation*}
$$

and the angular－motion part

$$
\begin{equation*}
E_{\varphi}=\frac{\hbar^{2} n^{2}}{2 m \rho^{2}} . \tag{3.150}
\end{equation*}
$$

Now let us notice that a similar separation exists in classical mechanics，${ }^{56}$ because the total energy of a particle moving in a central field may be presented，within the plane of motion，as

$$
\begin{equation*}
E=\frac{m}{2} v^{2}+U(\rho)=\frac{m}{2}\left(\dot{\rho}^{2}+\rho^{2} \dot{\varphi}^{2}\right)+U(\rho)=E_{\rho}+E_{\varphi} \tag{3.151}
\end{equation*}
$$

where

[^560]\[

$$
\begin{equation*}
E_{\rho} \equiv \frac{p_{\rho}^{2}}{2 m}+U(\rho), \quad E_{\varphi} \equiv \frac{L_{z}^{2}}{2 m \rho^{2}} . \tag{3.152}
\end{equation*}
$$

\]

The comparison of the latter relation with Eqs. (139) and (150) gives us grounds to suspect that the quantization rule $L_{z}=n \hbar$ may be valid for this problem as well, and may be in other cases as well. In Sec. 5.6 , we will see that this is indeed the case.

Returning to Eq. (147), on the basis of our experience with 1D wave mechanics we may expect that this ordinary, linear, second-order differential equation should have (for a motion confined to a certain final region of its argument $\rho$ ), for any fixed $n$, a discrete energy spectrum described by some other integer quantum number (say, $l$ ). This means that eigenfunctions (142), and corresponding eigenenergies (148) should be indexed by two quantum numbers. Note, however, that since the radial function obeys equation (147), which already depends on $n$, function X $\rho$ ) should carry both indices, so the variable separation is not so "clean" as it was for the rectangular quantum well. Normalizing the angular function to the full circle, $\Delta \varphi=2 \pi$, we may rewrite Eq. (142) as

$$
\begin{equation*}
\psi_{n, l}=R_{n, l}(\rho) F_{n}(\varphi)=\frac{1}{(2 \pi) 1 / 2} R_{n, l}(\rho) e^{i n \varphi} . \tag{3.153}
\end{equation*}
$$

A good (and important) example of a solvable problem of this type is a free 2D particle whose motion is rigidly confined to a disk of radius $R$ :

$$
U(\rho)=\left\{\begin{array}{l}
0, \quad \text { for } 0 \leq \rho<R  \tag{3.154}\\
+\infty, \quad \text { for } R<\rho
\end{array}\right.
$$

In this case, the solutions $\mathbb{R}_{n, l}(\rho)$ of Eq. (147) are proportional to the first-order Bessel functions $J_{n}\left(k_{l} \rho\right),{ }^{57}$ and the spectrum of possible values of parameter $k_{l}$ should found the boundary condition $R_{n, l}(R)=0$. Let me leave the detailed solution and analysis of this problem for reader's exercise.

### 3.6. Spherically-symmetric systems: Brute force approach

Now let us address the (mathematically more involved) case of 3D motion, with sphericallysymmetric potential

$$
\begin{equation*}
U(\mathbf{r})=U(r) . \tag{3.155}
\end{equation*}
$$

Let me start, again, with a rigid rotator - now a spherical rotator, i.e. a particle confined to move on the surface of a sphere of radius $R$. It has 2 degrees of freedom, because any position on the spherical surface is completely described by two coordinates - say, the polar angle $\theta$ and the azimuthal angle $\varphi$. In this case, the kinetic energy we need to consider is limited to its angular part, so that in the Laplace operator in spherical coordinates ${ }^{58}$ we may keep only those parts, with fixed $r=R$. Then the stationary Schrödinger equation becomes

[^561]\[

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m R^{2}}\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial}{\partial \theta}\right)+\frac{1}{\sin ^{2} \theta} \frac{\partial^{2}}{\partial \varphi^{2}}\right] \psi=E \psi \tag{3.156}
\end{equation*}
$$

\]

(Again, I abstain from attaching any indices to $\psi$ and $E$ for the time being.) With the usual variable separation assumption,

$$
\begin{equation*}
\psi=\Theta(\theta) F(\varphi) \tag{3.157}
\end{equation*}
$$

Eq. (156), with all terms multiplied by $\sin ^{2} \theta / \Theta F$, yields

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m R^{2}}\left[\frac{\sin \theta}{\Theta} \frac{d}{d \theta}\left(\sin \theta \frac{d \Theta}{d \theta}\right)+\frac{1}{F} \frac{d^{2} F}{d^{2} \varphi}\right]=E \sin ^{2} \theta \tag{3.158}
\end{equation*}
$$

Just as in Eq. (143), fraction $\left(d^{2} F / d x^{2}\right) / F$ may be a function of $\varphi$ only, and hence has to be constant, giving for it an equation similar to Eq. (144). So, the azimuthal functions are just the sine waves (146) again, and we can use the same periodicity condition (145) to write them in the normalized form ${ }^{59}$

$$
\begin{equation*}
F_{m}(\varphi)=\frac{1}{(2 \pi)^{1 / 2}} e^{i m \varphi} \tag{3.159}
\end{equation*}
$$

With that, fraction $\left(d^{2} F / d \varphi^{2}\right) / F$ equals $\left(-m^{2}\right)$, and Eq. (158), after multiplication by $\Theta / \sin ^{2} \theta$, is reduced to the following ordinary, linear differential equation for function $\Theta(\theta)$ :

$$
\begin{equation*}
-\frac{1}{\sin \theta} \frac{d}{d \theta}\left(\sin \theta \frac{d \Theta}{d \theta}\right)+\frac{m^{2}}{\sin ^{2} \theta} \Theta=\varepsilon \Theta, \quad \text { with } \quad \varepsilon \equiv E /\left(\frac{\hbar^{2}}{2 m R^{2}}\right), \tag{3.160}
\end{equation*}
$$

It is convenient to recast it into an equation for a new variable $P(\xi) \equiv \Theta(\theta)$, with $\xi \equiv \cos \theta$ :

$$
\begin{equation*}
\frac{d}{d \xi}\left[\left(1-\xi^{2}\right) \frac{d P}{d \xi}\right]+\left[l(l+1)-\frac{m^{2}}{1-\xi^{2}}\right] P=0 \tag{3.161}
\end{equation*}
$$

where a new notation for the normalized energy is introduced: $l(l+1) \equiv \varepsilon$. The motivation for such notation is that, according to a mathematical analysis, ${ }^{60}$ Eq. (161) with integer $m$, has solutions only if parameter $l$ is integer: $l=0,1,2, \ldots$, and only if that integer is not smaller than $|m|$, i.e. if

$$
\begin{equation*}
-l \leq m \leq+l . \tag{3.162}
\end{equation*}
$$

This immediately gives the following energy spectrum of the spherical rotator:

$$
\begin{equation*}
E_{l}=\frac{\hbar^{2} l(l+1)}{2 m R^{2}} \tag{3.163}
\end{equation*}
$$

[^562]so that the only effect of the magnetic quantum number $m$ here is imposing the restriction (162) on the orbital quantum number $l$. This means, in particular, that each of energy level (163) corresponds to ( $2 l+$ 1) different values of $m$, i.e. is $(2 l+1)$-degenerate.

To understand the physics of this degeneracy, we need to explore the corresponding eigenfunctions of Eq. (161). They are naturally numbered by two integers, $m$ and $l$, and are called the associated Legendre functions $P_{l}^{m}$. For the particular, simplest case $m=0$, these functions are just (Legendre) polynomials $P_{l}(\xi) \equiv P_{1}^{0}(\xi)$, which may be either defined as the solutions of the Legendre equation following from Eq. (161) at $m=0$ :

Legendre equation

$$
\begin{equation*}
\frac{d}{d \xi}\left[\left(1-\xi^{2}\right) \frac{d}{d \xi} P\right]+l(l+1) P=0 \tag{3.164}
\end{equation*}
$$

or calculated explicitly from the following Rodrigues formula: ${ }^{61}$

Rodrigues formula for Legendre polynomials

$$
\begin{equation*}
P_{l}(\xi)=\frac{1}{2^{l} l!} \frac{d^{l}}{d \xi^{l}}\left(\xi^{2}-1\right)^{l}, \quad l=0,1,2, \ldots \tag{3.165}
\end{equation*}
$$

Using this formula, it easy to spell out a few lowest Legendre polynomials:

$$
\begin{equation*}
P_{0}(\xi)=1, \quad P_{1}(\xi)=\xi, \quad P_{2}(\xi)=\frac{1}{2}\left(3 \xi^{2}-1\right), \quad P_{3}(\xi)=\frac{1}{2}\left(5 \xi^{3}-3 \xi\right), \ldots \tag{3.166}
\end{equation*}
$$

though such expressions become more and more bulky as $l$ is increased. As Fig. 18 shows, as argument $\xi$ is decreased, all these functions start in one point, $P_{l}(+1)=+1$, and end up either in the same point or in the opposite point: $P_{l}(-1)=(-1)^{l}$. On the way between these two end points, the $l^{\text {th }}$ polynomial crosses the horizontal axis exactly $l$ times, i.e. has $l$ roots. ${ }^{62}$ It may be shown that on the segment $[-1,+1]$, the Lagrange polynomials form a full orthogonal set of functions, with the following normalization rule:

$$
\begin{equation*}
\int_{-1}^{+1} P_{l}(\xi) P_{l^{\prime}}(\xi) d \xi=\frac{2}{2 l+1} \delta_{l l^{\prime}} . \tag{3.167}
\end{equation*}
$$



Fig. 3.18. A few lowest Legendre polynomials.

[^563]For $m>0$, the associated Legendre functions may be expressed via the Legendre polynomials (165) using the following formula, which reminds Eq. (165):

$$
\begin{equation*}
P_{l}^{m}(\xi)=(-1)^{m}\left(1-\xi^{2}\right)^{m / 2} \frac{d^{m}}{d \xi^{m}} P_{l}(\xi), \tag{3.168}
\end{equation*}
$$

while if the index $m$ is negative, the following simple relation may be used:

$$
\begin{equation*}
P_{l}^{-m}(\xi)=(-1)^{m} \frac{(l-m)!}{(l+m)!} P_{l}^{m}(\xi) \tag{3.169}
\end{equation*}
$$

On the segment $\xi=[-1,+1]$, each set of the associated Legendre functions with fixed index $m$ forms a full orthogonal set, with the normalization relation,

$$
\begin{equation*}
\int_{-1}^{+1} P_{l}^{m}(\xi) P_{l^{\prime}}^{m}(\xi) d \xi=\frac{2}{2 l+1} \frac{(l+m)!}{(l-m)!} \delta_{l l^{\prime}} \tag{3.170}
\end{equation*}
$$

which is evidently a generalization of Eq. (167) for arbitrary $m$.
Since the difference between angles $\theta$ and $\varphi$ is to some extent artificial (caused by the arbitrary direction of the polar axis), physicists prefer to use not the functions $\Theta(\theta) \propto P_{l}^{m}(\cos \theta)$ and $F_{m}(\varphi) \propto$ $\exp \{i m \varphi\}$ separately, but their products (157), which are called spherical harmonics:

$$
\begin{equation*}
Y_{l}^{m}(\theta, \varphi) \equiv\left[\frac{(2 l+1)}{4 \pi} \frac{(l-m)!}{(l+m)!}\right]^{1 / 2} P_{l}^{m}(\cos \theta) e^{i m \varphi} \tag{3.171}
\end{equation*}
$$

The specific coefficient in Eq. (171) is chosen in a way to simplify the following two relations: the equation for negative $m$,

$$
\begin{equation*}
Y_{l}^{-m}(\theta, \varphi)=(-1)^{m}\left[Y_{l}^{m}(\theta, \varphi)\right]^{*}, \tag{3.172}
\end{equation*}
$$

and the normalization relation

$$
\begin{equation*}
\oint Y_{l}^{m}(\theta, \varphi)\left[Y_{l^{\prime}}^{m^{\prime}}(\theta, \varphi)\right]^{*} d \Omega=\delta_{l l} \delta_{m m^{\prime}}, \tag{3.173}
\end{equation*}
$$

with integration over the whole solid angle $4 \pi$. The last relation shows that the spherical harmonics form an orthonormal set of functions. This set is also full, so that any function defined on a sphere may be uniquely presented as a linear combination of $Y_{l}^{m}$.

Despite a somewhat intimidating formulas given above, they yield rather simple expressions for the lowest spherical harmonics:

$$
\begin{align*}
& l=0: \quad Y_{0}^{0}=(1 / 4 \pi)^{1 / 2}  \tag{3.174}\\
& l=1: \quad\left\{\begin{array}{l}
Y_{1}^{1}=-(3 / 8 \pi)^{1 / 2} \sin \theta e^{i \varphi} \\
Y_{1}^{0}=(3 / 4 \pi)^{1 / 2} \cos \theta \\
Y_{1}^{-1}=+(3 / 8 \pi)^{1 / 2} \sin \theta e^{-i \varphi}
\end{array}\right. \tag{3.175}
\end{align*}
$$

$$
l=2:\left\{\begin{array}{l}
Y_{2}^{2}=+(15 / 32 \pi)^{1 / 2} \sin ^{2} \theta e^{2 i \varphi}  \tag{3.176}\\
Y_{2}^{1}=-(15 / 8 \pi)^{1 / 2} \sin \theta \cos \theta e^{i \varphi}, \\
Y_{2}^{0}=(3 / 16 \pi)^{1 / 2}\left(3 \cos ^{2} \theta-1\right) \\
Y_{2}^{-1}=+(15 / 8 \pi)^{1 / 2} \sin \theta \cos \theta e^{-i \varphi} \\
Y_{2}^{-2}=-(15 / 32 \pi)^{1 / 2} \sin ^{2} \theta e^{-2 i \varphi}
\end{array}\right.
$$

It is important to understand the symmetry of these functions. Since spherical functions with $m \neq$ 0 are complex, the most popular way of their graphical representation is first to form their real combinations corresponding to two opposite values of $m,{ }^{63}$

$$
Y_{l m} \equiv \frac{1}{\sqrt{2}}\left[Y_{l}^{|m|}+\operatorname{sgn}(m)(-1)^{m} Y_{l}^{-|m|}\right] \propto \begin{cases}\cos m \varphi, & \text { for } m>0,  \tag{3.177}\\ \sin m \varphi, & \text { for } m<0,\end{cases}
$$

(for $m=0, Y_{l 0} \equiv Y_{l}^{0}$ ), and then plot the magnitude of these combinations in spherical coordinates as the distance from the origin, while using two colors to show their sign - see Fig. 19.


[^564]Let us starting from the simplest case $l=0$. According to Eq. (162), there could be only one such $s$ state, ${ }^{64}$ with $m=0$. The spherical harmonic corresponding to that state is just a constant, so that the wavefunction is uniformly distributed over the sphere. Since the functions does not have gradient in any direction, the kinetic energy (163) of the particle equals is zero.

For $l=1$, there could be 3 different $p$ states, with $m=-1,0$, and +1 . As the second row in Fig. 19 shows, these states are essentially identical in structure, and are just differently oriented in space, thus explaining the 3 -fold degeneracy of the kinetic energy - see Eq. (163). This is not quite true for 5 different $d$ states $(l=2)$, shown in the bottom row of Fig. 19, as well as states with higher $l$ : despite their equal energies, they differ not only by their special orientation. The states with $m=0$ have gradient only in the $\theta$ direction, while the states with the ultimate values of $m(m= \pm l)$ change only gradually (as $\left.\sin ^{l} \theta\right)$ in the polar direction, while oscillating in the azimuthal direction. The states with intermediate values of $m$ provide a crossover between these two extremes, oscillating in both directions, stronger and stronger in the direction of $\varphi$ as $|m|$ is increased. Still, the magnetic quantum number, surprisingly, does not affect the energy for any $l$. Another surprising feature of the spherical harmonics follows from the comparison of Eq. (163) with the second of classical relations (152). These expressions coincide if we interpret constant

$$
\begin{equation*}
L^{2} \equiv \hbar^{2} l(l+1), \tag{3.178}
\end{equation*}
$$

as the value of the full angular momentum squared $L^{2}=|\mathbf{L}|^{2}$ (including its both $\theta$ and $\varphi$ components) in the eigenstate with eigenfunction $Y_{l}^{m}$. On the other hand, the structure of the azimuthal component $F(\varphi)$ of the wavefunction is exactly the same as in 2D axially-symmetric problems, suggesting that Eq. (139) still gives correct values (in our new notation, $L_{z}=m \hbar$ ) for the $z$-component of the angular momentum. If this is so, why for any state with $l>0,\left(L_{z}\right)^{2}=m^{2} \hbar^{2} \leq l^{2} \hbar^{2}$ is less than $L^{2}=l(l+1) \hbar^{2}$ ? In other words, what prevents the angular momentum vector to be fully aligned with axis $z$ ?

Besides that issue, though the above analysis of the spherical rotator is formally (mathematically) complete, it is as unsatisfactory on the physics level as the harmonic oscillator analysis in Sec. 2.6. In particular, it does not explain the meaning of the extremely simple relations for eigenvalues of energy and angular momentum on the backdrop of rather complicated wavefunctions.

We will obtain natural answers to all these questions and concerns in Sec. 5.6, but now let us complete our survey of wave mechanics by extending it to 3D motion in an arbitrary sphericallysymmetric potential (155). In this case we have to use the full form of the Laplace operator in spherical coordinates. The variable separation procedure is an evident generalization of what we have done before, with the particular solution

$$
\begin{equation*}
\psi=R(\rho) \Theta(\theta) F(\varphi), \tag{3.179}
\end{equation*}
$$

whose substitution into the stationary Schrödinger equation yields

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m r^{2}}\left[\frac{1}{尺} \frac{d}{d r}\left(r^{2} \frac{d 尺}{d r}\right)+\frac{1}{\Theta} \frac{1}{\sin \theta} \frac{d}{d \theta}\left(\sin \theta \frac{d \Theta}{d \theta}\right)+\frac{1}{\sin ^{2} \theta} \frac{1}{F} \frac{d^{2} F}{d \varphi^{2}}\right]+U(r)=E . \tag{3.180}
\end{equation*}
$$

[^565]It is evident that the angular part（the two last terms in square brackets）separates from the radial part，and for the former part we get Eq．（156）again，with the only change，$R \rightarrow r$ ．This change does not affect the fact that the eigenfunctions of that equation are the spherical harmonics（171），and the angular eigenenergy is given by Eq．（163），again with the replacement $R \rightarrow r$ ．This means that for the radial function，Eq．（180）gives the following equation，

$$
\begin{equation*}
-\frac{\hbar^{2}}{2 m r^{2}}\left[\frac{1}{尺} \frac{d}{d r}\left(r^{2} \frac{d 尺}{d r}\right)-l(l+1)\right]+U(r)=E . \tag{3.181}
\end{equation*}
$$

Note that no information about the magnetic quantum number $m$ has not crept into the radial equation （besides establishing the limitation（162）for possible values of $l$ ），so that this equation depends only on the latter quantum number．

The radial equation becomes rather simple for $U(r)=0$ ，and may be used，for example，to solve the eigenproblem for the free 3D motion of a particle inside the sphere of radius $R$ ．Leaving that problem for the reader＇s exercise，I will proceed to the most important Bohr atom problem，i．e．of motion in the so－called attractive Coulomb potential ${ }^{65}$

Attractive Coulomb potential

$$
\begin{equation*}
U(r)=-\frac{C}{r}, \quad \text { with } C>0 \tag{3.182}
\end{equation*}
$$

The natural scales of $r$ and $E$ are，respectively，${ }^{66}$

$$
\begin{equation*}
r_{0} \equiv \frac{\hbar^{2}}{m C} \quad \text { and } E_{0} \equiv \frac{\hbar^{2}}{m r_{0}^{2}} \equiv m\left(\frac{C}{\hbar}\right)^{2} \tag{3.183}
\end{equation*}
$$

In the normalized units $\varepsilon \equiv E / E_{0}$ and $\xi \equiv r / r_{0}$ ，Eq．（181）looks simpler，

$$
\begin{equation*}
\frac{d^{2} 尺}{d \xi^{2}}+\frac{2}{\xi} \frac{d 尺}{d \xi}-l(l+1) R+2\left(\varepsilon+\frac{1}{\xi}\right) 尺=0 \tag{3.184}
\end{equation*}
$$

but unfortunately its eigenfunctions may be called elementary only in the most generous meaning of the word．With the adequate normalization，

$$
\begin{equation*}
\int_{0}^{\infty} \mathbb{R}_{n, l} \mathbb{R}_{n^{\prime}, l} r^{2} d r=\delta_{n n^{\prime}}, \tag{3.185}
\end{equation*}
$$

these（mutually orthogonal）functions may be presented as

[^566]\[

$$
\begin{equation*}
\mathrm{R}_{n, l}(r)=-\left\{\left(\frac{2}{n r_{0}}\right)^{3} \frac{(n-l-1)!}{2 n[(n+l)!]^{3}}\right\}^{1 / 2} \exp \left\{-\frac{r}{n r_{0}}\right\}\left(\frac{2 r}{n r_{0}}\right)^{l} L_{n-l-1}^{2 l+1}\left(\frac{2 r}{n r_{0}}\right) \tag{3.186}
\end{equation*}
$$

\]

Bohr

Here $L_{p}^{q}(\xi)$ are the so-called associated Laguerre polynomials, which may be calculated as

$$
\begin{equation*}
L_{p}^{q}(\xi)=(-1)^{q} \frac{d^{q}}{d \xi^{q}} L_{p+q}(\xi) \tag{3.187}
\end{equation*}
$$

Associated Laguerre polynomials
from simple Laguerre polynomials $L_{p}(\xi) \equiv L_{p}{ }^{0}(\xi) .{ }^{67}$ In turn, the easiest way to obtain $L_{p}(\xi)$ is to use the following Rodrigues formula: 68

$$
\begin{equation*}
L_{p}(\xi)=e^{\xi} \frac{d^{p}}{d \xi^{p}}\left(\xi^{p} e^{-\xi}\right) \tag{3.188}
\end{equation*}
$$

Notice that in contrast with the associated Legendre functions $P_{l}^{m}$ participating in spherical harmonics, $L_{p}{ }^{q}$ are just polynomials, and those with small indices $p$ and $q$ are indeed simple.

Returning to Eq. (186), we see that the natural quantization of the radial equation (184) has brought us a new quantum number (integer) $n$. In order to understand its range, we should notice that according to Eq. (188), the highest power of terms in polynomial $L_{p+q}$ is $(p+q)$, and hence, according to Eq. (187), that of $L_{p}{ }^{q}$ is $p$, so that of the highest power in the polynomial participating in Eq. (186) is ( $n$ $-l-1$ ). Since the power cannot be negative (to avoid the unphysical divergence of wavefunctions at $r$ $\rightarrow 0$ ), the radial quantum number $n$ has to obey the restriction $n \geq l+1$. Since $l$, as we already know, may take values $l=0,1,2, \ldots$, we may conclude that $n$ may only take values

$$
\begin{equation*}
n=1,2, \ldots \tag{3.189}
\end{equation*}
$$

What makes this relation important is the following, most surprising result of the theory: the eigenenergies corresponding to wavefunctions (179), which are indexed with 3 quantum numbers:

$$
\begin{equation*}
\psi_{n, l . m}=R_{n, l}(r) Y_{l}^{m}(\theta, \varphi), \tag{3.190}
\end{equation*}
$$

depend only on $n$ and agree with Bohr's formula (1.8):

$$
\begin{equation*}
E_{n}=-\frac{E_{0}}{2 n^{2}}=-\frac{1}{2 n^{2}} m\left(\frac{C}{\hbar}\right)^{2} \tag{3.191}
\end{equation*}
$$

Because of this reason, $n$ is usually called the principal quantum number, and the above relation between it and "more subordinate" $l$ is rewritten as

$$
\begin{equation*}
l \leq n-1 . \tag{3.192}
\end{equation*}
$$

Together with inequality (162), this gives us the most important hierarchy of the 3 quantum numbers involved in the problem:

$$
\begin{equation*}
1 \leq n \leq \infty \quad \Rightarrow \quad 0 \leq l \leq n-1 \quad \Rightarrow \quad-l \leq m \leq+l \tag{3.193}
\end{equation*}
$$

Bohr atom's quantum numbers

[^567]Taking into account the $(2 l+1)$-degeneracy related to the magnetic number $m$, and using the well-known formula for the arithmetic progression, ${ }^{69}$ we see that each energy level (191) has the following orbital degeneracy:

$$
\begin{equation*}
g=\sum_{l=0}^{n-1}(2 l+1)=2 \sum_{l=0}^{n-1} l+\sum_{l=0}^{n-1} 1=2 \frac{n(n-1)}{2}+n=n^{2} . \tag{3.194}
\end{equation*}
$$

Due to its importance for applications, let us spell out the quantum number hierarchy of a few lowestenergy states, using the traditional notation in which the value of $n$ is followed by the letter that denotes the value of $l$ :

$$
\begin{array}{cccc}
n=1: & l=0 & \text { (one } 1 s \text { state) } & m=0 . \\
n=2: & l=0 & \text { (one } 2 s \text { state) } & m=0, \\
& l=1 & \text { (three } 2 p \text { states) } & m=0, \pm 1 . \\
n=3: & l=0 & \text { (one } 3 s \text { state) } & m=0 \\
& l=1 & \text { (three } 3 p \text { states) } & m=0, \pm 1  \tag{3.197}\\
& l=2 & \text { (five } 3 d \text { states) } & m=0, \pm 1, \pm 2 .
\end{array}
$$

Figure 20 shows plots of the radial functions (186) of the listed states. The most important of them is of course the ground (1s) state with $n=1$ and hence $E=-E_{0} / 2$, whose radial function (186) is just

$$
\begin{equation*}
\mathrm{R}_{1,0}(r)=\frac{2}{r_{0}^{3 / 2}} e^{-r / r_{0}} \tag{3.198}
\end{equation*}
$$

and the angular distribution is uniform - see Eq. (174). The gap between the ground energy and the energy $E=-E_{0} / 8$ of the lowest excited states (with $n=2$ ) in a hydrogen atom (in which $E_{0}=E_{\mathrm{H}} \approx 27.2$ eV ) is as large as $\sim 10 \mathrm{eV}$, so that their thermal excitation requires temperatures as high as $\sim 10^{5} \mathrm{~K}$, and the overwhelming part of all hydrogen atoms in the visible Universe are in their ground state. Since atomic hydrogen makes up about $75 \%$ of the "normal" matter, we are very fortunate that such simple formulas as Eqs. (174) and (198) describe the atomic states most frequently met in Mother Nature! ${ }^{70}$

The radial functions of the next states, $2 s$ and $2 p$, are also not too complex:

$$
\begin{equation*}
R_{2,0}(r)=\frac{1}{\left(2 r_{0}\right)^{3 / 2}}\left(2-\frac{r}{r_{0}}\right) e^{-r / 2 r_{0}}, \quad R_{2,1}(r)=\frac{1}{\left(2 r_{0}\right)^{3 / 2}} \frac{r}{3^{1 / 2} r_{0}} e^{-r / 2 r_{0}} \tag{3.199}
\end{equation*}
$$

(Note again that the former of these states $(2 s)$ can only have a uniform angular distribution, while three $2 p$ states have different values of $m=0, \pm 1$, and hence have different angular distributions - see Eq. (175) and the second row of Fig. 19.) The most important trend here is a larger radius of decay of the exponent ( $2 r_{0}$ for $n=2$ instead of $r_{0}$ for $n=1$ ), and hence the radial extension of the states. This trend is confirmed by the following general formula: ${ }^{71}$

[^568]\[

$$
\begin{equation*}
\langle r\rangle_{n, l}=\frac{r_{0}}{2}\left[3 n^{2}-l(l+1)\right] . \tag{3.200}
\end{equation*}
$$

\]

The second important trend is that at fixed $n$, the orbital quantum number $l$ determines how fast does the wavefunction change with $r$ near the origin, and how much it oscillates in the radial direction at larger $r$. For example, the $2 s$ eigenfunction $\mathbb{R}_{2,0}(r)$ is nonvanishing at $r=0$, and makes one "wiggle" (has one root) in the radial direction, while eigenfunctions $2 p$ equal zero at $r=0$, and do not oscillate at all in the radial direction. Instead, those wavefunctions always oscillate as functions of some angle - see the second row of Fig. 19. The same trend in clearly visible for $n=3$ (see Fig. 20), and continues for the higher values of $n$.


Fig. 3.20. The lowest radial functions of the Bohr atom problem.

The interpretation of these results is that the states with $l=l_{\text {max }}=n-1$ may be viewed as analogs of the circular motion of a particle in a plane whose orientation defines the quantum number $m$, with an almost fixed radius $r \approx r_{0}\left(n^{2} \pm n\right)$. On the other hand, the best classical image of an $s$-state $(l=0)$ is the purely radial motion of the particle to and from the attracting center. (The latter image is especially imperfect, because the motion would need to happen simultaneously in all radial directions.) The classical language becomes reasonable only for the so-called Rydberg states, with $n \gg 1$, whose linear superpositions may be used to compose wave packets closely following the classical, circular or elliptic trajectories of the particle - just as was discussed in Sec. 2.2 for the free 1D motion.

Besides Eq. (200), mathematics gives us several other simple relations for the radial functions $R_{n, l}$ (and, since the spherical harmonics are normalized to 1 , for the eigenfunctions as the whole), including those that we will use later in the course: ${ }^{72}$

$$
\begin{equation*}
\left\langle\frac{1}{r}\right\rangle_{n, l}=\frac{1}{n^{2} r_{0}}, \quad\left\langle\frac{1}{r^{2}}\right\rangle_{n, l}=\frac{1}{n^{3}(l+1 / 2) r_{0}^{2}}, \quad\left\langle\frac{1}{r^{3}}\right\rangle_{n, l}=\frac{1}{n^{3} l(l+1 / 2)(l+1) r_{0}^{3}} . \tag{3.201}
\end{equation*}
$$

In particular, the first of them means that for any eigenfunction $\psi_{n, l, m}$, with all its complicated radial and angular dependencies, there is a simple relation between the potential and full energies:

$$
\begin{equation*}
\langle U\rangle_{n, l}=-C\left\langle\frac{1}{r}\right\rangle_{n, l}=-\frac{C}{n^{2} r_{0}}=-\frac{E_{0}}{n^{2}}=2 E_{n}, \tag{3.202}
\end{equation*}
$$

so that the average kinetic energy of the particle, $\langle T\rangle_{n, l}=E_{n}-\langle U\rangle_{n, l}$, is equal to $\left|E_{n}\right|>0$.
These simple results are in a sharp contrast with the rather complicated expressions for the eigenfunctions, and motivate a search for more general methods of quantum mechanics, which would replace or at least complement our brute-force (wave-mechanics) approach, to reveal their real nature. Such an approach will be the main topic of the next chapter.

### 3.7. Atoms

Before proceeding to that chapter, let me show that, rather strikingly, the classification of quantum numbers in the simple potential well (182), carried out in the last section, together with very modest borrowings from the further theory, allows an semi-quantitative explanation of the whole system of chemical elements. The "only" two additions we need are the following facts:
(i) due to interaction with relatively low-temperature environments, atoms tend to relax into their lowest-energy state, and
(ii) due to the Pauli principle (valid for electrons as Fermi particles), each orbital eigenstate discussed above can be occupied with 2 electrons with opposite spins.

Of course, atomic electrons do interact, so that their quantitative description requires quantum mechanics of multiparticle systems, which is rather complex. (Its main concepts will be discussed in Chapter 8.) However, the lion's share of this interaction reduces to simple electrostatic screening, i.e. the partial compensation of the electric charge of the atomic nucleus, as felt by a particular electron, by other electrons of the atom. This screening changes the qualitative results (such as the energy scale) dramatically; however, the quantum number hierarchy, and hence their classification, is not affected.

The system of atoms is most often presented as the famous periodic table of chemical elements, ${ }^{73}$ whose simple version is shown in Fig. 21, while Fig. 22 presents a sequential list of the elements with their electron configurations. The numbers in table's cells (and the first column in the list) are the

[^569]atomic numbers $Z$, which physically are the numbers of protons in the atomic nucleus, and hence the numbers of electrons in the electrically neutral atom. The electron configuration in Fig. 22 follows the convention already used in Eqs. (195)-(197), with the additional upper index showing the number of electrons with the indicated values of quantum numbers $n$ and $l$.

The lightest atom, with $Z=1$, is hydrogen (chemical symbol H ) - the only atom for each the theory discussed in Sec. 6 is quantitatively correct. ${ }^{74}$ According to Eq. (191), the $1 s$ ground state of its only electron corresponds to quantum numbers $n=1, l=0$, and $m=0$ - see Eq. (196). In most versions of the periodic table, the cell of H is placed in the top left corner. In the next atom, helium ( $\mathrm{He}, Z=2$ ), the same orbital quantum state $(1 s)$ is filled with two electrons with different spins. ${ }^{75}$ Note that due to the twice higher electric charge of the nucleus, i.e. the twice higher value of constant $C$ in Eq. (182), resulting in a 4 -fold increase of constant $E_{0}$ (183), the binding energy of each electron is crudely 4 times higher than that of the hydrogen atom - though the electron interaction decreases it by about $25 \%$ - see Sec. 7.2. This is why taking one electron away (i.e. positive ionization) of the helium atom requires a very high energy, 23.4 eV , which is not available in usual chemical reactions. On the other hand, a neural helium atom cannot bind one more electron (i.e. form a negative ion) either. As a result, helium, and all other elements with fully completed electron shells (sets of states with eigenenergies well separated from higher energy levels) is a chemically inert noble gas, thus starting the whole right-most column of the periodic table, committed to such elements.


Lanthanides:
Actinides:

| 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| La | Ce | Pr | Nd | Pm | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu |
| 89 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 |
| Ac | Ac | Th | Pa | U | Np | Pu | Am | Cm | Bk | Cf | Es | Fm | Md | Lr |

Fig. 21. The periodic table of elements, showing their atomic numbers, as well as their basic physical/chemical properties at the so-called ambient (meaning usual laboratory) conditions.

[^570]| Atomic number | Atomic symbol | Electron states | Atomic number | Atomic symbol | Electron states | Atomic number | Atomic symbol | Electron states |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Period 1 |  |  | Period 5 |  | [ Kr ] shell, | 77 | Ir | $4 f^{14} 5 d^{7} 6 s^{2}$ |
|  |  |  |  |  | plus: | 78 | Pt | $4 f^{14} 5 d^{9} 6 s^{1}$ |
| 1 | H | $1 s^{1}$ | 37 | Rb | $5 s^{1}$ | 79 | Au | $44^{44} 5 d^{10} 6 s^{1}$ |
| 2 | He | $1 s^{2}$ | 38 | Sr | $5 s^{2}$ | 80 | Hg | $4 f^{14} 5 d^{10} 6 s^{2}$ |
| Period 2 |  | [ He$]$ shell, | 39 | Y | $4 d^{1} 5 s^{2}$ | 81 | Tl | $4 f^{\text {f }} 5 d^{10} 6 s^{2} 6 p^{1}$ |
|  |  | plus: | 40 | Zr | $4 d^{2} 5 s^{2}$ | 82 | Pb | $4 f^{14} 5 d^{10} 6 s^{2} 6 p^{2}$ |
| 3 | Li | $2 s^{1}$ | 41 | Nb | $4 d^{4} 5 s^{1}$ | 83 | Bi | $4 f^{14} 5 d^{10} 6 s^{2} 6 p^{3}$ |
| 4 | Be | $2 s^{2}$ | 42 | Mo | $4 d^{5} 5 s^{1}$ | 84 | Po | $4 f^{14} 5 d^{10} 6 s^{2} 6 p^{4}$ |
| 5 | B | $2 s^{2} 2 p^{1}$ | 43 | Tc | $4 d^{6} 5 s^{1}$ | 85 | At | $4 f^{14} 5 d^{10} 6 s^{2} 6 p^{5}$ |
| 6 | C | $2 s^{2} 2 p^{2}$ | 44 | Ru | $4 d^{7} 5 s^{1}$ | 86 | Rn | $4 f^{14} 5 d^{10} 6 s^{2} 6 p^{6}$ |
| 7 | N | $2 s^{2} 2 p^{3}$ | 45 | Rh | $4 d^{8} 5 s^{1}$ | Period 7 |  | [Rn] shell, |
| 8 | O | $2 s^{2} 2 p^{4}$ | 46 | Pd | $4 d^{10}$ |  |  | plus: |
| 9 | F | $2 s^{2} 2 p^{5}$ | 47 | Ag | $4 d^{10} 5 s^{1}$ | 87 | Fr | $7 s^{1}$ |
| 10 | Ne | $2 s^{2} 2 p^{6}$ | 48 | Cd | $4 d^{10} 5 s^{2}$ | 88 | Ra | $7 s^{2}$ |
| Period 3 |  | [ Ne ] shell, | 49 | In | $4 d^{10} 5 s^{2} 5 p^{1}$ | 89 | Ac | $6 d^{1} 7 s^{2}$ |
|  |  | plus: | 50 | Sn | $4 d^{10} 5 s^{2} 5 p^{2}$ | 90 | Th | $6 d^{2} 7 s^{2}$ |
| 11 | Na | $3 s^{1}$ | 51 | Sb | $4 d^{10} 5 s^{2} 5 p^{3}$ | 91 | Pa | $5 f^{2} 6 d^{1} 7 s^{2}$ |
| 12 | Mg | $3 s^{2}$ | 52 | Te | $4 d^{10} 5 s^{2} 5 p^{4}$ | 92 | U | $5 f^{3} 6 d^{1} 7 s^{2}$ |
| 13 | Al | $3 s^{2} 3 p^{1}$ | 53 | 1 | $4 d^{10} 5 s^{2} 5 p^{5}$ | 93 | Np | $5 f^{4} 6 d^{1} 7 s^{2}$ |
| 14 | Si | $3 s^{2} 3 p^{2}$ | 54 | Xe | $4 d^{10} 5 s^{2} 5 p^{6}$ | 94 | Pu | $5 f^{6} 7 s^{2}$ |
| 15 | P | $3 s^{2} 3 p^{3}$ | Period 6 |  | [Xe] shell, | 95 | Am | $5 f^{7} 7 s^{2}$ |
| 16 | S | $3 s^{2} 3 p^{4}$ |  |  | plus: | 96 | Cm | $5 f^{7} 6 d^{1} 7 s^{2}$ |
| 17 | Cl | $3 s^{2} 3 p^{5}$ | 55 | Cs | $6 s^{1}$ | 97 | Bk | $5 f^{9} 7 s^{2}$ |
| 18 | Ar | $3 s^{2} 3 p^{6}$ | 56 | Ba | $6 s^{2}$ | 98 | Cf | $5 f^{10} 7 s^{2}$ |
| Period 4 |  | [ Ar ] shell, | 57 | La | $5 d^{1} 6 s^{2}$ | 99 | Es | $5 f^{11} 7 s^{2}$ |
|  |  | plus: | 58 | Ce | $4 f^{1} 5 d^{1} 6 s^{2}$ | 100 | Fm | $5 f^{12} 7 s^{2}$ |
| 19 | K | $4 s^{1}$ | 59 | Pr | $4 f^{3} 6 s^{2}$ | 101 | Md | $5 f^{13} 7 s^{2}$ |
| 20 | Ca | $4 s^{2}$ | 60 | Nd | $4 f^{4} 6 s^{2}$ | 102 | No | $5 f^{14} 7 s^{2}$ |
| 21 | Sc | $3 d^{1} 4 s^{2}$ | 61 | Pm | $4 f^{5} 6 s^{2}$ | 103 | Lr | $5 f^{14} 6 d^{1} 7 s^{2}$ |
| 22 | Ti | $3 d^{2} 4 s^{2}$ | 62 | Sm | $4 f^{6} 6 s^{2}$ | 104 | Rf | $5 f^{14} 6 d^{2} 7 s^{2}$ |
| 23 | V | $3 d^{3} 4 s^{2}$ | 63 | Eu | $4 f^{7} 6 s^{2}$ | 105 | Db | $5 f^{14} 6 d^{3} 7 s^{2}$ |
| 24 | Cr | $3 d^{4} 4 s^{2}$ | 64 | Gd | $4 f^{7} 5 d^{1} 6 s^{2}$ | 106 | Sg | $5 f^{14} 6 d^{4} 7 s^{2}$ |
| 25 | Mn | $3 d^{5} 4 s^{2}$ | 65 | Tb | $4 f^{9} 6 s^{2}$ | 107 | Bh | $5 f^{14} 6 d^{5} 7 s^{2}$ |
| 26 | Fe | $3 d^{6} 4 s^{2}$ | 66 | Dy | $4 f^{10} 6 s^{2}$ | 108 | Hs | $5 f^{14} 6 d^{6} 7 s^{2}$ |
| 27 | Co | $3 d^{7} 4 s^{2}$ | 67 | Ho | $4 f^{11} 6 s^{2}$ | 109 | Mt | $5 f^{14} 6 d^{7} 7 s^{2}$ |
| 28 | Ni | $3 d^{8} 4 s^{2}$ | 68 | Er | $4 f^{12} 6 s^{2}$ | 110 | Ds | $5 f^{14} 6 d^{8} 7 s^{2}$ |
| 29 | Cu | $3 d^{9} 4 s^{1}$ | 69 | Tm | $4 f^{13} 6 s^{2}$ | 111 | Rg | $5 f^{14} 6 d^{9} 7 s^{2}$ |
| 30 | Zn | $3 d^{10} 4 s^{2}$ | 70 | Yb | $4 f^{14} 6 s^{2}$ | 112 | Cn | $5 f^{4} 6 d^{10} 7 s^{2}$ |
| 31 | Ga | $3 d^{10} 4 s^{2} 4 p^{1}$ | 71 | Lu | $4 f^{14} 5 d^{1} 6 s^{2}$ | 113 | Uut | $5 f^{14} 6 d^{10} 7 s^{2} 7 p^{1}$ |
| 32 | Ge | $3 d^{10} 4 s^{2} 4 p^{2}$ | 72 | Hf | $4 f^{14} 5 d^{2} 6 s^{2}$ | 114 | F1 | $5 f^{14} 6 d^{10} 7 s^{2} 7 p^{2}$ |
| 33 | As | $3 d^{10} 4 s^{2} 4 p^{3}$ | 73 | Ta | $4 f^{44} 5 d^{3} 6 s^{2}$ | 115 | Uup | $5 f^{44} 6 d^{10} 7 s^{2} 7 p^{3}$ |
| 34 | Se | $3 d^{10} 4 s^{2} 4 p^{4}$ | 74 | W | $4 f^{14} 5 d^{4} 6 s^{2}$ | 116 | Lv | $5 f^{14} 6 d^{10} 7 s^{2} 7 p^{4}$ |
| 35 | Br | $3 d^{10} 4 s^{2} 4 p^{5}$ | 75 | Re | $4 f^{14} 5 d^{5} 6 s^{2}$ | 117 | Uus | $5 f^{14} 6 d^{10} 7 s^{2} 7 p^{5}$ |
| 36 | Kr | $3 d^{10} 4 s^{2} 4 p^{6}$ | 76 | Os | $4 f^{44} 5 d^{6} 6 s^{2}$ | 118 | Uuo | $5 f^{44} 6 d^{10} 7 s^{2} 7 p^{6}$ |

Fig. 3.22. Atomic electron configurations. The upper index shows the number of electrons in states with the indicated quantum numbers $n$ (the first digit) and $l$ (letter-coded as listed above).

The situation changes dramatically as we move to the next element, lithium (Li), with $Z=3$ electrons. Two of them are still accommodated by the inner shell $n=1$ (listed in Fig. 22 as the helium shell $[\mathrm{He}])$, but the third one has to reside in the next shell with $n=2$ and $l=0$, i.e. in the $2 s$ state. According to Eq. (191), the binding energy of this electron is much lower, especially if we take into account that according to Eq. (200), the $1 s$ electrons of the [He] shell are much closer to the nucleus and almost completely compensate two thirds of its electric charge $+3 e$. As a result, the $2 s$ electron is reasonably well described by Eq. (199), with binding energy of just 5.39 eV , so that a lithium atom can give out that electron rather easily - to either atoms of other elements to form chemical compounds, or into the common conduction band of solid state lithium - and as a result it is a typical alkali metal. The similarity of chemical properties of lithium and hydrogen, with the chemical valence of one, ${ }^{76}$ places Li as the starting element of the second period (row), with the first period limited to only H and He .

In the next element, beryllium $(Z=4)$, the $2 s$ state $(n=2, l=0)$ picks up one more electron, with the opposite spin. Due to the higher electric charge of the nucleus, $Q=4 e$, with only half of it compensated by $1 s$ electrons of the [He] shell, the binding energy of the $2 s$ electrons is higher than in lithium, so that the ionization energy increases to 9.32 eV . As a result, beryllium is also chemically active but not as active as lithium, with the valence of two, and is also is metallic in its solid state phase, but does not conduct electric current as well as lithium.

Moving in this way along the second row of the periodic table (from $Z=3$ to $Z=10$ ), we see the gradual filling of all 4 different orbital states of the $n=2$ shell, by 2 electrons each, with gradually growing ionization potential (up to 21.6 eV in Ne with $Z=10$ ), i.e. the growing reluctance to have metallic conductance or form positive ions. However, the final elements of the row, such as oxygen (O, with $Z=8$ ) and especially fluorine ( F , with $Z=9$ ) can readily pick up extra electrons to fill their $2 p$ states, i.e. form negative ions. As a result, these elements are chemically active, with the double valence for oxygen and single valence for fluorine. However, the final element of this row, neon, has its $n=2$ shell full, and cannot form a stable negative ion. This is why it is a noble gas, like helium. Traditionally, in the periodic table it is placed right under helium (Fig. 21), to emphasize the similarity of their chemical and physical properties. But this necessitates making an at least 6 -cell gap in the $1^{\text {st }}$ row. (Actually, the gap is often made larger, to accommodate next rows - keep reading.)

Period 3, i.e. the $3^{\text {rd }}$ row of the table starts exactly like period 2 , with sodium ( Na , with $\mathrm{Z}=11$ ), also a chemically active alkali metal whose atom features 10 electrons filling shells with $n=1$ and $n=2$ (in Fig. 22 collectively called the neon shell, [Ne]), plus one electron in a $3 s$ state ( $n=3, l=0, m=0$ ), which may be reasonably well described by the hydrogen atom theory - see, e.g., the red trace on the last panel of Fig. 20. Naively we could expect that, according to Eq. (194), and with the account of double spin degeneracy, this period of the table should have $2 n^{2}=2 \times 3^{2}=18$ elements, with gradual filling of two $3 s$ states, six $3 p$ states, and ten $3 d$ states. However, here we run into a big surprise: after argon (Ar, with $Z=18$ ), a relatively inert element with ionization energy of 15.7 eV due to the fully filled $3 s$ and $3 p$ shells, the next element, potassium ( K , with $Z=19$ ) is an alkali metal again!

The reason for that is the difference of the actual electron energies from those of the hydrogen atom, which is due mostly to inter-electron interactions and gradually accumulates with the growth of $Z$. It may be semi-quantitatively understood from the results of Sec. 6. In hydrogen-like atoms, electron state energies do not depend on the quantum number $l$ (as well as $m$ ) - see Eq. (191). However, the

[^571]orbital quantum number does affect the wavefunction of an electron. As Fig. 20 shows, the larger $l$ the less the probability for an electron to be close to the nucleus, where its positive charge is less compensated by other electrons. As a result of this effect (and also the relativistic corrections to be discussed in Sec. 6.3), electron's energy grows with $l$. Actually, this effect was visible even in period 2: it manifests itself in the filling order ( $p$ states after $s$ states). However, for potassium ( K , with $\mathrm{Z}=19$ ) and calcium ( Ca , with $Z=20$ ), energies of $3 d$ states become so high that energies of two $4 s$ states (with opposite spins) are lower, and they are filled first. As described by factor 3 in the square brackets of Eq. (200), and also by Eq. (201), the effect of the principal number $n$ on the distance from the nucleus is stronger than that of $l<n$, so that $4 s$ wavefunctions of K and Ca are relatively far from the nucleus, and determine the chemical valence (equal to 1 and 2, correspondingly) of these elements. The next atoms, from $\mathrm{Sc}(Z=21)$ to $\mathrm{Zn}(Z=30)$, with the gradually filled "internal" $3 d$ states, are the so-called transition metals whose (comparable) ionization energies and chemical properties are determined by $4 s$ electrons.

This fact is the origin of the difference between various forms of the "periodic" table. In its most popular option, shown in Fig. 21, K is used to start the next, period 4, and then a new period is started each time and only when the first electron with the next principal quantum number ( $n$ ) appears. ${ }^{77}$ This topology provides a very clear mapping on the chemical properties of the first element of each period (an alkali metal), as well as its last element (a noble gas). This also automatically means making gaps in all previous rows. Usually, this gap is made between the atoms with completely filled $s$ states and with the first electron in a $p$ state, because here the properties of the elements make a somewhat larger step. (For example, the step from Be to B makes the material an insulator, but it is not large enough to make a similar difference between Mg to Al .) As a result, elements of the same column have approximately similar chemical valence and physical properties.

However, to accommodate longer lowest rows, such presentation is inconvenient, because the whole table would be too broad. This is why the so-called rare earths, including lanthanides (with $Z$ from 57 to 70 , of the $6^{\text {th }}$ row, with gradual filling of $4 f$ and $5 d$ states) and actinides ( Z from 89 to 103 , of the $7^{\text {th }}$ row, with gradual filling of $5 f$ and $6 d$ states), are presented as outlet lines (Fig. 21). This is quite acceptable for the purposes of standard chemistry, because chemical properties of elements within each group are rather close.

To summarize, the "periodic table of elements" is not periodic in the strict sense of the word. Nevertheless, it has had an enormous historic significance for chemistry, as well as atomic and solid state physics, and is still very convenient for many purposes. For our course, the most important aspect of its discussion is the surprising possibility to describe, at least for classification purposes, such a complex multi-electron system as an atom as a set of quasi-independent electrons in certain quantum states indexed with the same quantum numbers $n, l$, and $m$ as those of the hydrogen atom. This fact enables the use of various perturbation theories, which give more quantitative description of atomic properties. Some of these techniques will be reviewed in Chapters 6 and 8 of this course. ${ }^{78}$

[^572]
### 3.8. Exercise problems

3.1. A particle of energy $E$ is incident (in Fig. on the right, within the plane of drawing) on a sharp potential step:

$$
U(\mathbf{r})=\left\{\begin{array}{cc}
0, & \text { for } x<0 \\
U_{0}, & \text { for } 0<x .
\end{array}\right.
$$

Find the particle reflection probability $R$ as a function of the incidence angle $\theta$;
 sketch and discuss the function, for different magnitudes and signs of $U_{0}$.
3.2. Use the finite difference method with step $h=a / 2$ to calculate as many eigenenergies as possible, for a free particle confined to the interior of:
(i) a square with side $a$;
(ii) a cube with side $a$.

For the square, repeat the calculations, using a finer step: $h=a / 3$. Compare the results for different $h$, with the exact formula.

Hint: It is advisable to first solve (or review the solution of :-) the similar 1D problem in Chapter 1 , or start from reading about the finite difference method. ${ }^{79}$ Also, try to exploit problem's symmetry.
3.3. Use the variational method to estimate the ground state energy of a particle of mass $m$, moving in a spherically-symmetric potential

$$
U(\mathbf{r})=a r^{4} .
$$

3.4. In the classical version of the Landau level problem discussed in Sec. 2, the center of particle's orbit is an integral of motion, determined by initial conditions. Calculate the commutation relations between the quantum-mechanical operators corresponding to the Cartesian coordinates of the center, and to the sum of their squares.
3.5.* Analyze how are the Landau levels (3.50) modified by an additional constant electric field $\mathbf{E}$, directed along the particle plane. Contemplate the physical meaning of your result, and its implications for the quantum Hall effect in a gate-defined Hall bar. (The area $L \times W$ area of such a bar [see Fig. 3.6 of the lecture notes] is defined by metallic gate electrodes parallel to
 the 2D electron gas plane - see Fig. on the right. The negative voltage $V_{g}$, applied to the gates, chases the electrons gas out of the confinement plane at the remaining sample area.)
3.6. Analyze how are the Landau levels (50) modified if a 2D particle is confined in an additional 1D potential well $U(x)=m \omega_{0}{ }^{2} x^{2} / 2$

[^573]3.7. Find the eigenfunctions of a spinless, charged 3D particle moving in "crossed" (perpendicular), uniform electric and magnetic fields. For each eigenfunction, calculate the expectation value of particle's velocity in the direction perpendicular to both fields, and compare the result with the solution of the corresponding classical problem.

Hint: Generalize Landau's solution for 2D particles, discussed in Sec. 2.
3.8. Use the Born approximation to calculate the angular dependence and the full cross-section of scattering of an incident plane wave, propagating along axis $x$, by the following pair of point inhomogeneities:

$$
U(\mathbf{r})=W\left[\delta\left(\mathbf{r}-\mathbf{n}_{z} \frac{a}{2}\right)+\delta\left(\mathbf{r}+\mathbf{n}_{z} \frac{a}{2}\right)\right] .
$$

Analyze the results in detail. Derive the condition of the Born approximation's validity for such deltafunctional scatterers.
3.9. Use the Born approximation to calculate the differential and full cross-sections of a spherical scatterer:

$$
U(\mathbf{r})=\left\{\begin{array}{cc}
U_{0}, & \text { for } r<R \\
0, & \text { otherwise }
\end{array}\right.
$$

Analyze both results, especially the angular dependence of $d \sigma / d \Omega$, in detail, for $k R \ll 1$ and $k R \gg 1$.
3.10. Use the Born approximation to calculate differential and full cross-sections of electron scattering by a screened Coulomb field of a point charge $Z e$, with electrostatic potential

$$
\phi(\mathbf{r})=\frac{Z e}{4 \pi \varepsilon_{0} r} e^{-\lambda r}
$$

neglecting the spin interaction effects, and analyzed their dependence on the screening parameter $\lambda$. Compare the results with those given by the classical ("Rutherford") formula ${ }^{80}$ for the unscreened Coulomb potential ( $\lambda \rightarrow 0$ ), and formulate the condition of Born approximation's validity in this limit.
3.11. A quantum particle of mass $m$ with electric charge $Q$ is scattered by a localized distributed charge with a spherically-symmetric density $\rho(r)$ and zero total charge. Use the Born approximation to calculate the differential cross-section of forward scattering (with scattering angle $\theta=0$ ), and evaluate it for scattering of electrons by a hydrogen atom in its ground state.
3.12. Reformulate the Born approximation for the 1D case. Use the result to find the scattering and transfer matrices of a "rectangular" scatterer

$$
U(x)=\left\{\begin{aligned}
U_{0}, & \text { for }|x|<d / 2 \\
0, & \text { otherwise }
\end{aligned}\right.
$$

[^574]Compare the results with the those of the exact calculations carried out earlier in the course.
3.13. Use Eq. (88) to show that the Bragg rule for the diffraction wave maxima, $\mathbf{k}=\mathbf{k}_{0}+\mathbf{Q}$, where $\mathbf{Q}$ is any vector of the reciprocal lattice defined by Eq. (110), is valid not only for electromagnetic waves, but also for non-relativistic quantum particle scattering by a periodic (Bravais) lattice.
3.14. In the tight-binding approximation, calculate the eigenstates and eigenenergies of three similar, weakly coupled quantum wells located in the vertices of an equilateral triangle.
3.15. Figure on the right shows a fragment of a periodic 2D lattice, with open and solid points showing the location of different local potentials - say, different atoms.
(i) Find the reciprocal lattice and the $1^{\text {st }}$ Brillouin zone;
(ii) Find wave number $k$ of the monochromatic radiation incident along axis $x$, at which the lattice creates the first-order diffraction peak within the $[x, y]$ plane, and the direction towards this peak.

(iii) Semi-qualitatively, describe the evolution of the intensity of the peak if the local potentials represented by the open and solid points tend to each other.
3.16. For the 2D hexagonal lattice (Fig. 11b):
(i) find the reciprocal lattice $\mathbf{Q}$ and the $1^{\text {st }}$ Brillouin zone;
(ii) use the tight-binding approximation to calculate the dispersion relation $E(\mathbf{q})$ for a 2D particle moving in a potential with such periodicity, close to the eigenenergy of an axially-symmetric state quasi-localized at the potential minima;
(iii) analyze and sketch (or plot) the resulting dispersion relation $E(\mathbf{q})$ inside the $1^{\text {st }}$ Brillouin zone.
3.17. ${ }^{*}$ Complete the tight-binding approximation calculation of band structure of the honeycomb lattice, started in the end of Sec. 4. Analyze the results. Prove that the Dirac points $\mathbf{q}_{\mathrm{D}}$ are located in the corners of the $1^{\text {st }}$ Brillouin zone, and express the velocity $v_{n}$, participating in Eq. (122), in terms of the coupling energy $\delta_{n}$. Show that the final results do not change if the quasi-localized wavefunctions are not axially-symmetric, but are proportional to $\exp \{\operatorname{in} \varphi\}$ - as they are, with $n=1$, for the $2 p_{z}$ electrons of carbon atoms in graphene, which are responsible for its transport properties.
3.18. Examine basic properties of the so-called Wannier functions defined as

$$
\phi_{\mathbf{R}}(\mathbf{r})=\operatorname{const} \times \int_{B Z} \psi_{\mathbf{q}}(\mathbf{r}) e^{-i \mathbf{q} \cdot \mathbf{R}} d^{3} q
$$

where $\psi_{\mathbf{q}}(\mathbf{r})$ is the Bloch wavefunction (3.108), $\mathbf{R}$ is any vector of the Bravais lattice, and the integration over quasi-momentum $\mathbf{q}$ is extended over any (e.g., the first) Brillouin zone.
3.19. Evaluate the long-range electrostatic interaction (the so-called London dispersion force) between two similar, electrically-neutral but polarizable molecules, modeling them as isotropic 3D harmonic oscillators.

Hint: Using the classical expression for the interaction between two electric dipoles, ${ }^{81}$ try to present the total Hamiltonian of the system as a sum of Hamiltonians of several independent harmonic oscillators, and calculate their ground-state energy as a function of distance between the molecules.
3.20. Use the variable separation method to find expressions for the eigenfunctions and the corresponding eigenenergies of a free 2 D particle confined inside a thin round disk of radius $R$ :

$$
U=\left\{\begin{array}{l}
0, \quad \text { for } 0 \leq \rho<R, \\
+\infty, \quad \text { for } R<\rho,
\end{array}\right.
$$

where $\rho \equiv\{x, y, 0\}$. What is the level degeneracy? Calculate 5 lowest energy levels with accuracy better than $1 \%$.
3.21. Calculate the ground-state energy of a 2 D particle localized in a shallow flat-bottom potential well

$$
U(\rho)=\left\{\begin{array}{ll}
-U_{0}, & \text { for } \rho<R \\
0, & \text { for } \rho>R
\end{array}\right\}, \quad \text { with } 0<U_{0} \ll \frac{\hbar^{2}}{m R^{2}} .
$$

3.22. Spell out the explicit form of spherical harmonics $Y_{4}^{0}(\theta, \varphi)$ and $Y_{4}^{4}(\theta, \varphi)$.
3.23. Calculate $\langle x\rangle$ and $\left\langle x^{2}\right\rangle$ in the ground state of the planar and spherical rotators of radius $R$. What can you say about averages $\left\langle p_{x}\right\rangle$ and $\left\langle p_{x}{ }^{2}\right\rangle$ ?
3.24. According to the discussion in the beginning of Sec. 5, eigenfunctions of a 3D harmonic oscillator may be calculated as products of three 1D "Cartesian oscillators" - see, in particular Eq. (124), with $d=3$. However, according to the discussion in Sec. 3.6, wavefunctions of the type (190), proportional to spherical harmonics $Y_{l}^{m}$, are also eigenstates of this spherically-symmetric system. Represent:
(i) the ground state of the oscillator, and
(ii) each of its lowest excited states,
taken in the form (190), as linear combinations of products of 1D oscillator wavefunctions. Also, calculate the degeneracy of $n^{\text {th }}$ energy level of the oscillator.
3.25. A spherical rotator (with $r \equiv\left(x^{2}+y^{2}+z^{2}\right)^{1 / 2}=R=$ const) of mass $m$ is in the state with wavefunction

$$
\psi=\operatorname{const} \times\left(\frac{1}{3}+\sin ^{2} \theta\right)
$$

Calculate the system's energy.
3.26. ${ }^{*}$ Calculate the eigenfunctions and the energy spectrum of a 3 D particle free to move inside a sphere of radius $R$ :

[^575]\[

U=\left\{$$
\begin{array}{c}
0, \quad \text { for } 0 \leq r<R, \\
+\infty, \quad \text { for } R<r .
\end{array}
$$\right.
\]

Calculate 5 lowest energy levels with a $1 \%$ accuracy, and indicate the degeneracy of each level.
Hint: The solution of this problem requires the so-called spherical Bessel functions $j_{l}(\xi)$, whose description is available in most math handbooks. ${ }^{82}$
3.27. Find the smallest value of depth $U_{0}$ for that the spherical quantum well

$$
U=\left\{\begin{array}{c}
-U_{0}, \quad \text { for } r<R, \\
0, \quad \text { for } R<r,
\end{array}\right.
$$

has a bound (localized) eigenstate. Does such a state exist for a very narrow and deep well $U=-w \delta(\mathbf{r})$, with a positive and finite 20 .
3.28. Calculate the smallest value of depth $U_{0}$ for that the following spherically-symmetric quantum well,

$$
U(r)=-U_{0} e^{-r / R}, \quad \text { with } U_{0}, R>0
$$

has a bound (localized) eigenstate.
Hint: Try to introduce the following new variables: $f \equiv r \mathrm{R}$ and $\xi \equiv C e^{-r / 2 R}$, with an appropriate choice of constant $C$.
3.29. Calculate the lifetime of the lowest metastable state in the spherical-shell potential

$$
U(r)=w \delta(r-R), \quad \text { with } \quad w>0,
$$

in the limit of large $w$. Specify the limit of validity of your result.
3.30. Calculate the condition at which a particle of mass $m$, moving in the field of a very thin spherically-symmetric shell, with

$$
U(\mathbf{r})=-w \delta(r-R), \quad \text { with } w>0
$$

has at least one localized ("bound") stationary state. Compare the result with that for potential

$$
U_{0}(\mathbf{r})=-w_{0} \delta(\mathbf{r}), \quad \text { with } w_{0}>0
$$

Hint: Note that the first delta-function is one-dimensional, while the second one is threedimensional, so that parameters $w$ and $w_{0}$ have different dimensionalities.
3.31. A particle, moving in a central potential $U(r)$, with $U(r) \rightarrow 0$ at $r \rightarrow \infty$, has a stationary state with the following wavefunction:

$$
\psi=C r^{\alpha} e^{-\beta r} \cos \theta
$$

where $C, \alpha$, and $\beta$ are constants. Calculate:

[^576](i) probabilities of all possible values of quantum numbers $m$ and $l$,
(ii) the confining potential, and
(iii) state's energy.
3.32. Calculate the energy spectrum of a particle moving in a monotonic, but otherwise arbitrary attractive central potential $U(r)$, in the approximation of large orbital quantum numbers $l$. Formulate the quantitative condition(s) of validity of your theory. Check that for the Coulomb potential $U(r)=-C / r$, your result agrees with Eq. (191).
3.33. An electron had been in the ground state of a hydrogen-like atom/ion with nuclear charge $Z e$, when the charge suddenly changed to $(Z+1) e .{ }^{83}$ Calculate the probabilities for the electron of the changed system to be:
(i) in the ground state, and
(ii) in the lowest excited state.

Evaluate these probabilities for the particular case of the beta decay of tritium, with the formation of a single-positive ion of ${ }^{3} \mathrm{He}$.
3.34. Calculate $\left\langle x^{2}\right\rangle$ and $\left\langle p_{x}{ }^{2}\right\rangle$ in the ground state of a hydrogen-like atom. Compare the results with Heisenberg's uncertainty relation. What do these results tell about electron's velocity in the atom?
3.35. Apply to Eq. (181) the Hellmann-Feynman theorem (see Problem 1.4) to prove:
(i) the first of Eqs. (3.201), and
(ii) the fact that for a spinless particle in an arbitrary spherically-symmetric attractive potential $U(r)$, the ground state is always an $s$-state (with the orbital quantum number $l=0$ ).
3.36. For the ground state of a hydrogen atom, calculate the expectation values of $\varepsilon$ and $\varepsilon^{2}$, where $\varepsilon$ is the electric field created by the atom at distance $r \gg r_{0}$ from its nucleus. Interpret the resulting relation between $\langle\varepsilon\rangle^{2}$ and $\left\langle\varepsilon^{2}\right\rangle$ (at the same observation point).

[^577]

## Chapter 4. Bra-ket Formalism

The objective of this chapter is a discussion of Dirac's bra-ket formalism of quantum mechanics, which not only overcomes some inconveniences of wave mechanics, but also allows a natural description of such "internal" properties of particles as their spin. In the course of discussion of the formalism I will give several simple examples of its use, leaving more involved applications for the following chapters.

### 4.1. Motivation

We have seen that wave mechanics gives many results of primary importance. Moreover, it is fully (or mostly) sufficient for many applications, for example, for solid state electronics and device physics. However, in the course of our survey we have filed several grievances about this approach. Let me briefly summarize these complaints:
(i) Wave mechanics is focused on the spatial dependence of wavefunctions. On the other hand, our attempts to analyze the temporal evolution of quantum systems within this approach (beyond the trivial time behavior of the eigenfunctions, described by Eq. (1.61)), run into technical difficulties. For example, we could derive Eq. (2.159) describing time dynamics of the metastable state, or Eq. (2.185) describing quantum oscillations in coupled wells, only for the simplest potential profiles, though it is intuitively clear that these simple results should be common for all problem of this kind. Deriving the equations of such processes for arbitrary potential profiles is possible using perturbation theories (to be reviewed in Chapter 6), but that in the wave mechanics language they would require very bulky formulas.
(ii) The same is true concerning other issues that are conceptually addressable within wave mechanics, e.g., the Feynman path integral approach, description of coupling to environment, etc. Addressing them in wave mechanics would lead to formulas so bulky that I had (wisely :-) postponed them until we have got a more compact formalism on hand.
(iii) In the discussion of several key problems (for example the harmonic oscillator and spherically-symmetric potentials) we have run into rather complicated eigenfunctions coexisting with simple energy spectra - that infer some simple background physics. It is very important to get this physics revealed.
(iv) In the wave mechanics postulates, formulated in Sec. 1.2, quantum mechanical operators of the coordinate and momentum are treated very unequally - see Eqs. (1.26b). However, some key expressions, e.g., for the fundamental eigenfunction of a free-particle,

$$
\begin{equation*}
\exp \left\{i \frac{\mathbf{p} \cdot \mathbf{r}}{\hbar}\right\} \tag{4.1}
\end{equation*}
$$

or the harmonic oscillator's Hamiltonian,

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m} \hat{p}^{2}+\frac{m \omega_{0}^{2}}{2} \hat{r}^{2}, \tag{4.2}
\end{equation*}
$$

invite a similar treatment of momentum and coordinate.

However, the strongest motivation for a more general formalism comes from wave mechanics' conceptual incapability to describe elementary particles' spins and other internal quantum degrees of freedom, such as quark flavors or lepton numbers. In this context, let us review the basic facts on spin (which is a very representative and experimentally the most accessible of all internal quantum numbers), to understand what a more general formalism should explain - as a minimum.

Figure 1 shows the conceptual scheme of the simplest spin-revealing experiment, first carried out by O. Stern and W. Gerlach in 1922. ${ }^{1}$ A collimated beam of electrons is passed through a gap between poles of a strong magnet, where the magnetic field $B$, whose orientation is taken for axis $z$ in Fig. 1, is non-uniform, so that both $\mathcal{B}_{z}$ and $d \mathcal{B}_{z} / d z$ are not equal to zero. As a result, the beam splits into two parts of equal intensity.


Fig. 4.1. The simplest SternGerlach experiment.

This simplest experiment can be semi-quantitatively explained on classical, though somewhat phenomenological grounds by assuming that each electron has an intrinsic, permanent magnetic dipole moment $\mathbf{m}$. Indeed, classical electrodynamics ${ }^{2}$ tells us that the potential energy $U$ of a magnetic dipole in an external magnetic field is equal to $(-\mathbf{m} \cdot \boldsymbol{B})$, so that the force acting on the particle,

$$
\begin{equation*}
\mathbf{F}=-\nabla U=-\nabla(-\mathbf{m} \cdot \boldsymbol{B}), \tag{4.3}
\end{equation*}
$$

has a nonvanishing vertical component

$$
\begin{equation*}
F_{z}=-\frac{\partial}{\partial z}\left(-m_{z} \cdot \mathcal{B}_{z}\right)=m_{z} \frac{\partial \mathcal{B}_{z}}{\partial z} . \tag{4.4}
\end{equation*}
$$

Hence if we further postulate the existence of two possible, discrete values of $m_{\mathrm{z}}= \pm \mu$, this explains the Stern-Gerlach effect qualitatively, as a result of the incident electrons having a random sign, but similar magnitude of $m_{z}$. A quantitative explanation of the beam splitting angle requires the magnitude of $\mu$ to be equal (or close) to the so-called Bohr magneton ${ }^{3}$

$$
\begin{equation*}
\mu_{\mathrm{B}} \equiv \frac{\hbar e}{2 m_{e}} \approx 0.9274 \times 10^{-23} \frac{\mathrm{~J}}{\mathrm{~T}} \tag{4.5}
\end{equation*}
$$

Bohr magneton

As we will see below, this value cannot be explained by any internal motion of the electron, say its rotation about axis $z$.

[^578]Much more importantly, this semi-classical language cannot explain the results of the following set of multi-stage Stern-Gerlach experiments, shown in Fig. 2 - even qualitatively. In the first of the experiments, the electron beam is first passed through a magnetic field oriented (together with its gradient) along axis $z$, just as in Fig. 1. Then one of the two resulting beams is absorbed (or otherwise removed from the setup), while the other one is passed through a similar but $x$-oriented field. The experiment shows that this beam is split again into two components of equal intensity. A classical explanation of this experiment would require a very unnatural suggestion that the initial electrons had random but discrete components of the magnetic moment simultaneously in two directions, $z$ and $x$.

However, even this assumption cannot explain the results of the three-stage Stern-Gerlach experiment shown on the middle panel of Fig. 2. Here, the previous two-state setup is complemented with one more absorber and one more magnet, now with the $z$-orientation again. Completely counterintuitively, it again gives two beams of equal intensity, as if we have not yet filtered out the electrons with $m_{z}$ corresponding to the lower beam, in the first, $z$-stage.


Fig. 4.2. Three multi-stage Stern-Gerlach experiments.
 Boxes SG (...) denote magnets similar to one shown in Fig. 1, with the axis oriented in the indicated direction.

The only way to save the classical explanation here is to say that maybe, electrons somehow interact with the magnetic field, so that the $x$-polarized (non-absorbed) beam becomes spontaneously depolarized again somewhere between magnetic stages. But any hope for such explanation is ruined by the control experiment shown on the bottom panel of Fig. 2, whose results indicate that no such depolarization happens.

We will see below that all these (and many more) results find a natural explanation in the matrix mechanics pioneered by W. Heisenberg, M. Born and P. Jordan in 1925. However, the matrix formalism is inconvenient for the solution of most problems discussed in Chapters 1-3, and for a time it was eclipsed by Schrödinger's wave mechanics, which had been put forward just a few months later. However, very soon P. A. M. Dirac introduced a more general bra-ket formalism, which provides a generalization of both approaches and proves their equivalence. Let me describe it.

### 4.2. States, state vectors, and linear operators

The basic notion of the general formulation of quantum mechanics is the quantum state of a system. ${ }^{4}$ To get some gut feeling of this notion, if a quantum state $\alpha$ of a particle may be adequately described by wave mechanics, this description is given by the corresponding wavefunction $\Psi_{\alpha}(\mathbf{r}, t)$. Note, however, the state as such is not a mathematical object (such as a function), ${ }^{5}$ and can participate in mathematical formulas only as a "pointer" - e.g., the index of function $\Psi_{\alpha \text {. On the other hand, the }}$ wavefunction is not a state, but a mathematical object (a complex function of space and time) giving a quantitative description of the state - just as the radius-vector as a function of time is a mathematical object describing the motion of a classical particle - see Fig. 3. Similarly, in the Dirac formalism a certain quantum state $\alpha$ is described by either of two mathematical objects, called the state vectors: the ket-vector $|\alpha\rangle$ and bra-vector $\langle\alpha| .{ }^{6}$

One should be cautions with the term "vector" here. Usual "geometric" vectors are defined in the usual geometric (say, Euclidean) space. In contrast, bra- and ket-vectors are defined in abstract Hilbert spaces of a given system, ${ }^{7}$ and, despite certain similarities with the geometric vectors, are new mathematical objects, so that we need new rules for handling them. The primary rules are essentially postulates and are justified only the correct description/prediction of all experimental observations their corollaries. While these is a general consensus among physicists what the corollaries are, there are many possible ways to carve from them the basic postulate sets. Just as in Sec. 1.2, I will not try too hard to beat the number of the postulates to the smallest possible minimum, trying instead to keep their physical meaning transparent.


Fig. 4.3. Particle's state and its descriptions.
(i) Ket-vectors. Let us start with ket-vectors - sometimes called just kets for short. Perhaps the most important property of the vectors concerns their linear superposition. Namely, if several ketvectors $\left|\alpha_{j}\right\rangle$ describe possible states of a quantum system, then any linear combination (superposition)

$$
\begin{equation*}
|\alpha\rangle=\sum_{j} c_{j}\left|\alpha_{j}\right\rangle \tag{4.6}
\end{equation*}
$$

[^579]where $c_{j}$ are any (possibly complex) $c$-numbers, also describes a possible state of the same system. (One may say that vector $|\alpha\rangle$ belongs to the same Hilbert space as all $\left|\alpha_{j}\right\rangle$.) Actually, since ket-vectors are new mathematical objects, the exact meaning of the right-hand part of Eq. (6) becomes clear only after we have postulated the following rules of summation of these vectors,
\[

$$
\begin{equation*}
\left|\alpha_{j}\right\rangle+\left|\alpha_{j^{\prime}}\right\rangle=\left|\alpha_{j^{\prime}}\right\rangle+\left|\alpha_{j}\right\rangle, \tag{4.7}
\end{equation*}
$$

\]

and their multiplication by $c$-numbers:

$$
\begin{equation*}
c_{j}\left|\alpha_{j}\right\rangle=\left|\alpha_{j}\right\rangle c_{j} . \tag{4.8}
\end{equation*}
$$

Note that in the set of wave mechanics postulates, statements parallel to (7) and (8) were unnecessary, because wavefunctions are the usual (albeit complex) functions of space and time, and we know from the usual algebra that such relations are valid.

As evident from Eq. (6), the complex coefficient $c_{j}$ may be interpreted as the "weight" of state $\alpha_{j}$ in the linear superposition $\alpha$. One important particular case is $c_{j}=0$, showing that state $\alpha_{j}$ does not participate in the superposition $\alpha$. By the way, the corresponding term of sum (6), i.e. product

Null-state
vector

$$
\begin{equation*}
0\left|\alpha_{j}\right\rangle \tag{4.9}
\end{equation*}
$$

has a special name: the null-state vector. (It is important to avoid confusion between the null-state corresponding to vector (9), and the ground state of the system, which is frequently denoted by ketvector $|0\rangle$. In some sense, the null-state does not exist at all, while the ground state does - and frequently is the most important quantum state of the system.)
(ii) Bra-vectors and inner ("scalar") products. Bra-vectors $\langle\alpha|$, which obey the rules similar to Eqs. (7) and (8), are not new, independent objects: if a ket-vector $|\alpha\rangle$ is known, the corresponding bravector $\langle\alpha|$ describes the same state. In other words, there is a unique dual correspondence between $|\alpha\rangle$ and $\langle\alpha|,{ }^{8}$ very similar (though not identical) to that between a wavefunction $\Psi$ and its complex conjugate $\Psi^{*}$. The correspondence between these vectors is described by the following rule: if a ket-vector of a linear superposition is described by Eq. (6), then the corresponding bra-vector is

Linear
superposition of bra-vectors

$$
\begin{equation*}
\langle\alpha|=\sum_{j} c_{j}^{*}\left\langle\alpha_{j}\right|=\sum_{j}\left\langle\alpha_{j}\right| c_{j}^{*} \tag{4.10}
\end{equation*}
$$

The mathematical convenience of using two types of vectors, rather than just one, becomes clear from the notion of their inner product (also called the short bracket):

Inner bra-ket product

$$
\begin{equation*}
\langle\beta \| \alpha\rangle \equiv\langle\beta \mid \alpha\rangle . \tag{4.11}
\end{equation*}
$$

This is a (generally, complex) ${ }^{9}$ scalar, whose main property is the linearity with respect to any of its component vectors. For example, if a linear superposition $\alpha$ is described by the ket-vector (6), then

[^580]\[

$$
\begin{equation*}
\langle\beta \mid \alpha\rangle=\sum_{j} c_{j}\left\langle\beta \mid \alpha_{j}\right\rangle \tag{4.12}
\end{equation*}
$$

\]

while if Eq. (10) is true, then

$$
\begin{equation*}
\langle\alpha \mid \beta\rangle=\sum_{j} c_{j}^{*}\left\langle\alpha_{j} \mid \beta\right\rangle . \tag{4.13}
\end{equation*}
$$

In plain English, $c$-numbers may be moved either into, or out of the inner products.
The second key property of the inner product is

$$
\begin{equation*}
\langle\alpha \mid \beta\rangle=\langle\beta \mid \alpha\rangle^{*} \tag{4.14}
\end{equation*}
$$

It is compatible with Eq. (10); indeed, the complex conjugation of both parts of Eq. (12) gives:

$$
\begin{equation*}
\langle\beta \mid \alpha\rangle^{*}=\sum_{j} c_{j}^{*}\left\langle\beta \mid \alpha_{j}\right\rangle^{*}=\sum_{j} c_{j}^{*}\left\langle\alpha_{j} \mid \beta\right\rangle=\langle\alpha \mid \beta\rangle . \tag{4.15}
\end{equation*}
$$

Finally, one more rule: the inner product of the bra- and ket-vectors describing the same state (called the norm squared) is real and non-negative,

$$
\begin{equation*}
\|\alpha\|^{2} \equiv\langle\alpha \mid \alpha\rangle \geq 0 \tag{4.16}
\end{equation*}
$$

Inner product's complex conjugate

In order to give the reader some feeling about the meaning of this rule: we will show below that if state $\alpha$ may be described by wavefunction $\Psi_{\alpha}(\mathbf{r}, t)$, then

$$
\begin{equation*}
\langle\alpha \mid \alpha\rangle=\int \Psi_{\alpha}^{*} \Psi_{\alpha} d^{3} r \geq 0 \tag{4.17}
\end{equation*}
$$

Hence the role of the bra-ket is very similar to the complex conjugation of the wavefunction, and Eq. (10) emphasizes this similarity. (Note that, by convention, there is no conjugation sign in the bra-part of the inner product; its role is played by the angular bracket inversion.)
(iii) Operators. One more key notion of the Dirac formalism are quantum-mechanical linear operators. Just as for the operators discussed in wave mechanics, the function of an operator is the "generation" of one state from another: if $|\alpha\rangle$ is a possible ket of the system, and $\hat{A}$ is a legitimate operator, then the following combination,

$$
\begin{equation*}
\hat{A}|\alpha\rangle \tag{4.18}
\end{equation*}
$$

is also a ket-vector describing a possible state of the system, i.e. a ket-vector in the same Hilbert space as the initial vector $|\alpha\rangle$. As follows from the adjective "linear", the main rules governing the operators is their linearity with respect to both any superposition of vectors:

$$
\begin{equation*}
\hat{A}\left(\sum_{j} c_{j}\left|\alpha_{j}\right\rangle\right)=\sum_{j} c_{j} \hat{A}\left|\alpha_{j}\right\rangle \tag{4.19}
\end{equation*}
$$

and any superposition of operators:

$$
\begin{equation*}
\left(\sum_{j} c_{j} \hat{A}_{j}\right)|\alpha\rangle=\sum_{j} c_{j} \hat{A}_{j}|\alpha\rangle \tag{4.20}
\end{equation*}
$$

These rules are evidently similar to Eqs. (1.53)-(1.54) of wave mechanics.
The above rules imply that an operator "acts" on the ket-vector on its right; however, a combination of the type $\langle\alpha| \hat{A}$ is also legitimate and presents a new bra-vector. It is important that, generally, this vector does not represent the same state as ket-vector (18); instead, the bra-vector isomorphic to ket-vector (18) is

Hermitian conjugate operator

Hermitian operator's definition

$$
\begin{equation*}
\langle\alpha| \hat{A}^{\dagger} \tag{4.21}
\end{equation*}
$$

This statement serves as the definition of the Hermitian conjugate (or "Hermitian adjoint") $\hat{A}^{\dagger}$ of the initial operator $\hat{A}$. For an important class of operators, called the Hermitian operators, the conjugation is inconsequential, i.e. for them

$$
\begin{equation*}
\hat{A}^{\dagger}=\hat{A} . \tag{4.22}
\end{equation*}
$$

(This equality, as well as any other operator equation below, means that these operators act similarly on any bra- or ket-vector.) ${ }^{10}$

To proceed further, we need an additional postulate, called the associative axiom of multiplication: into any legitimate bra-ket expression, ${ }^{11}$ not including an explicit summation, we may insert or remove parentheses (just in the ordinary product of scalars), meaning as usual that the operation inside the parentheses is performed first. The first two examples of this postulate are given by Eqs. (19) and (20), but the associative axiom is more general and says, for example:

$$
\begin{equation*}
\langle\beta|(\hat{A}|\alpha\rangle)=(\langle\beta| \hat{A})|\alpha\rangle \equiv\langle\beta| \hat{A}|\alpha\rangle, \tag{4.23}
\end{equation*}
$$

This equality serves as the definition of the last form, called the long bracket (evidently, also a scalar), with an operator sandwiched between a bra-vector and a ket-vector. This definition, when combined with the definition of the Hermitian conjugate and Eq. (14), yields an important corollary:

$$
\begin{equation*}
\langle\beta| \hat{A}|\alpha\rangle=\langle\beta|(\hat{A}|\alpha\rangle)=\left(\left(\langle\alpha| \hat{A}^{\dagger}\right)|\beta\rangle\right)^{*}=\langle\alpha| \hat{A}^{\dagger}|\beta\rangle^{*} \tag{4.24}
\end{equation*}
$$

which is most frequently rewritten as

$$
\begin{equation*}
\langle\alpha| \hat{A}|\beta\rangle^{*}=\langle\beta| \hat{A}^{\dagger}|\alpha\rangle \tag{4.25}
\end{equation*}
$$

The associative axiom also enables to readily explore the following definition of one more, outer product of bra- and ket-vectors:

[^581]\[

$$
\begin{equation*}
|\beta\rangle\langle\alpha| \tag{4.26}
\end{equation*}
$$

\]

In contrast to the inner product (12), which is a scalar, this mathematical construct is an operator. Indeed, the associative axiom allows us to remove parentheses in the following expression:

$$
\begin{equation*}
(|\beta\rangle\langle\alpha|) \gamma\rangle=|\beta\rangle\langle\alpha \mid \gamma\rangle . \tag{4.27}
\end{equation*}
$$

But the last bra-ket is just a scalar; hence the mathematical object (26) acting on a ket-vector (in this case, $|\gamma\rangle$ ) gives a new ket-vector, which is the essence of operator's action. Very similarly,

$$
\begin{equation*}
\langle\delta|(|\beta\rangle\langle\alpha|)=\langle\delta \mid \beta\rangle\langle\alpha| \tag{4.28}
\end{equation*}
$$

- again a typical operator's action on a bra-vector.

Now let us perform the following calculation. We may use the parentheses insertion into the braket equality following from Eq. (14),

$$
\begin{equation*}
\langle\gamma \mid \alpha\rangle\langle\beta \mid \delta\rangle=(\langle\delta \mid \beta\rangle\langle\alpha \mid \gamma\rangle)^{*}, \tag{4.29}
\end{equation*}
$$

to transform it to the following form:

$$
\begin{equation*}
\langle\gamma|(|\alpha\rangle\langle\beta|)|\delta\rangle=(\langle\delta|(|\beta\rangle\langle\alpha|)|\gamma\rangle)^{*} . \tag{4.30}
\end{equation*}
$$

Since this equation should be valid for any vectors $\langle\gamma|$ and $|\beta\rangle$, its comparison with Eq. (25) gives the following operator equality

$$
\begin{equation*}
(|\alpha\rangle\langle\beta|)^{\dagger}=|\beta\rangle\langle\alpha| . \tag{4.31}
\end{equation*}
$$

This is the conjugate rule for outer products; it reminds rule (14) for inner products, but involves the Hermitian (rather than the usual complex) conjugation.

The associative axiom is also valid for the operator "multiplication":

$$
\begin{equation*}
(\hat{A} \hat{B})|\alpha\rangle=\hat{A}(\hat{B}|\alpha\rangle), \quad\langle\beta|(\hat{A} \hat{B})=(\langle\beta| \hat{A}) \hat{B} \tag{4.32}
\end{equation*}
$$

showing that the action of an operator product on a state vector is nothing more than the sequential action of the operands. However, we have to be rather careful with the operator products; generally they do not commute: $\hat{A} \hat{B} \neq \hat{B} \hat{A}$. This is why the commutator, the operator defined as

$$
\begin{equation*}
[\hat{A}, \hat{B}] \equiv \hat{A} \hat{B}-\hat{B} \hat{A} \tag{4.33}
\end{equation*}
$$

is a very useful option. Another similar notion is the anticommutator: ${ }^{12}$

$$
\begin{equation*}
\{\hat{A}, \hat{B}\} \equiv \hat{A} \hat{B}+\hat{B} \hat{A} . \tag{4.34}
\end{equation*}
$$

Finally, the bra-ket formalism broadly uses two special operators: the null operator $\hat{0}$ defined by the following relations:

[^582]Identity
operator

Expansion over
basis vectors

$$
\begin{equation*}
\hat{0}|\alpha\rangle \equiv 0|\alpha\rangle, \quad\langle\alpha| \hat{0} \equiv\langle\alpha| 0, \tag{4.35}
\end{equation*}
$$

for an arbitrary state $\alpha$; we may say that the null operator "kills" any state, turning it into the null-state. Another elementary operator is the identity operator, which is also defined by its action (or rather "inaction" :-) on an arbitrary state vector:


$$
\begin{equation*}
\hat{I}|\alpha\rangle \equiv|\alpha\rangle, \quad\langle\alpha| \hat{I} \equiv\langle\alpha| \tag{4.36}
\end{equation*}
$$

### 4.3. State basis and matrix representation

While some operations in quantum mechanics may be carried out in the general bra-ket formalism outlined above, most calculations are done for specific quantum systems that feature at least one full and orthonormal set $\{u\}$ of states $u_{j}$, frequently called a basis. These terms mean that any state vector of the system may be represented as a unique sum of the type (6) or (10) over its basis vectors:

$$
\begin{equation*}
|\alpha\rangle=\sum_{j} \alpha_{j}\left|u_{j}\right\rangle, \quad\langle\alpha|=\sum_{j} \alpha_{j}^{*}\left\langle u_{j}\right| \tag{4.37}
\end{equation*}
$$

(so that, in particular, if $\alpha$ is one of the basis states, say $u_{j}$, then $\alpha_{j}=\delta_{j j}$,), and that

For the systems that may be described by wave mechanics, examples of the full orthonormal bases are
represented by any orthonormal set of eigenfunctions calculated in the previous 3 chapters - as the
For the systems that may be described by wave mechanics, examples of the full orthonormal bases are
represented by any orthonormal set of eigenfunctions calculated in the previous 3 chapters - as the simplest example, see Eq. (1.76).

Due to the uniqueness of expansion (37), the full set of coefficients $\alpha_{j}$ gives a complete description of state $\alpha$ (in a fixed basis $\{u\}$ ), just as the usual Cartesian components $A_{x}, A_{y}$, and $A_{z}$ give a complete description of a usual geometric 3D vector A (in a fixed reference frame). Still, let me emphasize some differences between the quantum-mechanical bra- and ket-vectors and the usual geometric vectors:
(i) a basis set may have a large or even infinite number of states $u_{j}$, and
(ii) the expansion coefficients $\alpha_{j}$ may be complex.

With these reservations in mind, the analogy with geometric vectors may be pushed even further.
inner-multiply both parts of the first of Eqs. (37) by a bra-vector $\left\langle u_{j^{\prime}}\right\rangle$ and then transform the
With these reservations in mind, the analogy with geometric vectors may be pushed even further.
Let us inner-multiply both parts of the first of Eqs. (37) by a bra-vector $\left\langle u_{j}{ }^{\prime}\right|$ and then transform the relation using the linearity rules discussed in the previous section, and Eq. (38):

$$
\begin{equation*}
\left\langle u_{j^{\prime}} \mid \alpha\right\rangle=\left\langle u_{j^{\prime}}\right| \sum_{j} \alpha_{j}\left|u_{j}\right\rangle=\sum_{j} \alpha_{j}\left\langle u_{j^{\prime}} \mid u_{j}\right\rangle=\alpha_{j^{\prime}}, \tag{4.39}
\end{equation*}
$$

Together with Eq. (14), this means that any of the expansion coefficients in Eq. (37) may be presented as an inner product:

Expansion coefficients as inner products

$$
\begin{equation*}
\left\langle u_{j} \mid u_{j^{\prime}}\right\rangle=\delta_{j j^{\prime}} \tag{4.38}
\end{equation*}
$$


七-
these relations are analogs of equalities $A_{j}=\mathbf{n}_{j} \cdot \mathbf{A}$ of the usual vector algebra. Using these important relations (which we will use on numerous occasions), expansions (37) may be rewritten as

$$
\begin{equation*}
|\alpha\rangle=\sum_{j}\left|u_{j}\right\rangle\left\langle u_{j} \mid \alpha\right\rangle \equiv \sum_{j} \hat{\Lambda}_{j}|\alpha\rangle, \quad\langle\alpha|=\sum_{j}\left\langle\alpha \mid u_{j}\right\rangle\left\langle u_{j}\right| \equiv \sum_{j}\langle\alpha| \hat{\Lambda}_{j}, \tag{4.41}
\end{equation*}
$$

A comparison of these relations with Eq. (26) shows that the outer product defined as

$$
\begin{equation*}
\hat{\Lambda}_{j} \equiv\left|u_{j}\right\rangle\left\langle u_{j}\right|, \tag{4.42}
\end{equation*}
$$

is a legitimate linear operator. Such an operator, acting on any state vector of the type (37), singles out just one of its components, for example,

$$
\begin{equation*}
\hat{\Lambda}_{j}|\alpha\rangle=\left|u_{j}\right\rangle\left\langle u_{j} \mid \alpha\right\rangle=\alpha_{j}\left|u_{j}\right\rangle, \tag{4.43}
\end{equation*}
$$

i.e. kills all components of the linear superposition but one. In the geometric analogy, such operator "projects" the state vector on its ( $j^{\text {th }}$ ) "direction", hence its name - the projection operator. Probably, the most important property of the projection operators, called the closure (or completeness) relation, immediately follows from Eq. (41): their sum over the full basis is equivalent to the identity operator:

$$
\begin{equation*}
\sum_{j}\left|u_{j}\right\rangle\left\langle u_{j}\right|=\hat{I} \tag{4.44}
\end{equation*}
$$

This means in particular that we may insert the left-hand part of Eq. (44) into any bra-ket relation, at any place - the trick that we will use again and again.

Let us see how expansions (37) transform all the notions introduced in the last section, starting from the short bra-ket (11) (the inner product of two state vectors):

$$
\begin{equation*}
\langle\beta \mid \alpha\rangle=\sum_{j, j^{\prime}}\left\langle u_{j}\right| \beta_{j}^{*} \alpha_{j^{\prime}}\left|u_{j^{\prime}}\right\rangle=\sum_{j, j^{\prime}} \beta_{j}^{*} \alpha_{j^{\prime}} \delta_{j j^{\prime}}=\sum_{j} \beta_{j}^{*} \alpha_{j} . \tag{4.45}
\end{equation*}
$$

Besides the complex conjugation, this expression is similar to the scalar product of the usual vectors. Now, let us explore the long bra-ket (23):

$$
\begin{equation*}
\langle\beta| \hat{A}|\alpha\rangle=\sum_{j, j^{\prime}} \beta_{j}^{*}\left\langle u_{j}\right| \hat{A}\left|u_{j^{\prime}}\right\rangle \alpha_{j^{\prime}} \equiv \sum_{j, j^{\prime}} \beta_{j}^{*} A_{j j^{\prime}} \alpha_{j^{\prime}} . \tag{4.46}
\end{equation*}
$$

Here, the last step uses a very important notion of matrix elements of the operator, defined as

$$
\begin{equation*}
A_{j j^{\prime}} \equiv\left\langle u_{j}\right| \hat{A}\left|u_{j^{\prime}}\right\rangle \tag{4.47}
\end{equation*}
$$


while for the identity operator $\hat{I}$, defined by Eqs. (36), we readily get

$$
\begin{equation*}
I_{i j^{\prime}}=\left\langle u_{j}\right| \hat{I}\left|u_{j^{\prime}}\right\rangle=\left\langle u_{j} \mid u_{j^{\prime}}\right\rangle=\delta_{j j^{\prime}}, \tag{4.49}
\end{equation*}
$$

i.e. its matrix (called the identity matrix) is diagonal - also in any basis:

Identity matrix

$$
\mathrm{I} \equiv\left(\begin{array}{ccc}
1 & 0 & \ldots  \tag{4.50}\\
0 & 1 & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right) .
$$

The convenience of the matrix language extends well beyond the presentation of particular operators. For example, let us use definition (47) to calculate matrix elements for a product of two operators:

$$
\begin{equation*}
(A B)_{j j^{\prime \prime}}=\left\langle u_{j}\right| \hat{A} \hat{B}\left|u_{j^{\prime \prime}}\right\rangle . \tag{4.51}
\end{equation*}
$$

Here we can use Eq. (44) for the first (but not the last!) time, inserting the identity operator between the two operators, and then expressing it via a sum of projection operators:

Matrix element of an operator product

$$
\begin{equation*}
(A B)_{j j^{\prime \prime}}=\left\langle u_{j}\right| \hat{A} \hat{B}\left|u_{j^{\prime \prime}}\right\rangle=\left\langle u_{j}\right| \hat{A} \hat{I} \hat{B}\left|u_{j^{\prime \prime}}\right\rangle=\sum_{j^{\prime}}\left\langle u_{j}\right| \hat{A}\left|u_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}}\right| \hat{B}\left|u_{j^{\prime \prime}}\right\rangle=\sum_{j^{\prime}} A_{j j^{\prime}} B_{j j^{\prime \prime}} \tag{4.52}
\end{equation*}
$$

This result corresponds to the standard "row by column" rule of calculation of an arbitrary element of the matrix product

$$
\mathrm{AB}=\left(\begin{array}{ccc}
A_{11} & A_{12} & \ldots  \tag{4.53}\\
A_{21} & A_{22} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{ccc}
B_{11} & B_{12} & \ldots \\
B_{21} & B_{22} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right) .
$$

Hence the product of operators may be presented (in a fixed basis!) by that of their matrices (in the same basis). This is so convenient that the same language is often used to present not only the long bracket,

Long
bracket
as a matrix product

Short bracket as a matrix product

$$
\langle\beta| \hat{A}|\alpha\rangle=\sum_{j^{\prime}} \beta_{j}^{*} A_{j j} \alpha_{j^{\prime}}=\left(\beta_{1}^{*}, \beta_{2}^{*}, \ldots\right)\left(\begin{array}{ccc}
A_{11} & A_{12} & \ldots  \tag{4.54}\\
A_{21} & A_{22} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{c}
\alpha_{1} \\
\alpha_{2} \\
\ldots
\end{array}\right)
$$

but even the simpler short bracket:

$$
\langle\beta \mid \alpha\rangle=\sum_{j} \beta_{j}^{*} \alpha_{j}=\left(\beta_{1}^{*}, \beta_{2}^{*}, \ldots\right)\left(\begin{array}{c}
\alpha_{1}  \tag{4.55}\\
\alpha_{2} \\
\ldots
\end{array}\right)
$$

although these equalities require the use of non-square matrices: rows of (complex-conjugate!) expansion coefficients for the presentation of bra-vectors, and columns of these coefficients for the presentation of ket-vectors. With that, the mapping of states and operators on matrices becomes completely general.

Now let us have a look at the outer product operator (26). Its matrix elements are just

$$
\begin{equation*}
(|\alpha\rangle\langle\beta|)_{i j^{\prime}}=\left\langle u_{j} \mid \alpha\right\rangle\left\langle\beta \mid u_{j^{\prime}}\right\rangle=\alpha_{j} \beta_{j^{\prime}}^{*} . \tag{4.56}
\end{equation*}
$$

These are elements of a very special square matrix, whose filling requires the knowledge of just 2 N scalars (where $N$ is the basis set size), rather than $N^{2}$ scalars as for an arbitrary operator. However, a simple generalization of such outer product may present an arbitrary operator. Indeed, let us insert two identity operators (44), with different summation indices, on both sides of any operator:

$$
\begin{equation*}
\hat{A}=\hat{I} \hat{A} \hat{I}=\left(\sum_{j}\left|u_{j}\right\rangle\left\langle u_{j}\right|\right) \hat{A}\left(\sum_{j^{\prime}}\left|u_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}}\right|\right), \tag{4.57}
\end{equation*}
$$

and use the associative axiom to rewrite this expression as

$$
\begin{equation*}
\hat{A}=\sum_{j, j^{\prime}}\left|u_{j}\right\rangle\left\langle u_{j}\right| \hat{A}\left|u_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}}\right| . \tag{4.58}
\end{equation*}
$$

But the expression in the middle long bracket is just the matrix element (47), so that we may write

$$
\begin{equation*}
\hat{A}=\sum_{j, j^{\prime}}\left|u_{j}\right\rangle A_{j j^{\prime}}\left\langle u_{j^{\prime}}\right| . \tag{4.59}
\end{equation*}
$$

Operator's expression via its matrix elements
The reader has to agree that this formula, which is a natural generalization of Eq. (44), is extremely elegant. Also note the following parallel: if we consider the matrix element definition (47) as some sort of analog of Eq. (40), then Eq. (59) is a similar analog of the expansion expressed by Eq. (37).

The matrix presentation is so convenient that it makes sense to move it by one level lower - from state vector products to "bare" state vectors resulting from operator's action upon a given state. For example, let us use Eq. (59) to present the ket-vector (18) as

$$
\begin{equation*}
\left.\left|\alpha^{\prime}\right\rangle \equiv \hat{A}|\alpha\rangle=\left(\sum_{j, j^{\prime}}\left|u_{j}\right\rangle A_{i j^{\prime}}\left\langle u_{j^{\prime}}\right|\right) \alpha\right\rangle=\sum_{j, j^{\prime}}\left|u_{j}\right\rangle A_{j j^{\prime}}\left\langle u_{j^{\prime}} \mid \alpha\right\rangle . \tag{4.60}
\end{equation*}
$$

According to Eq. (40), the last short bracket is just $\alpha_{j}$, so that

$$
\begin{equation*}
\left|\alpha^{\prime}\right\rangle=\sum_{j, j^{\prime}}\left|u_{j}\right\rangle A_{i j j^{\prime}} \alpha_{j^{\prime}}=\sum_{j}\left(\sum_{j^{\prime}} A_{i j^{\prime}} \alpha_{j^{\prime}}\right)\left|u_{j}\right\rangle \tag{4.61}
\end{equation*}
$$

But expression in middle parentheses is just the coefficient $\alpha_{j}^{\prime}$ of expansion (37) of the resulting ketvector (60) in the same basis, so that

$$
\begin{equation*}
\alpha_{j}^{\prime}=\sum_{j^{\prime}} A_{j j^{\prime}} \alpha_{j^{\prime}} \tag{4.62}
\end{equation*}
$$

This result corresponds to the usual rule of multiplication of a matrix by a column, so that we may represent any ket-vector by its column matrix, with the operator action looking like

$$
\left(\begin{array}{c}
\alpha_{1}^{\prime}  \tag{4.63}\\
\alpha_{2}^{\prime} \\
\ldots
\end{array}\right)=\left(\begin{array}{ccc}
A_{11} & A_{12} & \ldots \\
A_{21} & A_{22} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{c}
\alpha_{1} \\
\alpha_{2} \\
\ldots
\end{array}\right) .
$$

Absolutely similarly, the operator action on the bra-vector (21), represented by its row-matrix, is

$$
\left({\alpha_{1}^{\prime *}}^{*}, \alpha_{2}^{\prime *}, \ldots\right)=\left(\alpha_{1}^{*}, \alpha_{2}^{*}, \ldots\right)\left(\begin{array}{ccc}
\left(A^{\dagger}\right)_{11} & \left(A^{\dagger}\right)_{12} & \ldots  \tag{4.64}\\
\left(A^{\dagger}\right)_{21} & \left(A^{\dagger}\right)_{22} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right) .
$$

By the way, Eq. (64) naturally raises the following question: what are the elements of the matrix in its right-hand part, or more exactly, what is the relation between the matrix elements of an operator and its Hermitian conjugate? The simplest way to get an answer is to use Eq. (25) with two arbitrary states (say, $u_{j}$ and $u_{j}$ ) of the same basis in the role of $\alpha$ and $\beta$. Together with the orthonormality relation (38), this immediately gives ${ }^{13}$

Hermitian conjugate's matrix elements

$$
\begin{equation*}
\left(\hat{A}^{\dagger}\right)_{i j j^{\prime}}=\left(A_{j^{\prime} j}\right)^{*} \tag{4.65}
\end{equation*}
$$

Thus, the matrix of the Hermitian conjugate operator is the complex conjugated and transposed matrix of the initial operator. This result exposes very clearly the essence of the Hermitian conjugation. It also shows that for the Hermitian operators, defined by Eq. (22),

$$
\begin{equation*}
A_{j j^{\prime}}=A_{j^{\prime} j}^{*}, \tag{4.66}
\end{equation*}
$$

i.e. any pair of their matrix elements, symmetric about the main diagonal, should be complex conjugate of each other. As a corollary, the main-diagonal elements have to be real:

$$
\begin{equation*}
A_{i j}=A_{i j}^{*} \text {, i.e. } \operatorname{Im} A_{j j}=0 \tag{4.67}
\end{equation*}
$$

(Matrix (50) evidently satisfies Eq. (66), so that the identity operator is Hermitian.)
In order to fully appreciate the special role played by Hermitian operators in the quantum theory, let us introduce the key notions of eigenstates $a_{j}$ (described by their eigenvectors $\left\langle a_{j}\right|$ and $\left|a_{j}\right\rangle$ ) and eigenvalues (c-numbers) $A_{j}$ of an operator $\hat{A}$, defined by the equation they have to satisfy: ${ }^{14}$

Operator's eigenstates eigenvalues

Hermitian operator's eigenvalues

Let us prove that eigenvalues of any Hermitian operator are real, ${ }^{15}$

$$
\begin{equation*}
A_{j}=A_{j}^{*}, \quad \text { for } j=1,2, \ldots, N \tag{4.69}
\end{equation*}
$$

[^583]while the eigenstates corresponding to different eigenvalues are orthogonal:
\[

$$
\begin{equation*}
\left\langle a_{j} \mid a_{j^{\prime}}\right\rangle=0, \quad \text { if } A_{j} \neq A_{j^{\prime}} . \tag{4.70}
\end{equation*}
$$

\]

The proof of both statements is surprisingly simple. Let us inner-multiply both sides of Eq. (68) by bra-vector $\left\langle a_{j}\right\rangle$. In the right-hand part of the result, the eigenvalue $A_{j}$, as a $c$-number, may be taken out of the bra-ket, giving

$$
\begin{equation*}
\left\langle a_{j^{\prime}}\right| \hat{A}\left|a_{j}\right\rangle=A_{j}\left\langle a_{j^{\prime}} \mid a_{j}\right\rangle . \tag{4.71}
\end{equation*}
$$

This equality should hold for any pair of eigenstates, so that we may swap the indices in Eq. (71), and complex-conjugate the result:

$$
\begin{equation*}
\left\langle a_{j}\right| \hat{A}\left|a_{j^{\prime}}\right\rangle^{*}=A_{j^{\prime}}^{*}\left\langle a_{j} \mid a_{j^{\prime}}\right\rangle^{*} . \tag{4.72}
\end{equation*}
$$

Now using Eqs. (14) and (25), together with the Hermitian operator definition (22), we may transform Eq. (72) to the following form:

$$
\begin{equation*}
\left\langle a_{j^{\prime}}\right| \hat{A}\left|a_{j}\right\rangle=A_{j^{\prime}}^{*}\left\langle a_{j^{\prime}} \mid a_{j}\right\rangle . \tag{4.73}
\end{equation*}
$$

Subtracting this equation from Eq. (71), we get

$$
\begin{equation*}
0=\left(A_{j}-A_{j^{\prime}}^{*}\right)\left\langle a_{j^{\prime}} \mid a_{j}\right\rangle . \tag{4.74}
\end{equation*}
$$

There are two possibilities to satisfy this equation. If indices $j$ and $j$ ' are equal (denote the same eigenstate), then the bra-ket is the state's norm squared, and cannot be equal to zero. Then the left parentheses (with $j=j^{\prime}$ ) have to be zero, i.e. Eq. (69) is valid. On the other hand, if $j$ and $j$ ' correspond to different eigenvalues of $\hat{A}$, the parentheses cannot equal zero (we have just proved that all $A_{j}$ are real!), and hence the state vectors indexed by $j$ and $j$ ' should be orthogonal, e.g., Eq. (70) is valid.

As will be discussed below, these properties make Hermitian operators suitable for the description of physical observables.

### 4.4. Change of basis and matrix diagonalization

From the discussion of last section, it may look that the matrix language is fully similar to, and in many instances more convenient than the general bra-ket formalism. In particular, Eqs. (52), (54), (55) show that any part of any bra-ket expression may be directly mapped on the similar matrix expression, with the only slight inconvenience of using not only columns, but also rows (with their elements complex-conjugated), for state vector presentation. In this context, why do we need the bra-ket language at all? The answer is that the elements of the matrices depend on the particular choice of the basis set, very much like the Cartesian components of a usual vector depend on the particular choice of reference frame orientation (Fig. 4), and very frequently it is convenient to use two or more different basis sets for the same system.

With this motivation, let us study what happens if we change from one basis, $\{u\}$, to another one, $\{v\}$ - both full and orthonormal. First of all, let us prove that for each such pair of bases, there exists such an operator $\hat{U}$ that, first,

Basis transform

$$
\begin{equation*}
\left|v_{j}\right\rangle=\hat{U}\left|u_{j}\right\rangle \tag{4.75}
\end{equation*}
$$

and, second,

Unitary operator's definition

Unitary operator of basis transform

$$
\begin{equation*}
\hat{U} \hat{U}^{\dagger}=\hat{U}^{\dagger} \hat{U}=\hat{I} \tag{4.76}
\end{equation*}
$$

(Due to the last property, ${ }^{16} \hat{U}$ is called a unitary operator, and Eq. (75), a unitary transformation.)


Fig. 4.4. Transformation of components of a 2 D vector at a reference frame rotation.

A very simple proof of both statements may be achieved by construction. Indeed, let us take

$$
\begin{equation*}
\hat{U} \equiv \sum_{j^{\prime}}\left|v_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}}\right| \tag{4.77}
\end{equation*}
$$

- an evident generalization of Eq. (44). Then

$$
\begin{equation*}
\hat{U}\left|u_{j}\right\rangle=\sum_{j^{\prime}}\left|v_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}} \mid u_{j}\right\rangle=\sum_{j^{\prime}}\left|v_{j^{\prime}}\right\rangle \delta_{j^{\prime} j}=\left|v_{j}\right\rangle, \tag{4.78}
\end{equation*}
$$

so that Eq. (75) has been proved. Now, applying Eq. (31) to each term of sum (77), we get

$$
\begin{equation*}
\hat{U}^{\dagger} \equiv \sum_{j^{\prime}}\left|u_{j^{\prime}}\right\rangle\left\langle v_{j^{\prime}}\right| \tag{4.79}
\end{equation*}
$$

so that

$$
\begin{equation*}
\hat{U} \hat{U}^{\dagger}=\sum_{j, j^{\prime}}\left|v_{j}\right\rangle\left\langle u_{j} \mid u_{j^{\prime}}\right\rangle\left\langle v_{j^{\prime}}\right|=\sum_{j, j^{\prime}}\left|v_{j}\right\rangle \delta_{j j^{\prime}}\left\langle v_{j^{\prime}}\right|=\sum_{j}\left|v_{j}\right\rangle\left\langle v_{j}\right| . \tag{4.80}
\end{equation*}
$$

But according to the closure relation (44), the last expression is just the identity operator, q.e.d. ${ }^{17}$ (The proof of the second equality in Eq. (76) is absolutely similar.)

As a by-product of our proof, we have also got another important expression (79). It implies, in particular, that while, according to Eq. (77), operator $\hat{U}$ performs the transform from the "old" basis $u_{j}$ to the "new" basis $v_{j}$, its Hermitian adjoint $\hat{U}^{\dagger}$ performs the reciprocal unitary transform:

Reciprocal
basis transform

$$
\begin{equation*}
\hat{U}^{\dagger}\left|v_{j}\right\rangle=\sum_{j^{\prime}}\left|u_{j^{\prime}}\right\rangle \delta_{j^{\prime} j}=\left|u_{j}\right\rangle . \tag{4.81}
\end{equation*}
$$

[^584]Now, let us see how do the matrix elements of the unitary transform operators look like. Generally, as was stated above, operator's elements depend on the basis we calculate them in, so we should be careful - initially. For example, let us calculate the elements in basis $\{u\}$ :

$$
\begin{equation*}
U_{i j^{\prime} \mid \text { in } u} \equiv\left\langle u_{j}\right| \hat{U}\left|u_{j^{\prime}}\right\rangle=\left\langle u_{j}\right|\left(\sum_{k}\left|v_{k}\right\rangle\left\langle u_{k}\right|\right)\left|u_{j^{\prime}}\right\rangle=\left\langle u_{j} \mid v_{j^{\prime}}\right\rangle . \tag{4.82}
\end{equation*}
$$

Now performing a similar calculation in basis $\{v\}$, we get

$$
\begin{equation*}
\left.U_{i j^{\prime}}\right|_{\text {in } v} \equiv\left\langle v_{j}\right| \hat{U}\left|v_{j^{\prime}}\right\rangle=\left\langle v_{j}\right|\left(\sum_{k}\left|v_{k}\right\rangle\left\langle u_{k}\right|\right)\left|v_{j^{\prime}}\right\rangle=\left\langle u_{j} \mid v_{j^{\prime}}\right\rangle . \tag{4.83}
\end{equation*}
$$

Surprisingly, the result is the same! This is of course true for the Hermitian conjugate of the unitary transform operator as well:

$$
\begin{equation*}
\left.U_{i j^{\prime}}^{\dagger}\right|_{\text {in } u}=\left.U_{i j^{\prime}}^{\dagger}\right|_{\text {in } v}=\left\langle v_{j} \mid u_{j^{\prime}}\right\rangle . \tag{4.84}
\end{equation*}
$$

These expressions may be used, first of all, to rewrite Eq. (75) in a more direct form. Applying the first of Eqs. (41) to state $v_{j}$ ' of the "new" basis, we get

$$
\begin{equation*}
\left|v_{j^{\prime}}\right\rangle=\sum_{j}\left|u_{j}\right\rangle\left\langle u_{j} \mid v_{j^{\prime}}\right\rangle=\sum_{j} U_{i j^{\prime}}\left|u_{j}\right\rangle \tag{4.85}
\end{equation*}
$$

Similarly, the reciprocal transform is

$$
\begin{equation*}
\left|u_{j^{\prime}}\right\rangle=\sum_{j}\left|v_{j}\right\rangle\left\langle v_{j} \mid u_{j^{\prime}}\right\rangle=\sum_{j} U_{j j^{\prime}}^{\dagger}\left|v_{j}\right\rangle \tag{4.86}
\end{equation*}
$$

These equations are very convenient for applications; we will use them already later in this section.
Next, we may use Eqs. (83), (84) to express the effect of the unitary transform on expansion coefficients (37) of vectors of an arbitrary state $\alpha$. In the "old" basis $\{u\}$, they are given by Eq. (40). Similarly, in the "new" basis $\{v\}$,

$$
\begin{equation*}
\left.\alpha_{j}\right|_{\text {in } v}=\left\langle v_{j} \mid \alpha\right\rangle . \tag{4.87}
\end{equation*}
$$

Again inserting the identity operator in the form of closure (44), with internal index $j^{\prime}$, and then using Eq. (84), we get

$$
\begin{equation*}
\left.\alpha_{j}\right|_{\text {in } v}=\left\langle v_{j}\right|\left(\sum_{j^{\prime}}\left|u_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}}\right|\right)|\alpha\rangle=\sum_{j^{\prime}}\left\langle v_{j} \mid u_{j^{\prime}}\right\rangle\left\langle u_{j^{\prime}} \mid \alpha\right\rangle=\sum_{j^{\prime}} U_{j j^{\prime}}^{\dagger}\left\langle u_{j^{\prime}} \mid \alpha\right\rangle=\sum_{j^{\prime}} U_{j j^{\prime}}^{\dagger} \alpha_{j^{\prime} \mid \text { in } u} . \tag{4.88}
\end{equation*}
$$

The reciprocal transform is (of course) performed by matrix elements of operator $\hat{U}$ :

$$
\begin{equation*}
\left.\alpha_{j}\right|_{\text {in } u}=\sum_{j^{\prime}} U_{j j^{\prime}},\left.\alpha_{j^{\prime}}\right|_{\text {in } v} \tag{4.89}
\end{equation*}
$$

Both structurally and philosophically, these expressions are similar to the transformation of components of a usual vector at coordinate frame rotation. For example, in two dimensions (Fig. 4):

$$
\binom{\alpha_{x}^{\prime}}{\alpha_{y}^{\prime}}=\left(\begin{array}{cc}
\cos \varphi & \sin \varphi  \tag{4.90}\\
-\sin \varphi & \cos \varphi
\end{array}\right)\binom{\alpha_{x}}{\alpha_{y}}
$$

(In this analogy, the equality to 1 of the determinant of the rotation matrix in Eq. (90) corresponds to the unitary property (76) of the unitary transform operators.) Please pay attention here: while the transform (75) from the "old" basis $\{u\}$ to the "new" basis $\{v\}$ is performed by the unitary operator, the change (88) of a state vectors components at this transformation requires its Hermitian conjugate. Actually, this is also natural from the point of view of the geometric analog of the unitary transform (Fig. 4): if the "new" reference frame $\left\{x, y^{\prime}\right\}$ is obtained by a counterclockwise rotation of the "old" frame $\{x, y\}$ by some angle $\varphi$, for the observer rotating with the frame, vector $\alpha$ (which is itself unchanged) rotates clockwise. Due to the analogy between expressions (88) and (89) on one hand, and our old friend Eq. (62) on the other hand, it is tempting to skip indices in our new results by writing

$$
\begin{equation*}
|\alpha\rangle_{\text {in } v}=\hat{U}^{\dagger}|\alpha\rangle_{\text {in } u}, \quad|\alpha\rangle_{\text {in } u}=\hat{U}|\alpha\rangle_{\text {in } v} . \tag{4.91}
\end{equation*}
$$

Since matrix elements of $\hat{U}$ and $\hat{U}^{\dagger}$ do not depend on basis, such language is not too bad; still, the symbolic Eq. (91) should not be confused with genuine (basis-independent) bra-ket equalities.

Now let us use the same trick of identity operator insertion, repeated twice, to find the transformation rule for matrix elements of an arbitrary operator:

$$
\begin{equation*}
\left.A_{j j^{\prime}}\right|_{\text {in } v} \equiv\left\langle v_{j}\right| \hat{A}\left|v_{j^{\prime}}\right\rangle=\left\langle v_{j}\right|\left(\sum_{k}\left|u_{k}\right\rangle\left\langle u_{k}\right|\right) \hat{A}\left(\sum_{k^{\prime}}\left|u_{k^{\prime}}\right\rangle\left\langle u_{k^{\prime}}\right|\right)\left|v_{j^{\prime}}\right\rangle=\left.\sum_{k, k^{\prime}} U_{j k}^{\dagger} A_{k k^{\prime}}\right|_{\text {in } u} U_{k j^{\prime}} ; \tag{4.92}
\end{equation*}
$$

Matrix elements' transforms
absolutely similarly, we can get

$$
\begin{equation*}
A_{i j^{\prime}} \mid \text { in } u \sum_{k, k^{\prime}} U_{j k} A_{k k^{\prime} \mid \text { in } v} U_{k j^{\prime}}^{\dagger} \tag{4.93}
\end{equation*}
$$

In the spirit of Eq. (91), we may present these results symbolically as well, in a compact bra-ket form:

$$
\begin{equation*}
\left.\hat{A}\right|_{\text {in } v}=\left.\hat{U}^{\dagger} \hat{A}\right|_{\text {in } u} \hat{U},\left.\quad \hat{A}\right|_{\text {in } u}=\left.\hat{U} \hat{A}\right|_{\text {in } v} \hat{U}^{\dagger} . \tag{4.94}
\end{equation*}
$$

As a sanity check, let us apply this result to the identity operator:

$$
\begin{equation*}
\left.\hat{I}\right|_{\text {in } v}=\left(\hat{U}^{\dagger} \hat{I} \hat{U}\right)_{\text {in } u}=\left(\hat{U}^{\dagger} \hat{U}\right)_{\text {in } u}=\left.\hat{I}\right|_{\text {in } u} \tag{4.95}
\end{equation*}
$$

- as it should be. One more invariant of the basis change is the trace of any operator, defined as the sum of the diagonal terms of its matrix in a certain basis:

Operator/
matrix trace

$$
\begin{equation*}
\operatorname{Tr} \hat{A} \equiv \operatorname{Tr} \mathrm{~A} \equiv \sum_{j} A_{i j} \tag{4.96}
\end{equation*}
$$

The (easy) proof of this fact, using the relations we have already discussed, is left for reader's exercise.
So far, I have implied that both state bases $\{u\}$ and $\{v\}$ are known, and the natural question is where does this information comes from in quantum mechanics of actual physical systems. To get a partial answer to this question, let us return to Eq. (68) that defines eigenstates and eigenvalues of an
operator. Let us assume that the eigenstates $a_{j}$ of a certain operator $\hat{A}$ form a full and orthonormal set, and find the matrix elements of the operator in the basis of these states. For that, it is sufficient to innermultiply both sides of Eq. (68), written for index $j^{\prime}$, by the bra-vector of an arbitrary state $a_{j}$ of the same set:

$$
\begin{equation*}
\left\langle a_{j}\right| \hat{A}\left|a_{j^{\prime}}\right\rangle=\left\langle a_{j}\right| A_{j^{\prime}}\left|a_{j^{\prime}}\right\rangle . \tag{4.97}
\end{equation*}
$$

The left-hand part is just the matrix element $A_{j j}$, we are looking for, while the right hand part is just $A_{j} \cdot \delta_{j j}$. As a result, we see that the matrix is diagonal, with the diagonal consisting of eigenvalues:

$$
\begin{equation*}
A_{i j^{\prime}}=A_{j} \delta_{j j^{\prime}} \tag{4.98}
\end{equation*}
$$

In particular, in the eigenstate basis (but not necessarily in an arbitrary basis!), $A_{j j}$ means the same as $A_{j}$. Thus the most important problem of finding the eigenvalues and eigenstates of an operator is equivalent to the diagonalization of its matrix, ${ }^{18}$ i.e. finding the basis in which the corresponding operator acquires the diagonal form (98); then the diagonal elements are the eigenvalues, and the basis itself is the desirable set of eigenstates.

Let us modify the above calculation by inner-multiplying Eq. (68) by a bra-vector of a different basis - say, the one, denoted $\{u\}$, in which we know the matrix elements $A_{j j}$. The multiplication gives

$$
\begin{equation*}
\left\langle u_{k}\right| \hat{A}\left|a_{j}\right\rangle=\left\langle u_{k}\right| A_{j}\left|a_{j}\right\rangle . \tag{4.99}
\end{equation*}
$$

In the left-hand part we can (as usual :-) insert the identity operator, between the operator and the ketvector, and then use the closure relation (44), while in the right-hand part, we can move the eigenvalue $A_{j}$ out of the bra-ket, and then insert a summation over a new index, compensating it with the proper Kronecker delta symbol:

$$
\begin{equation*}
\left\langle u_{k}\right| \hat{A} \sum_{k^{\prime}}\left|u_{k^{\prime}}\right\rangle\left\langle u_{k^{\prime}} \mid a_{j}\right\rangle=A_{j} \sum_{k^{\prime}}\left\langle u_{k^{\prime}} \mid a_{j}\right\rangle \delta_{k k^{\prime}} \tag{4.100}
\end{equation*}
$$

Moving out the sign of summation over $k$ ', and using definition (47) of the matrix elements, we get

$$
\begin{equation*}
\sum_{k^{\prime}}\left(A_{k k^{\prime}}-A_{j} \delta_{k k^{\prime}}\right)\left\langle u_{k^{\prime}} \mid a_{j}\right\rangle=0 . \tag{4.101}
\end{equation*}
$$

But the set of such equalities, for all $N$ possible values of index $k$, is just a system of linear, homogeneous equations for unknown $c$-numbers $\left\langle u_{k} \mid a_{j}\right\rangle$. But according to Eqs. (82)-(84), these numbers are nothing else than the matrix elements $U_{k^{\prime} j}$ of a unitary matrix providing the required transformation from the initial basis $\{u\}$ to the basis $\{a\}$ that diagonalizes matrix A. The system may be presented in the matrix form:

$$
\left(\begin{array}{ccc}
A_{11}-A_{j} & A_{12} & \ldots  \tag{4.102}\\
A_{21} & A_{22}-A_{j} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right)\left(\begin{array}{c}
U_{1 j} \\
U_{2 j} \\
\ldots
\end{array}\right)=0
$$

$\qquad$

and the usual condition of its consistency,

$$
\left|\begin{array}{ccc}
A_{11}-A_{j} & A_{12} & \ldots  \tag{4.103}\\
A_{21} & A_{22}-A_{j} & \ldots \\
\ldots & \ldots & \ldots
\end{array}\right|=0,
$$

plays the role of the characteristic equation of the system. This equation has $N$ roots $A_{j} ;$; plugging each of them back into system (102), we can use it to find $N$ matrix elements $U_{k j}(k=1,2, \ldots N)$ corresponding to this particular eigenvalue. However, since equations (103) are homogeneous, they allow finding $U_{k j}$ only to a constant multiplier. In order to ensure their normalization, i.e. the unitary character of matrix $U$, we may use the condition that all eigenvectors are normalized (just as the basis vectors are):

$$
\begin{equation*}
\left\langle a_{j} \mid a_{j}\right\rangle=\sum_{k}\left\langle a_{j} \mid u_{k}\right\rangle\left\langle u_{k} \mid a_{j}\right\rangle=\sum_{k}\left|U_{k j}\right|^{2}=1, \tag{4.104}
\end{equation*}
$$

for each $j$. This normalization completes the diagonalization. ${ }^{19}$
Now (at last!) I can give the reader some examples. As a simple but very important case, let us diagonalize the operators described (in a certain 2-function basis $\{u\}$ ) by the so-called Pauli matrices

Pauli

$$
\sigma_{x} \equiv\left(\begin{array}{ll}
0 & 1  \tag{4.105}\\
1 & 0
\end{array}\right), \quad \sigma_{y} \equiv\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right), \quad \sigma_{z} \equiv\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right) .
$$

Though introduced by a physicist, with a specific purpose to describe electron's spin, these matrices have a general mathematical significance, because together with the $2 \times 2$ identity matrix I, they provide a full, linearly-independent $2 \times 2$ basis - meaning that an arbitrary $2 \times 2$ matrix may be presented as

$$
\left(\begin{array}{ll}
A_{11} & A_{12}  \tag{4.106}\\
A_{21} & A_{22}
\end{array}\right)=a_{0} \mathrm{I}+a_{x} \sigma_{x}+a_{y} \sigma_{y}+a_{z} \sigma_{z},
$$

with a unique set of 4 coefficients $a$.
Let us start with diagonalizing matrix $\sigma_{x}$. For it, the characteristic equation (103) is evidently

$$
\left|\begin{array}{cc}
-A_{j} & 1  \tag{4.107}\\
1 & -A_{j}
\end{array}\right|=0
$$

and has two roots, $A_{1,2}= \pm 1$. (Again, the numbering is arbitrary!) The reader may readily check that the eigenvalues of matrices $\sigma_{y}$ and $\sigma_{z}$ are similar. However, the eigenvectors of the operators corresponding to all these matrices are different. To find them for $\sigma_{x}$, let us plug its first eigenvalue, $A_{1}=+1$, back into equations (101), written for this particular case:

$$
\begin{array}{r}
-\left\langle u_{1} \mid a_{1}\right\rangle+\left\langle u_{2} \mid a_{1}\right\rangle=0  \tag{4.108}\\
\left\langle u_{1} \mid a_{1}\right\rangle-\left\langle u_{2} \mid a_{1}\right\rangle=0 .
\end{array}
$$

[^585]The equations are compatible (of course, because the used eigenvalue $A_{1}=+1$ satisfies the characteristic equation), and any of them gives

$$
\begin{equation*}
\left\langle u_{1} \mid a_{1}\right\rangle=\left\langle u_{2} \mid a_{1}\right\rangle, \text { i. e. } \quad U_{11}=U_{21} . \tag{4.109}
\end{equation*}
$$

With that, the normalization condition (104) yields

$$
\begin{equation*}
\left|U_{11}\right|^{2}=\left|U_{21}\right|^{2}=\frac{1}{2} . \tag{4.110}
\end{equation*}
$$

Although the normalization is insensitive to the simultaneous multiplication of $U_{11}$ and $U_{21}$ by the same phase factor $\exp \{i \varphi\}$ with any real $\varphi$, it is convenient to keep the coefficients real, for example taking $\varphi$ $=0$, i.e. to get

$$
\begin{equation*}
U_{11}=U_{21}=\frac{1}{\sqrt{2}} . \tag{4.111}
\end{equation*}
$$

Performing an absolutely similar calculation for the second characteristic value, $A_{2}=-1$, we get $U_{12}=-U_{22}$, and we may choose the common phase to get

$$
\begin{equation*}
U_{12}=-U_{22}=\frac{1}{\sqrt{2}}, \tag{4.112}
\end{equation*}
$$

so that the whole unitary matrix for diagonalization of the operator corresponding to $\sigma_{x}$ is ${ }^{20}$

$$
\mathrm{U}_{x}=\mathrm{U}_{x}^{\dagger}=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & 1  \tag{4.113}\\
1 & -1
\end{array}\right)
$$

For what follows, it will be convenient to have this result expressed in the ket-relation form - see Eqs. (85)-(86):

$$
\begin{array}{ll}
\left|a_{1}\right\rangle=U_{11}\left|u_{1}\right\rangle+U_{21}\left|u_{2}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|u_{1}\right\rangle+\left|u_{2}\right\rangle\right), & \left|a_{2}\right\rangle=U_{12}\left|u_{1}\right\rangle+U_{22}\left|u_{2}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|u_{1}\right\rangle-\left|u_{2}\right\rangle\right), \\
\left|u_{1}\right\rangle=U_{11}^{\dagger}\left|a_{1}\right\rangle+U_{21}^{\dagger}\left|a_{2}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|a_{1}\right\rangle+\left|a_{2}\right\rangle\right), & \left|u_{2}\right\rangle=U_{12}^{\dagger}\left|a_{1}\right\rangle+U_{22}^{\dagger}\left|a_{2}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|a_{1}\right\rangle-\left|a_{2}\right\rangle\right), \tag{4.115}
\end{array}
$$

These results are already sufficient to understand the Stern-Gerlach experiments described in Sec. 1 - with two additional postulates. The first of them is that particle's interaction with external magnetic field may be described by the following vector operator of the dipole magnetic moment: ${ }^{21}$

$$
\begin{equation*}
\hat{\mathbf{m}}=\gamma \hat{\mathbf{S}} \tag{4.116}
\end{equation*}
$$

where the coefficient $\gamma$, specific for every particle type, is called the gyromagnetic ratio, ${ }^{22}$ and $\hat{\mathbf{S}}$ is the vector operator of spin. For the so-called spin- $1 / 2$ particles (including the electron), this operator may be represented, in the so-called $z$-basis, by the following 3D vector of the Pauli matrices (105):

[^586]\[

\mathbf{S}=\frac{\hbar}{2}\left(\mathbf{n}_{x} \sigma_{x}+\mathbf{n}_{y} \sigma_{y}+\mathbf{n}_{z} \sigma_{z}\right)=\frac{\hbar}{2}\left($$
\begin{array}{cc}
\mathbf{n}_{z} & \mathbf{n}_{x}-i \mathbf{n}_{y}  \tag{4.117}\\
\mathbf{n}_{x}+i \mathbf{n}_{y} & -\mathbf{n}_{z}
\end{array}
$$\right),
\]

and $\mathbf{n}_{x, y, z}$ are the usual Cartesian unit vectors in 3D space. (In the quantum-mechanics sense, they are just $c$-numbers, or rather " $c$-vectors".) The $z$-basis, in which Eq. (177) is valid, is defined as an orthonormal basis of two states, frequently denoted $\uparrow$ an $\downarrow$, in which the $z$-component of the vector operator of spin is diagonal, with eigenvalues $+\hbar / 2$ and $-\hbar / 2$. Note that we do not "understand" what exactly these states are, ${ }^{23}$ but loosely associate them with a certain internal rotation of the electron about $z$-axis, with either positive or negative angular momentum component $S_{z}$. However, any attempt to use such classical interpretation for quantitative predictions runs into fundamental difficulties - see Sec. 5.7 below.

The second new postulate describes the general relation between the bra-ket formalism and experiment. ${ }^{24}$ Namely, in quantum mechanics, each real observable $A$ is represented by a Hermitian operator $\hat{A}=\hat{A}^{\dagger}$, and a result of its measurement in a quantum state $\alpha$, described by a linear superposition of the eigenstates $a_{j}$ of the operator,

$$
\begin{equation*}
|\alpha\rangle=\sum_{j} \alpha_{j}\left|a_{j}\right\rangle, \quad \text { with } \alpha_{j}=\left\langle a_{j} \mid \alpha\right\rangle, \tag{4.118}
\end{equation*}
$$

may be only one of corresponding eigenvalues $A_{j} \cdot{ }^{25}$ If state (118) and all eigenstates $\alpha_{j}$ are normalized to unity,

$$
\begin{equation*}
\langle\alpha \mid \alpha\rangle=1, \quad\left\langle a_{j} \mid a_{j}\right\rangle=1 \tag{4.119}
\end{equation*}
$$

then the probability of outcome $A_{j}$ is ${ }^{26}$

Quantum measurement potulate

$$
\begin{equation*}
W_{j}=\left|\alpha_{j}\right|^{2}=\alpha_{j}^{*} \alpha_{j}=\left\langle\alpha \mid a_{j}\right\rangle\left\langle a_{j} \mid \alpha\right\rangle, \tag{4.120}
\end{equation*}
$$

This relation is evidently a generalization of Eq. (1.22) in wave mechanics. As a sanity check, let us assume that the set of eigenstates $a_{j}$ is full, and calculate the sum of all the probabilities:

$$
\begin{equation*}
\sum_{j} W_{j}=\sum_{j}\left\langle\alpha \mid a_{j}\right\rangle\left\langle a_{j} \mid \alpha\right\rangle=\langle\alpha| \hat{I}|\alpha\rangle=1 . \tag{4.121}
\end{equation*}
$$

Now returning to the Stern-Gerlach experiment, conceptually the description of the first ( $z$ oriented) experiment shown in Fig. 1 is the hardest for us, because the statistical ensemble describing the unpolarized electron beam at its input is mixed ("incoherent"), and cannot be described by a pure

[^587]("coherent") superposition of the type (6) that have been the subject of our studies so far. (We will discuss the mixed ensembles in Chapter 7.) However, it is intuitively clear that its results, and in particular Eq. (6), are compatible with the description of its two output beams as sets of electrons in pure states $\uparrow$ and $\downarrow$, respectively. The absorber following that first stage (Fig. 2) just takes all spin-down electrons out of the picture, producing an output beam of polarized electrons in a pure $\uparrow$ state. For such beam, probabilities (120) are $W_{\uparrow}=1$ and $W_{\downarrow}=0$. This is certainly compatible with the result of the "control" experiment shown on the bottom panel of Fig. 2: the repeated SG $(z)$ stage does not split such a beam, keeping the probabilities the same.

Now let us discuss the double Stern-Gerlach experiment shown on the top panel of Fig. 2. For that, let us present the $z$-polarized beam in another basis of two states (I will denote them as $\rightarrow$ and $\leftarrow$ ) in which, by definition, the matrix of operator $\hat{S}_{x}$ is diagonal. But this is exactly the set we called $a_{1,2}$ in the $\sigma_{x}$ matrix diagonalization problem solved above. On the other hand, states $\uparrow$ and $\downarrow$ are exactly what we called $u_{1,2}$ in that problem, because in this basis, matrices $\sigma_{z}$ and hence $\mathrm{S}_{z}$ are diagonal. Hence, in application to the electron spin problem, we may rewrite Eqs. (114)-(115) as

$$
\begin{array}{ll}
|\rightarrow\rangle=\frac{1}{\sqrt{2}}(|\uparrow\rangle+|\downarrow\rangle), & |\leftarrow\rangle=\frac{1}{\sqrt{2}}(|\uparrow\rangle-|\downarrow\rangle), \\
|\uparrow\rangle=\frac{1}{\sqrt{2}}(|\rightarrow\rangle+|\leftarrow\rangle), & |\downarrow\rangle=\frac{1}{\sqrt{2}}(|\rightarrow\rangle-|\leftarrow\rangle), \tag{4.123}
\end{array}
$$

Relation between eigenvectors of operators $S_{x}$ and $S_{z}$

Currently, for us the first of Eqs. (123) is most important, because it shows that the quantum state of electrons entering the $\mathrm{SG}(x)$ stage may be presented as a coherent superposition of electrons with $S_{x}=+\hbar / 2$ and $S_{x}=-\hbar / 2$. Notice that the beams have equal probability amplitude moduli, so that according to Eq. (122), the split beams $\rightarrow$ and $\leftarrow$ have equal intensities, in accordance with experiment. (The minus sign before the second ket-vector is of no consequence here, though it may have an impact on outcome of other experiments - for example if the $\rightarrow$ and $\leftarrow$ beams are brought together again.)

Now, let us discuss the most mysterious (from the classical point of view) multi-stage SG experiment shown on the middle panel of Fig. 2. After the second absorber has taken out all electrons in, say, the $\leftarrow$ state, the remaining electrons in state $\rightarrow$ are passed to the final, SG (z), stage. But according to the first of Eqs. (122), this state may be presented as a (coherent) linear superposition of the $\uparrow$ and $\downarrow$ states, with equal amplitudes. The stage separates these two states into separate beams, with equal probabilities $W_{\uparrow}=W_{\downarrow}=1 / 2$ to find an electron in each of them, thus explaining the experimental results.

To conclude our discussion of the multistage Stern-Gerlach experiment, let me note that though it cannot be explained in terms of wave mechanics (which operates with scalar de Broglie waves), it has an analogy in classical theories of vector fields, such as the classical electrodynamics. Let a plane electromagnetic wave propagate perpendicular to the plane of drawing in Fig. 5, and pass through linear polarizer 1. Similarly to the initial SG (z) stages (including the following absorbers) shown in Fig. 2, the polarizer produces a wave linearly polarized in one direction - the vertical direction in Fig. 5. Its electric field vector has no horizontal component, as may be revealed by wave's full absorption in a perpendicular polarizer 3. However, let us pass the wave through polarizer 2 first. In this case, the output wave does acquire a horizontal component, as can be, again, revealed by passing it through polarizer 3. If angles between polarization direction 1 and 2 , and between 2 and 3 , are both equal $\pi / 4$, each polarizer reduces the wave amplitude by a factor of $\sqrt{ } 2$, and hence intensity by a factor of 2 , exactly
like in the multistage SG experiment, with polarizer 2 playing the role of the $\mathrm{SG}(x)$ stage. The "only" difference is that the necessary angle is $\pi / 4$, rather than by $\pi / 2$ for the Stern-Gerlach experiment. In quantum electrodynamics (see Chapter 9 below), which confirms the classical predictions for this experiment, this difference is explained by that between the integer spin of the electromagnetic field quanta, photons, and the half-integer spin of electrons.


Fig. 4.5. Light polarization sequence similar to the 3 -stage Stern-Gerlach experiment shown on the middle panel of Fig. 2.

### 4.5. Observables: Expectation values and uncertainties

After this particular (and hopefully very inspiring) example, let us discuss the general relation between the Dirac formalism and experiment in more detail. The expectation value of an observable over any statistical ensemble (not necessarily coherent) may be always calculated using the general rule (1.37). For the particular case of a coherent superposition (118), we can combine that definition with Eq. (120) and the second of Eqs. (118), and then use Eqs. (59) and (98) to write

$$
\begin{equation*}
\langle A\rangle=\sum_{j} A_{j} W_{j}=\sum_{j} \alpha_{j}^{*} A_{j} \alpha_{j}=\sum_{j}\left\langle\alpha \mid a_{j}\right\rangle A_{j}\left\langle a_{j} \mid \alpha\right\rangle=\sum_{j, j^{\prime}}\left\langle\alpha \mid a_{j}\right\rangle\left\langle a_{j}\right| \hat{A}\left|a_{j^{\prime}}\right\rangle\left\langle a_{j^{\prime}} \mid \alpha\right\rangle . \tag{4.124}
\end{equation*}
$$

Now using the completeness relation (44) twice, with indices $j$ and $j^{\prime}$, we arrive at a very simple and important formula ${ }^{27}$

This is a clear analog of the wave-mechanics formula (1.23) - and as we will see in the next chapter, may be used to derive it. A huge advantage of Eq. (125) is that it does not explicitly involve the eigenvector set of the corresponding operator, and allows the calculation to be performed in any convenient basis. ${ }^{28}$

For example, let us consider an arbitrary state $\alpha$ of spin- $1 / 2$, and calculate the expectation values of its components. The calculations are easiest in the $z$-basis, because we know the operators of the components in that basis - see Eq. (117). Representing the ket- and bra-vectors of our state as linear superpositions of vectors of the basis states $\uparrow$ and $\downarrow$,

$$
\begin{equation*}
|\alpha\rangle=\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle, \quad\langle\alpha|=\langle\uparrow| \alpha_{\uparrow}^{*}+\langle\downarrow| \alpha_{\downarrow}^{*} . \tag{4.126}
\end{equation*}
$$

[^588]and plugging these expressions to Eq. (125) written for observable $S_{z}$, we get
\[

$$
\begin{align*}
\left\langle S_{z}\right\rangle & =\left(\langle\uparrow| \alpha_{\uparrow}^{*}+\langle\downarrow| \alpha_{\downarrow}^{*}\right) \hat{S}_{z}\left(\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle\right)  \tag{4.127}\\
& =\alpha_{\uparrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{z}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{z}|\downarrow\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{z}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{z}|\downarrow\rangle .
\end{align*}
$$
\]

Now there are two equivalent ways (both very simple :-) to calculate the bra-kets in this expression. The first one is to represent each of them in the matrix form in the $z$-basis, in which bra- and ket-vectors of states $\uparrow$ and $\downarrow$ are, respectively, matrix-rows $(1,0)$ and $(0,1)$, or the similar matrixcolumns. Another (perhaps more elegant) way is to use the general Eq. (59), for the $z$-basis, to write

$$
\begin{equation*}
\hat{S}_{x}=\frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow|+|\downarrow\rangle\langle\uparrow|), \quad \hat{S}_{y}=-i \frac{\hbar}{2}(|\uparrow\rangle\langle\downarrow|-|\downarrow\rangle\langle\uparrow|), \quad \hat{S}_{z}=\frac{\hbar}{2}(|\uparrow\rangle\langle\uparrow|-|\downarrow\rangle\langle\downarrow|) \tag{4.128}
\end{equation*}
$$

For our particular calculation, we may plug the last of these expressions into Eq. (127), and to use the orthonormality conditions (119):

$$
\begin{equation*}
\langle\uparrow \mid \uparrow\rangle=\langle\downarrow \mid \downarrow\rangle=1, \quad\langle\uparrow \mid \downarrow\rangle=\langle\downarrow \mid \uparrow\rangle=0 . \tag{4.129}
\end{equation*}
$$

Both calculations give (of course) the same result:

$$
\begin{equation*}
\left\langle S_{z}\right\rangle=\frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\uparrow}^{*}-\alpha_{\downarrow} \alpha_{\downarrow}^{*}\right) . \tag{4.130}
\end{equation*}
$$

This particular result might be also obtained using Eq. (120) for probabilities $W_{\uparrow}=\alpha \uparrow \alpha \uparrow^{*}$ and $W_{\downarrow}=$ $\alpha \downarrow \downarrow_{\downarrow}{ }^{*}$ :

$$
\begin{equation*}
\left\langle S_{z}\right\rangle=W_{\uparrow}\left(+\frac{\hbar}{2}\right)+W_{\downarrow}\left(-\frac{\hbar}{2}\right)=\alpha_{\uparrow} \alpha_{\uparrow}^{*}\left(+\frac{\hbar}{2}\right)+\alpha_{\downarrow} \alpha_{\downarrow}^{*}\left(-\frac{\hbar}{2}\right) . \tag{4.131}
\end{equation*}
$$

The formal way (127), based on using Eq. (125), has, however, an advantage of being applicable, without any change, to finding the observables whose operators are not diagonal in the $z$-basis, as well. In particular, absolutely similar calculations give

$$
\begin{align*}
& \left\langle S_{x}\right\rangle=\alpha_{\uparrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{x}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{x}|\downarrow\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{x}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{x}|\downarrow\rangle=\frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\downarrow}^{*}+\alpha_{\downarrow} \alpha_{\uparrow}^{*}\right),  \tag{4.132}\\
& \left\langle S_{y}\right\rangle=\alpha_{\uparrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{y}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{y}|\downarrow\rangle+\alpha_{\uparrow} \alpha_{\downarrow}^{*}\langle\downarrow| \hat{S}_{y}|\uparrow\rangle+\alpha_{\downarrow} \alpha_{\uparrow}^{*}\langle\uparrow| \hat{S}_{y}|\downarrow\rangle=i \frac{\hbar}{2}\left(\alpha_{\uparrow} \alpha_{\downarrow}^{*}-\alpha_{\downarrow} \alpha_{\uparrow}^{*}\right), \tag{4.133}
\end{align*}
$$

Similarly, we can express, via the same coefficients $\alpha \uparrow$ and $\alpha \downarrow$, the r.m.s. fluctuations of all spin components. For example, let us have a good look at the spin state $\uparrow$. According to Eq. (126), in this state $\alpha \uparrow=1$ and $\alpha_{\downarrow}=0$, so that Eqs. (130)-(133) yield:

$$
\begin{equation*}
\left\langle S_{z}\right\rangle=\frac{\hbar}{2}, \quad\left\langle S_{x}\right\rangle=\left\langle S_{y}\right\rangle=0 . \tag{4.134}
\end{equation*}
$$

Now let us use the same Eq. (125) to calculate the spin component uncertainties. According to Eqs. (105) and (117), operators of spin component squared are equal to $(\hbar / 2)^{2} \hat{I}$, so that the general Eq. (1.33) yields

$$
\begin{gather*}
\left(\delta S_{z}\right)^{2}=\left\langle S_{z}^{2}\right\rangle-\left\langle S_{z}\right\rangle^{2}=\langle\uparrow| \hat{S}_{z}^{2}|\uparrow\rangle-\left(\frac{\hbar}{2}\right)^{2}=\left(\frac{\hbar}{2}\right)^{2}\langle\uparrow| \hat{I}|\uparrow\rangle-\left(\frac{\hbar}{2}\right)^{2}=0,  \tag{4.135a}\\
\left(\delta S_{x}\right)^{2}=\left\langle S_{x}^{2}\right\rangle-\left\langle S_{x}\right\rangle^{2}=\langle\uparrow| \hat{S}_{x}^{2}|\uparrow\rangle-0=\left(\frac{\hbar}{2}\right)^{2}\langle\uparrow| \hat{I}|\uparrow\rangle=\left(\frac{\hbar}{2}\right)^{2},  \tag{4.135b}\\
\left(\delta S_{y}\right)^{2}=\left\langle S_{y}^{2}\right\rangle-\left\langle S_{y}\right\rangle^{2}=\langle\uparrow| \hat{S}_{y}^{2}|\uparrow\rangle-0=\left(\frac{\hbar}{2}\right)^{2}\langle\uparrow| \hat{I}|\uparrow\rangle=\left(\frac{\hbar}{2}\right)^{2} . \tag{4.135c}
\end{gather*}
$$

While Eqs. (134) and (135a) are compatible with the classical notion of the spin being "definitely in the $\uparrow$ state", this correspondence should not be overstretched to the interpretation of this state as a certain $(z)$ orientation of electron's magnetic moment $\mathbf{m}$, because such classical picture cannot explain Eqs. (135b) and (135c). The best (but still imprecise!) classical image I can offer is the magnetic moment $\mathbf{m}$ oriented, on the average, in the $z$-direction, but still having $x$ - and $y$-components strongly "wobbling" about their zero average values.

It is straightforward to verify that in the $x$-polarized and $y$-polarized states the situation is similar, with the corresponding change of indices. Thus, in neither state may all 3 components of the spin have exact values. Let me show that this is not just an occasional fact, but reflects the most profound property of quantum mechanics, the uncertainty relations. Consider 2 observables, $A$ and $B$, that may be measured in the same quantum state. There are two possibilities here. If operators corresponding to the observables commute,

$$
\begin{equation*}
[\hat{A}, \hat{B}]=0 \tag{4.136}
\end{equation*}
$$

then all the matrix elements of the commutator in any orthogonal basis (in particular, in the basis of eigenstates $a_{j}$ of operator $A$ ) are also zero. From here, we get

$$
\begin{equation*}
\left\langle a_{j}\right|[\hat{A}, \hat{B}]\left|a_{j^{\prime}}\right\rangle=\left\langle a_{j}\right| \hat{A} \hat{B}\left|a_{j^{\prime}}\right\rangle-\left\langle a_{j}\right| \hat{B} \hat{A}\left|a_{j^{\prime}}\right\rangle=0 . \tag{4.137}
\end{equation*}
$$

In the first bra-ket of the middle expression, let us act by operator $\hat{A}$ on the bra-vector, while in the second one, on the ket-vector. According to Eq. (68), such action turns operators into the corresponding eigenvalues, so that we get

$$
\begin{equation*}
A_{j}\left\langle a_{j}\right| \hat{B}\left|a_{j^{\prime}}\right\rangle-A_{j^{\prime}}\left\langle a_{j}\right| \hat{B}\left|a_{j^{\prime}}\right\rangle=\left(A_{j}-A_{j^{\prime}}\right)\left\langle a_{j}\right| \hat{B}\left|a_{j^{\prime}}\right\rangle=0 \tag{4.138}
\end{equation*}
$$

This means that if eigenstates of operator $\hat{A}$ are non-degenerate (i.e. $A_{j} \neq A_{j}$, if $j \neq j$ '), the matrix of operator $\hat{B}$ has to be diagonal in basis $a_{j}$, i.e., the eigenstate sets of operators $\hat{A}$ and $\hat{B}$ coincide. Such pairs of observables, that share their eigenstates, are called compatible. For example, in wave mechanics of a particle, momentum (1.26) and the kinetic energy (1.27) are compatible, sharing eigenfunctions (1.29). Now we see that this is not occasional, because each Cartesian component of the kinetic energy is proportional to the square of the corresponding component of the momentum, and any operator commutes with an arbitrary power of itself:

$$
\begin{equation*}
\left[\hat{A}, \hat{A}^{n}\right] \equiv[\hat{A}, \underbrace{\hat{A} \hat{A} \ldots \hat{A}}_{n}]=\hat{A} \underbrace{\hat{A} \hat{A} \ldots}_{n} \hat{A}-\underbrace{\hat{A} \hat{A} \ldots \hat{A}}_{n} \hat{A}=0 . \tag{4.139}
\end{equation*}
$$

Now, what if operators $\hat{A}$ and $\hat{B}$ do not commute? Then the following general uncertainty relation is valid: ${ }^{29}$

$$
\delta A \delta B \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle| .
$$

General uncertainty relation

Schwartz inequality

The proof may be started by using postulate (16) - that the norm of any legitimate state of the system cannot be negative. Let us apply this postulate to the state with the following ket-vector:

$$
\begin{equation*}
|\delta\rangle \equiv|\alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}|\beta\rangle \tag{4.142}
\end{equation*}
$$

where $\alpha$ and $\beta$ are possible, non-null states of the system, so that the denominator in Eq. (142) is not equal to zero. For this case, Eq. (16) gives

$$
\begin{equation*}
\left(\langle\alpha|-\frac{\langle\alpha \mid \beta\rangle}{\langle\beta \mid \beta\rangle}\langle\beta|\right)\left(|\alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}|\beta\rangle\right) \geq 0 \tag{4.143}
\end{equation*}
$$

Opening the parentheses, we get

$$
\begin{equation*}
\langle\alpha \mid \alpha\rangle-\frac{\langle\alpha \mid \beta\rangle}{\langle\beta \mid \beta\rangle}\langle\beta \mid \alpha\rangle-\frac{\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle}\langle\alpha \mid \beta\rangle+\frac{\langle\alpha \mid \beta\rangle\langle\beta \mid \alpha\rangle}{\langle\beta \mid \beta\rangle^{2}}\langle\beta \mid \beta\rangle \geq 0 \tag{4.144}
\end{equation*}
$$

After the cancellation of one inner product $\langle\beta \mid \beta\rangle$ in the numerator and denominator of the last term, it cancels with the $2^{\text {rd }}$ (or $3^{\text {rd }}$ ) term, proving the Schwartz inequality (141).

Now let us apply this inequality to states

$$
\begin{equation*}
|\alpha\rangle \equiv \hat{\widetilde{A}}|\gamma\rangle \text { and }|\beta\rangle \equiv \hat{\widetilde{B}}|\gamma\rangle \tag{4.145}
\end{equation*}
$$

where, in both relations, $\gamma$ is the same (but otherwise arbitrary) possible state of the system, and the deviations operators are defined similarly to observable deviations (see Sec. 1.2), for example,

$$
\begin{equation*}
\hat{\tilde{A}} \equiv \hat{A}-\langle A\rangle \tag{4.146}
\end{equation*}
$$

With this substitution, and taking into account that the observable operators $\hat{A}$ and $\hat{B}$ are Hermitian, Eq. (141) yields

$$
\begin{equation*}
\left.\langle\gamma| \hat{\tilde{A}}^{2}|\gamma\rangle\langle\gamma| \hat{\widetilde{B}}^{2}|\gamma\rangle \geq|\langle\gamma| \hat{\tilde{A}} \hat{\tilde{B}}| \gamma\right\rangle\left.\right|^{2} \tag{4.147}
\end{equation*}
$$

[^589]Since state $\gamma$ is arbitrary, we may use Eq. (125) to rewrite this relation as an operator inequality:

$$
\begin{equation*}
\delta A \delta B \geq|\langle\hat{\tilde{A}} \hat{\tilde{B}}\rangle| . \tag{4.148}
\end{equation*}
$$

Actually, this is already an uncertainty relation, even "better" (stronger) than its standard form (140); moreover, it is more convenient in some cases. In order to proceed to Eq. (140), we need a couple more steps. First, let us notice that the operator product in Eq. (148) may be recast as

$$
\begin{equation*}
\hat{\widetilde{A}} \hat{\widetilde{B}}=\frac{1}{2}\{\hat{\widetilde{A}}, \hat{\widetilde{B}}\}-\frac{i}{2} \hat{C}, \quad \text { where } \hat{C} \equiv i[\hat{\widetilde{A}}, \hat{\widetilde{B}}] \tag{4.149}
\end{equation*}
$$

Any anticommutator of Hermitian operators, including that in Eq. (149), is a Hermitian operator, and its eigenvalues are purely real, so that its expectation value (in any state) is also purely real. On the other hand, the commutator part of Eq. (149) is just

$$
\begin{equation*}
\hat{C} \equiv i[\hat{\tilde{A}}, \hat{\widetilde{B}}]=i(\hat{A}-\langle A\rangle)(\hat{B}-\langle B\rangle)-i(\hat{B}-\langle B\rangle)(\hat{A}-\langle A\rangle)=i(\hat{A} \hat{B}-\hat{B} \hat{A})=i[\hat{A}, \hat{B}] . \tag{4.150}
\end{equation*}
$$

Second, according to Eqs. (52) and (65), the Hermitian conjugate of any product of Hermitian operators $\hat{A}$ and $\hat{B}$ is just the product of swapped operators. Using the fact, we may write

$$
\begin{equation*}
\hat{C}^{\dagger}=(i[\hat{A}, \hat{B}])^{\dagger}=-i(\hat{A} \hat{B})^{\dagger}+i(\hat{B} \hat{A})^{\dagger}=-i \hat{B} \hat{A}+i \hat{A} \hat{B}=i[\hat{A}, \hat{B}]=\hat{C} \tag{4.151}
\end{equation*}
$$

so that operator $\hat{C}$ is also Hermitian, i.e. its eigenvalues are also real, and thus its average is purely real as well. As a result, the square of the average of the operator product (149) may be presented as

$$
\begin{equation*}
\langle\hat{\tilde{A}} \hat{\tilde{B}}\rangle^{2}=\left\langle\frac{1}{2}\{\hat{\tilde{A}}, \hat{\tilde{B}}\}\right\rangle^{2}+\left\langle\frac{1}{2} \hat{C}\right\rangle^{2} . \tag{4.152}
\end{equation*}
$$

Since the first term in the right-hand part of this equality cannot be negative,

$$
\begin{equation*}
\langle\hat{\widetilde{A}} \hat{\tilde{B}}\rangle^{2} \geq\left\langle\frac{1}{2} \hat{C}\right\rangle^{2}=\left\langle\frac{i}{2}[\hat{A}, \hat{B}]\right\rangle^{2} \tag{4.153}
\end{equation*}
$$

and we can continue Eq. (148) as

$$
\begin{equation*}
\delta A \delta B \geq|\langle\hat{\tilde{A}} \hat{\tilde{B}}\rangle| \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|, \tag{4.154}
\end{equation*}
$$

thus proving Eq. (140).
For the particular case of operators $\hat{x}$ and $\hat{p}_{x}$ (or a similar pair of operators for another Cartesian coordinate), we can readily combine Eq. (140) with Eq. (2.14b) and to prove the original Heisenberg's uncertainty relation (2.13). For the spin-1/2 operators defined by Eq. (117), it is straightforward (and highly recommended to the reader) to show that

$$
\begin{equation*}
\left[\hat{S}_{x}, \hat{S}_{y}\right]=i \hbar \hat{S}_{z} \tag{4.155}
\end{equation*}
$$

with similar relations for other pairs of indices taken in the "correct" order (from $x$ to $y$ to $z$ to $x$, etc.). As a result, the uncertainty relations (140) for spin- $1 / 2$ particles, notably including electrons, are

$$
\begin{equation*}
\delta S_{x} \delta S_{y} \geq \frac{\hbar}{2}\left|\left\langle S_{z}\right\rangle\right|, \text { etc. } \tag{4.156}
\end{equation*}
$$

In particular, in the $\uparrow$ state, the right-hand part of this relation equals $(\hbar / 2)^{2}$, and neither of the uncertainties $\delta S_{x}, \delta S_{y}$ can equal zero. As a reminder, our direct calculation earlier in this section has shown that each of these uncertainties is equal to $\hbar / 2$, i.e. their product equals to the lowest value allowed by the uncertainty relation (156). In this aspect, the spin-polarized states are similar to the Gaussian wave packets studied in Sec. 2.2.

### 4.6. Quantum dynamics: Three pictures

So far in this chapter, I shied away from the discussion of system dynamics, implying that the bra- and ket-vectors of the system are their "snapshots" at a certain instant $t$. Now we are sufficiently prepared to examine their time dependence. One of the most beautiful features of quantum mechanics is that the time evolution may be described using either of three alternative "pictures", giving exactly the same final results for expectation values of all observables.

From the standpoint of our wave mechanics experience, the Schrödinger picture is the most natural. In this picture, the operators corresponding to time-independent observables (e.g., to the Hamiltonian function $H$ of an isolated system) are also constant, while the bra- and ket-vectors of the quantum state of the system evolve in time as

$$
\begin{equation*}
\langle\alpha(t)|=\left\langle\alpha\left(t_{0}\right)\right| \hat{u}^{\dagger}\left(t, t_{0}\right), \quad|\alpha(t)\rangle=\hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle, \tag{4.157}
\end{equation*}
$$

where $\hat{u}\left(t, t_{0}\right)$ is the time-evolution operator, which obeys the following differential equation:

$$
\begin{equation*}
i \hbar \dot{\hat{u}}=\hat{H} \hat{u} \tag{4.158}
\end{equation*}
$$

where $\hat{H}$ is the Hamiltonian operator of the system (that is always Hermitian, $\hat{H}^{\dagger}=\hat{H}$ ), and the dot means the differentiation is over argument $t$, but not $t_{0}$. While this equation is a very natural replacement of the wave-mechanical equation (1.25), and is also frequently called the Schrödinger equation, ${ }^{31}$ it still should be considered as a new, more general postulate, which finds its final justification (as it is usual in physics) in the agreement between its corollaries with experiment - more exactly, in having not a single credible contradiction with experiment.

Starting the discussion of Eqs. (157)-(158), let us first consider the case of a system described by a time-independent Hamiltonian, whose eigenstates $a_{n}$ and eigenvalues $E_{n}$ obey Eq. (68), ${ }^{32}$

$$
\begin{equation*}
\hat{H}\left|a_{n}\right\rangle=E_{n}\left|a_{n}\right\rangle, \tag{4.159}
\end{equation*}
$$

and hence are also time-independent. (Similarly to the wavefunctions $\psi_{n}$ defined by Eq. (1.60), $a_{n}$ are called the stationary states of the system.) Let us use Eqs. (157)-(159) to calculate the law of time evolution of the expansion coefficients $\alpha_{n}$, defined by Eq. (118), in the stationary state basis:

[^590]\[

$$
\begin{align*}
\dot{\alpha}_{n}(t) & =\frac{d}{d t}\left\langle a_{n} \mid \alpha(t)\right\rangle=\frac{d}{d t}\left\langle a_{n}\right| \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\left\langle a_{n}\right| \dot{\hat{u}}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle  \tag{4.160}\\
& =\left\langle a_{n}\right| \frac{1}{i \hbar} \hat{H} \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\frac{E_{n}}{i \hbar}\left\langle a_{n}\right| \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\frac{E_{n}}{i \hbar}\left\langle a_{n} \mid \alpha(t)\right\rangle=-\frac{i}{\hbar} E_{n} \alpha_{n} .
\end{align*}
$$
\]

This is the same simple equation as Eq. (1.59), and its integration yields a similar result - cf. Eq. (1.61), just with the initial time $t_{0}$ rather than 0 :


Pauli
Hamiltonian: operator

$$
\begin{equation*}
\alpha_{n}(t)=\alpha_{n}\left(t_{0}\right) \exp \left\{-\frac{i}{\hbar} E_{n}\left(t-t_{0}\right)\right\} \tag{4.161}
\end{equation*}
$$

In order to illustrate how does this result work, let us consider spin- $1 / 2$ dynamics in a timeindependent, uniform external magnetic field $B$, taking its direction for axis $z$. To construct the system's Hamiltonian, we may apply the correspondence principle to the classical expression for the energy of a magnetic moment $\mathbf{m}$ in the external magnetic field $\mathcal{B}, 33$

$$
\begin{equation*}
U=-\mathbf{m} \cdot \boldsymbol{B} . \tag{4.162}
\end{equation*}
$$

In quantum mechanics, the operator corresponding to the moment $\mathbf{m}$ is given by Eq. (116) (suggested by W. Pauli), so that the spin-field interaction is described by the so-called Pauli Hamiltonian:

$$
\begin{equation*}
\hat{H}=-\hat{\mathbf{m}} \cdot \boldsymbol{B}=-\hat{\boldsymbol{S}} \cdot \boldsymbol{B}=-\gamma \boldsymbol{B} \hat{S}_{z} \tag{4.163}
\end{equation*}
$$

where $\hat{S}_{z}$ is the operator of the $z$-component of electron's spin. According to Eq. (117), in the $z$-basis of states $\uparrow$ and $\downarrow$, the matrix of operator (163) is

$$
\begin{equation*}
\mathrm{H}=-\frac{\gamma \hbar B}{2} \sigma_{z}=\frac{\hbar \Omega}{2} \sigma_{z}, \quad \text { with } \Omega \equiv-\gamma B \text {. } \tag{4.164}
\end{equation*}
$$

The constant $\Omega$ so defined coincides with the classical frequency of the precession of a symmetric top, with an angular momentum $\mathbf{S}$ and magnetic moment $\mathbf{m}=\gamma \mathbf{S}$, about axis $z$, induced by external torque $\tau$ $=\mathbf{m} \times$ B: 34

$$
\begin{equation*}
\Omega=-\frac{\tau}{S}=-\frac{m B}{S}=-\gamma B . \tag{4.165a}
\end{equation*}
$$

For an electron, with its negative gyromagnetic ratio $\gamma_{e}=-g_{e} e / 2 m_{e}$, neglecting the minor difference between factors $g_{e}$ and 2 , we get

$$
\begin{equation*}
\Omega=\frac{e}{m_{e}} \mathcal{B}, \tag{4.165b}
\end{equation*}
$$

i.e. the frequency's magnitude coincides with that of the cyclotron frequency $\omega_{c}$ - see Eq. (3.48).

In order to apply the general Eq. (161), at this stage we would need to find the eigenstates $a_{n}$ and eigenenergies $E_{n}$ of our Hamiltonian. However, with our (smart :-) choice of the direction of axis $z$, the Hamiltonian matrix is already diagonal:

[^591]\[

\mathrm{H}=-\frac{\hbar \Omega}{2} \sigma_{z}=\frac{\hbar \Omega}{2}\left($$
\begin{array}{cc}
1 & 0  \tag{4.166}\\
0 & -1
\end{array}
$$\right)
\]

meaning that $\uparrow$ and $\downarrow$ are the eigenstates of the system, with eigenenergies, respectively,

$$
\begin{equation*}
E_{\uparrow}=+\frac{\hbar \Omega}{2} \quad \text { and } \quad E_{\downarrow}=-\frac{\hbar \Omega}{2} . \tag{4.167}
\end{equation*}
$$

(Note that their difference,

$$
\begin{equation*}
\Delta E \equiv\left|E_{\uparrow}-E_{\downarrow}\right|=\hbar|\Omega|=\hbar|\gamma \mathcal{B}|, \tag{4.168}
\end{equation*}
$$

corresponds to the classical energy $2 \mid m$ 耳 of flipping the magnetic dipole with moment $m=\gamma \hbar / 2$, oriented along the direction of field B. ${ }^{35}$ ) With that, Eq. (161) immediately yields following expressions for the time evolution of the expansion coefficients:

$$
\begin{equation*}
\alpha_{\uparrow}(t)=\alpha_{\uparrow}\left(t_{0}\right) \exp \left\{-\frac{i}{2} \Omega\left(t-t_{0}\right)\right\}, \quad \alpha_{\downarrow}(t)=\alpha_{\downarrow}\left(t_{0}\right) \exp \left\{\frac{i}{2} \Omega\left(t-t_{0}\right)\right\}, \tag{4.169}
\end{equation*}
$$

allowing a ready calculation of time evolution of the expectation values of any observable.
In particular, we can calculate the expectation value of $S_{z}$ as a function of time by applying Eq. (130) to an arbitrary time moment $t$ :

$$
\begin{equation*}
\left\langle S_{z}\right\rangle(t)=\frac{\hbar}{2}\left[\alpha_{\uparrow}(t) \alpha_{\uparrow}^{*}(t)-\alpha_{\downarrow}(t) \alpha_{\downarrow}^{*}(t)\right]=\frac{\hbar}{2}\left[\alpha_{\uparrow}(0) \alpha_{\uparrow}^{*}(0)-\alpha_{\downarrow}(0) \alpha_{\downarrow}^{*}(0)\right]=\left\langle S_{z}\right\rangle(0) . \tag{4.170}
\end{equation*}
$$

Thus the expectation value of the spin component parallel to the applied magnetic field remains constant, regardless of the initial state of the system. However, this is not true for the components perpendicular to the field. For example, Eq. (132), applied to moment $t$, gives

$$
\begin{equation*}
\left\langle S_{x}\right\rangle(t)=\frac{\hbar}{2}\left[\alpha_{\uparrow}(t) \alpha_{\downarrow}^{*}(t)+\alpha_{\downarrow}(t) \alpha_{\uparrow}^{*}(t)\right]=\frac{\hbar}{2}\left[\alpha_{\uparrow}(0) \alpha_{\downarrow}^{*}(0) e^{-i \Omega\left(t-t_{0}\right)}+\alpha_{\downarrow}(0) \alpha_{\uparrow}^{*}(0) e^{i \Omega\left(t-t_{0}\right)}\right] . \tag{4.171}
\end{equation*}
$$

Clearly, this expression describes sinusoidal oscillations with frequency (165). The amplitude and phase of these oscillations depend on initial conditions. Indeed, solving Eqs. (132)-(133) for the expansion coefficient products, we get relations

$$
\begin{equation*}
\hbar \alpha_{\downarrow}(t) \alpha_{\uparrow}^{*}(t)=\left\langle S_{x}\right\rangle(t)+i\left\langle S_{y}\right\rangle(t), \quad \hbar \alpha_{\uparrow}(t) \alpha_{\downarrow}^{*}(t)=\left\langle S_{x}\right\rangle(t)-i\left\langle S_{y}\right\rangle(t) \tag{4.172}
\end{equation*}
$$

valid for any time $t$. Plugging their values for $t=0$ into Eq. (171), we get

$$
\begin{align*}
\left\langle S_{x}\right\rangle(t) & =\frac{1}{2}\left[\left\langle S_{x}\right\rangle(0)+i\left\langle S_{y}\right\rangle(0)\right] e^{i \Omega\left(t-t_{0}\right)}+\frac{1}{2}\left[\left\langle S_{x}\right\rangle(0)-i\left\langle S_{y}\right\rangle(0)\right] e^{-i \Omega\left(t-t_{0}\right)}  \tag{4.173}\\
& \equiv\left\langle S_{x}\right\rangle(0) \cos \Omega t-\left\langle S_{y}\right\rangle(0) \sin \Omega t
\end{align*}
$$

An absolutely similar calculation using Eq. (133) gives

[^592]\[

$$
\begin{equation*}
\left\langle S_{y}\right\rangle(t)=\left\langle S_{y}\right\rangle(0) \cos \Omega t+\left\langle S_{x}\right\rangle(0) \sin \Omega t . \tag{4.174}
\end{equation*}
$$

\]

These formulas show, for example, if at moment $t=0$ the spin's state was $\uparrow$, i.e. $\left\langle S_{x}\right\rangle(0)=\left\langle S_{y}\right\rangle(0)$ $=0$, then the amplitude of oscillation of the both "lateral" component of spin vanishes. On the other hand, if the spin was initially in state $\rightarrow$, i.e. had the definite, maximum possible value of $S_{x}$, equal to $\hbar / 2$ (in classics, we would say "the spin $\hbar / 2$ was oriented in direction $x$ "), then both expectation values $\left\langle S_{x}\right\rangle$ and $\left\langle S_{y}\right\rangle$ oscillate in time ${ }^{36}$ with this amplitude, with the phase shift $\pi / 2$ between them. These formulas may be interpreted as the torque-induced precession of the Cartesian components of the spin vector of length $S=\hbar / 2$, confined in plane $[x, y]$, with classical frequency $\Omega=\gamma B$ about axis $z$ (counterclockwise if $\gamma \mathcal{B}>0$ ).

Thus, the gyromagnetic ratio is just the angular frequency of the torque-induced precession of spin (about field's direction) per unit magnetic field; for electrons, $\left|\gamma_{e}\right| \approx 1.761 \times 10^{11} \mathrm{~s}^{-1} \mathrm{~T}^{-1}$; for protons, the ratio is much smaller because of their larger mass: $\gamma_{p} \approx 2.675 \times 10^{8} \mathrm{~s}^{-1} \mathrm{~T}^{-1}$, and for larger spin- $1 / 2$ nuclei, $\gamma$ may be much smaller still - e.g., $8.681 \times 10^{6} \mathrm{~s}^{-1} \mathrm{~T}^{-1}$ for the ${ }^{57} \mathrm{Fe}$ nucleus. ${ }^{37}$

Note, however, that this classical language does not describe large quantum-mechanical uncertainties of these observables, which are absent in the classical picture of the precession - at least when it starts from a definite orientation of the angular momentum vector.

Now let us return to the discussion of the general Schrödinger equation (158) and prove the following fascinating fact: it is possible to write the general solution of this operator equation. In the easiest case when the Hamiltonian is time-independent, this solution is an exact analog of Eq. (161),

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right)=\hat{u}\left(t_{0}, t_{0}\right) \exp \left\{-\frac{i}{\hbar} \hat{H}\left(t-t_{0}\right)\right\}=\hat{I} \exp \left\{-\frac{i}{\hbar} \hat{H}\left(t-t_{0}\right)\right\} . \tag{4.175}
\end{equation*}
$$

To start its proof we should, first of all, understand what does a function (in this case, the exponent) of an operator mean. In the operator (and matrix) algebra, such functions are defined by their Taylor expansions; in particular, Eq. (175) means that

$$
\begin{align*}
\hat{u}\left(t, t_{0}\right) & =\hat{I}+\sum_{k=1}^{\infty} \frac{1}{k!}\left(-\frac{i}{\hbar} \hat{H} t\right)^{k} \\
& =\hat{I}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right) \hat{H}\left(t-t_{0}\right)+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^{2} \hat{H}^{2}\left(t-t_{0}\right)^{2}+\frac{1}{3!}\left(-\frac{i}{\hbar}\right)^{3} \hat{H}^{3}\left(t-t_{0}\right)^{3}+\ldots \tag{4.176}
\end{align*}
$$

where $\hat{H}^{2} \equiv \hat{H} \hat{H}, \hat{H}^{3} \equiv \hat{H} \hat{H} \hat{H}$, etc. Working with such series of operator products is not as hard as one could imagine, due to their regular structure. For example, let us differentiate Eq. (176) over $t$ :

[^593]\[

$$
\begin{align*}
\dot{\hat{u}}\left(t, t_{0}\right) & =\hat{0}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right) \hat{H}+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^{2} \hat{H}^{2} 2\left(t-t_{0}\right)+\frac{1}{3!}\left(-\frac{i}{\hbar}\right)^{2} \hat{H}^{3} 3\left(t-t_{0}\right)^{2}+\ldots \\
& =\left(-\frac{i}{\hbar}\right) \hat{H}\left[\hat{I}+\frac{1}{1!}\left(-\frac{i}{\hbar}\right) \hat{H}\left(t-t_{0}\right)+\frac{1}{2!}\left(-\frac{i}{\hbar}\right)^{2} \hat{H}^{2}\left(t-t_{0}\right)^{2}\right]+\ldots=-\frac{i}{\hbar} \hat{H} \hat{u}\left(t, t_{0}\right), \tag{4.177}
\end{align*}
$$
\]

so that the differential equation (158) is indeed satisfied. On the other hand, Eq. (175) also satisfies the initial condition

$$
\begin{equation*}
\hat{u}\left(t_{0}, t_{0}\right)=\hat{u}^{\dagger}\left(t_{0}, t_{0}\right)=\hat{I}, \tag{4.178}
\end{equation*}
$$

which immediately follows from the definition (157) of the evolution operator, so it is indeed the (unique) solution for the time evolution operator - in the Schrödinger picture.

Now let us allow operator $\hat{H}$ to be a function of time, but with the condition that its "values" (in fact, operators) at different instants commute with each other:

$$
\begin{equation*}
\left\lfloor\hat{H}\left(t^{\prime}\right), \hat{H}\left(t^{\prime \prime}\right)\right\rfloor=0, \quad \text { for any } t^{\prime}, t^{\prime \prime} \tag{4.179}
\end{equation*}
$$

(An important example of such a Hamiltonian is that of a particle under the effect of a classical, timedependent force $\mathbf{F}(t)$ :

$$
\begin{equation*}
\hat{H}_{F}=-\mathbf{F}(t) \cdot \hat{\mathbf{r}} . \tag{4.180}
\end{equation*}
$$

Indeed, the radius-vector operator $\hat{\mathbf{r}}$ does not depend explicitly on time and hence commutes with itself, as well as with $c$-numbers $\mathbf{F}\left(t^{\prime}\right)$ and $\mathbf{F}\left(t^{\prime \prime}\right)$.) In this case it is sufficient to replace, in all above formulas, product $\hat{H}\left(t-t_{0}\right)$ with the corresponding integral over time; in particular, Eq. (175) is generalized as

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right)=\hat{I} \exp \left\{-\frac{i}{\hbar} \int_{t_{0}}^{t} \hat{H}\left(t^{\prime}\right) d t^{\prime}\right\} \tag{4.181}
\end{equation*}
$$

Evolution operator: expression

This replacement means that the first form of Eq. (176) should be replaced with

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right)=\hat{I}+\sum_{k=1}^{\infty} \frac{1}{k!}\left(-\frac{i}{\hbar}\right)^{k}\left(\int_{t_{0}}^{t} \hat{H}\left(t^{\prime}\right) d t^{\prime}\right)^{k}=\hat{I}+\sum_{k=1}^{\infty}\left(-\frac{i}{\hbar}\right)^{k} \int_{t_{0}}^{t} d t_{1} \int_{t_{0}}^{t} d t_{2} \ldots \int_{t_{0}}^{t} d t_{k} \hat{H}\left(t_{1}\right) \hat{H}\left(t_{2}\right) \ldots \hat{H}\left(t_{k}\right) . \tag{4.182}
\end{equation*}
$$

The proof that the first form of Eq. (182) satisfies Eq. (158) is absolutely similar to the one carried out above.

We may now use Eq. (181) to show that the time-evolution operator is unitary at any moment, even for the time-dependent Hamiltonian. Indeed, from that formula,

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right) \hat{u}^{\dagger}\left(t, t_{0}\right)=\hat{I} \exp \left\{-\frac{i}{\hbar} \int_{t_{0}}^{t} \hat{H}\left(t^{\prime}\right) d t^{\prime}\right\} \hat{I} \exp \left\{+\frac{i}{\hbar} \int_{t_{0}}^{t} \hat{H}\left(t^{\prime \prime}\right) d t^{\prime \prime}\right\} . \tag{4.183}
\end{equation*}
$$

Since each of the exponents may be presented with the Taylor series (182), and, thanks to Eq. (179), different components of these sums may be swapped at will, expression (183) may be manipulated exactly as the product of $c$-number exponents, in particular rewritten it as

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right) \hat{u}^{\dagger}\left(t, t_{0}\right)=\hat{I} \exp \left\{-\frac{i}{\hbar}\left[\int_{t_{0}}^{t} \hat{H}\left(t^{\prime}\right) d t^{\prime}-\int_{t_{0}}^{t} \hat{H}\left(t^{\prime \prime}\right) d t^{\prime \prime}\right]\right\}=\hat{I} \exp \{\hat{0}\}=\hat{I} . \tag{4.184}
\end{equation*}
$$

This property ensures, in particular, that the system state's normalization does not depend on time:

$$
\begin{equation*}
\langle\alpha(t) \mid \alpha(t)\rangle=\left\langle\alpha\left(t_{0}\right)\right| \hat{u}^{\dagger}\left(t, t_{0}\right) \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\left\langle\alpha\left(t_{0}\right) \mid \alpha\left(t_{0}\right)\right\rangle . \tag{4.185}
\end{equation*}
$$

The most difficult cases for the explicit solution of Eq. (158) are those when Eq. (179) is violated. ${ }^{38}$ It may be proven that in these cases the integral limits in the last form of Eq. (182) should be truncated, giving the so-called Dyson series

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right)=\hat{I}+\sum_{k=1}^{\infty}\left(-\frac{i}{\hbar}\right)^{k} \int_{t_{0}}^{t} d t_{1} \int_{t_{0}}^{t_{1}} d t_{2} \ldots \int_{t_{0}}^{t_{k-1}} d t_{k} \hat{H}\left(t_{1}\right) \hat{H}\left(t_{2}\right) \ldots \hat{H}\left(t_{k}\right) . \tag{4.186}
\end{equation*}
$$

Since we would not have time to use this relation in our course, I will skip its proof. ${ }^{39}$
Let me now return to the general discussion of quantum dynamics to outline its alternative, Heisenberg picture. For that, let us recall that according to Eq. (125), in quantum mechanics the expectation value of any observable $A$ is a long bra-ket. Below we will see that other quantities (say, the rates of quantum transitions between pairs of different states, say $\alpha$ and $\beta$ ) may also be measured in experiment; the most general form for all such measurable quantities is the following long bracket:

$$
\begin{equation*}
\langle\alpha| \hat{A}|\beta\rangle \tag{4.187}
\end{equation*}
$$

As has been discussed above, in the Schrödinger picture the bra- and ket-vectors of the states are timedependent, while the variable operators stay constant (if the corresponding variables do not explicitly depend on time), so that Eq. (187), applied to moment $t$, may be presented as

$$
\begin{equation*}
\langle\alpha(t)| \hat{A}_{\mathrm{s}}|\beta(t)\rangle \tag{4.188}
\end{equation*}
$$

where index "S" emphasizes the Schrödinger picture. Let us apply to the bra- and ket-vectors in this expression the evolution law (157):

$$
\begin{equation*}
\langle\alpha| \hat{A}|\beta\rangle=\left\langle\alpha\left(t_{0}\right)\right| \hat{u}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{s}} \hat{u}\left(t, t_{0}\right)\left|\beta\left(t_{0}\right)\right\rangle . \tag{4.189}
\end{equation*}
$$

This equality means that if we form a long bracket with bra- and ket-vectors of the initial-time states, together with the following time-dependent Heisenberg operator ${ }^{40}$

$$
\begin{equation*}
\hat{A}_{\mathrm{H}}(t) \equiv \hat{u}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{S}} \hat{u}\left(t, t_{0}\right)=\hat{u}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{H}}\left(t_{0}\right) \hat{u}\left(t, t_{0}\right), \tag{4.190}
\end{equation*}
$$

all experimentally measurable results will remain the same as in the Schrödinger picture:

[^594]Let us see how does the Heisenberg picture work for the same simple (but very important!) problem of the spin- $1 / 2$ precession in a $z$-oriented magnetic field, described (in the $z$-basis) by the Hamiltonian matrix (164). In that basis, Eq. (158) for the time-evolution operator reads

$$
i \hbar\left(\begin{array}{cc}
\dot{u}_{11} & \dot{u}_{12}  \tag{4.192}\\
\dot{u}_{21} & \dot{u}_{22}
\end{array}\right)=\frac{\hbar \Omega}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\left(\begin{array}{ll}
u_{11} & u_{12} \\
u_{21} & u_{22}
\end{array}\right)=\frac{\hbar \Omega}{2}\left(\begin{array}{cc}
u_{11} & u_{12} \\
-u_{21} & -u_{22}
\end{array}\right) \text {. }
$$

We see that in this simple case the equations for different matrix elements of the evolution operator matrix are decoupled, and readily solvable, using the universal initial condition (178):41

$$
\mathrm{u}(t, 0)=\left(\begin{array}{cc}
e^{i \Omega t / 2} & 0  \tag{4.193}\\
0 & e^{-i \Omega t / 2}
\end{array}\right) \equiv \mathrm{I} \cos \frac{\Omega t}{2}-i \sigma_{z} \sin \frac{\Omega t}{2} .
$$

Now we can use Eq. (190) to find the Heisenberg-picture operators of spin components. Dropping index "H" for brevity (the Heisenberg-picture operators are clearly marked by their dependence on time anyway, we get

$$
\begin{align*}
\mathrm{S}_{x}(t) & =\mathrm{u}^{\dagger}(t, 0) \mathrm{S}_{x}(0) \mathrm{u}(t, 0)=\frac{\hbar}{2} \mathrm{u}^{\dagger}(t, 0) \sigma_{x} \mathrm{u}(t, 0) \\
& =\frac{\hbar}{2}\left(\begin{array}{cc}
e^{i \Omega t / 2} & 0 \\
0 & e^{-i \Omega t / 2}
\end{array}\right)\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right)\left(\begin{array}{cc}
e^{i-\Omega t / 2} & 0 \\
0 & e^{i \Omega t / 2}
\end{array}\right)  \tag{4.194}\\
& =\frac{\hbar}{2}\left(\begin{array}{cc}
0 & e^{i \Omega t} \\
e^{-i \Omega t} & 0
\end{array}\right)=\frac{\hbar}{2}\left[\sigma_{x} \cos \Omega t-\sigma_{y} \sin \Omega t\right] \equiv \mathrm{S}_{x}(0) \cos \Omega t-\mathrm{S}_{\mathrm{y}}(0) \sin \Omega t .
\end{align*}
$$

Absolutely similar calculations of the other spin components yield

$$
\begin{align*}
\mathrm{S}_{y}(t)=\frac{\hbar}{2}\left(\begin{array}{cc}
0 & -i e^{i \Omega t} \\
i e^{-i \Omega t} & 0
\end{array}\right) & =\frac{\hbar}{2}\left[\sigma_{y} \cos \Omega t+\sigma_{x} \sin \Omega t\right] \equiv \mathrm{S}_{y}(0) \cos \Omega t+\mathrm{S}_{x}(0) \sin \Omega t  \tag{4.195}\\
\mathrm{~S}_{z}(t) & =\frac{\hbar}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)=\frac{\hbar}{2} \sigma_{z}=S_{z}(0) . \tag{4.196}
\end{align*}
$$

A practical advantage of these formulas is that they describe system's evolution for arbitrary initial conditions, thus making the analysis of the initial state effects very simple. Indeed, since in the Heisenberg picture the expectation values of observables are calculated using Eq. (191) (with $\beta=\alpha$ ), with time-independent bra- and ket vectors, such averaging of Eqs. (194)-(196) immediately returns us to Eqs. (170), (173), and (174), obtained in the Schrödinger picture. Moreover, these equations for the Heisenberg operators formally coincide with the classical equations of the torque-induced precession for $c$-number variables. (In the next chapter, we will see that the same exact mapping is valid for the Heisenberg picture of the orbital motion.)

[^595]In order to see that the last fact is by no means a coincidence, let us combine Eqs. (158) and (190) to form an explicit differential equation of the Heisenberg operator evolution. For that, let us differentiate Eq. (190) over time:

$$
\begin{equation*}
\frac{d}{d t} \hat{A}_{\mathrm{H}}=\frac{\partial \hat{u}^{\dagger}}{\partial t} \hat{A}_{\mathrm{s}} \hat{u}+\hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\hat{u}^{\dagger} \hat{A}_{\mathrm{s}} \frac{\partial \hat{u}}{\partial t} . \tag{4.197}
\end{equation*}
$$

Plugging in the derivatives of the time evolution operator from Eq. (158) and its Hermitian conjugate, and multiplying both parts of the equation by $i \hbar$, we get

$$
\begin{equation*}
i \hbar \frac{d}{d t} \hat{A}_{\mathrm{H}}=-\hat{u}^{\dagger} \hat{H} \hat{A}_{\mathrm{s}} \hat{u}+\hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\hat{u}^{\dagger} \hat{A}_{\mathrm{S}} \hat{H} \hat{u} \tag{4.198a}
\end{equation*}
$$

If for the Schrödinger-picture Hamiltonian the condition similar to Eq. (179) is satisfied, then, according to Eqs. (177) or (182), the Hamiltonian commutes with the time evolution operator and its Hermitian conjugate, and may be swapped with any of them. ${ }^{42}$ Hence, we may rewrite Eq. (198a) as

$$
\begin{equation*}
i \hbar \frac{d}{d t} \hat{A}_{\mathrm{H}}=-\hat{H} \hat{u}^{\dagger} \hat{A}_{\mathrm{s}} \hat{u}+i \hbar \hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\hat{u}^{\dagger} \hat{A}_{\mathrm{s}} \hat{u} \hat{H}=i \hbar \hat{u}^{\dagger} \frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \hat{u}+\left[\hat{u}{ }^{\dagger} \hat{A}_{\mathrm{S}} \hat{u}, \hat{H}\right] . \tag{4.198b}
\end{equation*}
$$

Now using the definition (190) again, for both terms in the right-hand part, we may write

Heisenberg equation of motion

$$
\begin{equation*}
i \hbar \frac{d}{d t} \hat{A}_{\mathrm{H}}=i \hbar\left(\frac{\partial \hat{A}}{\partial t}\right)_{\mathrm{H}}+\left[\hat{A}_{\mathrm{H}}, \hat{H}\right] . \tag{4.199}
\end{equation*}
$$

This is the so-called Heisenberg equation of motion. ${ }^{43}$
Let us see how does this equation look for the same problem of spin- $1 / 2$ precession in a $z$ oriented, time-independent magnetic field, described in the $z$-basis by the Hamiltonian matrix (164), which does not depend on time. In this basis, Eq. (199) for the vector operator of spin reads ${ }^{44}$

$$
i \hbar\left(\begin{array}{ll}
\dot{\mathbf{S}}_{11} & \dot{\mathbf{S}}_{12}  \tag{4.200}\\
\dot{\mathbf{S}}_{21} & \dot{\mathbf{S}}_{22}
\end{array}\right)=\frac{\hbar \Omega}{2}\left[\left(\begin{array}{ll}
\mathbf{S}_{11} & \mathbf{S}_{12} \\
\mathbf{S}_{21} & \mathbf{S}_{22}
\end{array}\right),\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\right]=\hbar \Omega\left(\begin{array}{cc}
0 & -\mathbf{S}_{12} \\
\mathbf{S}_{21} & 0
\end{array}\right) .
$$

Once again, the equations for different matrix elements are decoupled, and their solution is elementary:

$$
\begin{align*}
& \mathbf{S}_{11}(t)=\mathbf{S}_{11}(0)=\text { const }, \quad \mathbf{S}_{22}(t)=\mathbf{S}_{22}(0)=\text { const }, \\
& \mathbf{S}_{12}(t)=\mathbf{S}_{12}(0) e^{i \Omega t}, \quad \mathbf{S}_{21}(t)=\mathbf{S}_{21}(0) e^{-i \Omega t} \tag{4.201}
\end{align*}
$$

[^596]According to Eq. (190), the initial "values" of the Heisenberg-picture matrix elements are just the Schrödinger-picture ones, so that using Eq. (117) we may rewrite this solution in either of two forms:

$$
\begin{gather*}
\mathbf{S}(t)=\frac{\hbar}{2}\left[\mathbf{n}_{x}\left(\begin{array}{cc}
0 & e^{i \Omega t} \\
e^{-i \Omega t} & 0
\end{array}\right)+\mathbf{n}_{y}\left(\begin{array}{cc}
0 & -i e^{i \Omega t} \\
i e^{-i \Omega t} & 0
\end{array}\right)+\mathbf{n}_{z}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\right] \\
=\frac{\hbar}{2}\left(\begin{array}{cc}
\mathbf{n}_{z} & \mathbf{n}_{-} e^{i \Omega t} \\
\mathbf{n}_{+} e^{-i \Omega} & -\mathbf{n}_{z}
\end{array}\right), \quad \text { with } \mathbf{n}_{ \pm} \equiv \mathbf{n}_{x} \pm i \mathbf{n}_{y} . \tag{4.202}
\end{gather*}
$$

The simplicity of the last expression is spectacular. (Remember, it covers any initial conditions, and all 3 spatial components of spin!) On the other hand, for some purposes the former expression may be more convenient; in particular, its Cartesian components immediately give our earlier results (194)(196).

One of advantages is that the Heisenberg picture is that it provides a more clear link between the classical and quantum mechanics. Indeed, analytical classical mechanics may be used to derive the following equation of time evolution of an arbitrary function $A\left(q_{j}, p_{j}, t\right)$ of generalized coordinates and momenta of the system, and time: ${ }^{45}$

$$
\begin{equation*}
\frac{d A}{d t}=\frac{\partial A}{\partial t}-\{A, H\} \tag{4.203}
\end{equation*}
$$

where $H$ is the classical Hamiltonian function of the system, and $\{. ., .$.$\} is the so-called Poisson bracket$ defined, for two arbitrary functions $A\left(q_{j}, p_{j}, t\right)$ and $B\left(q_{j}, p_{j}, t\right)$, as

$$
\begin{equation*}
\{A, B\} \equiv \sum_{j}\left(\frac{\partial A}{\partial p_{j}} \frac{\partial B}{\partial q_{j}}-\frac{\partial A}{\partial q_{j}} \frac{\partial B}{\partial p_{j}}\right) \tag{4.204}
\end{equation*}
$$

Comparing Eq. (203) with Eq. (199), we see that the correspondence between the classical and quantum mechanics (in the Heisenberg picture) is provided by the following symbolic relation ${ }^{46}$

$$
\begin{equation*}
\{A, B\} \leftrightarrow \frac{i}{\hbar}[\hat{A}, \hat{B}] . \tag{4.205}
\end{equation*}
$$

[^597]This relation may be used, in particular, for finding appropriate operators for system's observables, if their form is not immediately evident from the correspondence principle. We will develop this argumentation further in the next chapter where we revisit the wave mechanics, and also in Chapter 9.

Finally, let us discuss one more alternative picture of quantum dynamics. It is also attributed to P. A. M. Dirac, and is called either the "Dirac picture", or (more frequently) the interaction picture. The last name stems from the fact that this picture is very useful for the perturbative (approximate) approaches to systems whose Hamiltonians may be partitioned into two parts,

$$
\begin{equation*}
\hat{H}=\hat{H}_{0}+\hat{H}_{\mathrm{int}} \tag{4.206}
\end{equation*}
$$

where $\hat{H}_{0}$ is the sum of relatively simple Hamiltonians of non-interacting component sub-systems, while their second term in Eq. (206) represents their weak interaction. (Note, however, that the relations in the balance of this section are exact and not based on these assumptions.) In this case, it is natural to consider, together with the genuine unitary operator $\hat{u}\left(t, t_{0}\right)$ of the time evolution of the system, which obeys Eq. (158), a similarly defined unitary operator of evolution of the "unperturbed system" described by Hamiltonian $\hat{H}_{0}$ alone:

$$
\begin{equation*}
i \hbar \dot{\hat{u}}_{0}=\hat{H}_{0} \hat{u}_{0} \tag{4.207}
\end{equation*}
$$

and also the following interaction evolution operator,

Interaction evolution operator

$$
\begin{equation*}
\hat{u}_{I} \equiv \hat{u}_{0}^{\dagger} \hat{u} \tag{4.208}
\end{equation*}
$$

The sense of this definition becomes more clear if we insert the reciprocal relation,

$$
\begin{equation*}
\hat{u} \equiv \hat{u}_{0} \hat{u}_{0}^{\dagger} \hat{u}=\hat{u}_{0} \hat{u}_{I} \tag{4.209}
\end{equation*}
$$

and its Hermitian conjugate,

$$
\begin{equation*}
\hat{u}^{\dagger}=\left(\hat{u}_{0} \hat{u}_{I}\right)^{\dagger}=\hat{u}_{I}^{\dagger} \hat{u}_{0}^{\dagger}, \tag{4.210}
\end{equation*}
$$

into the basic Eq. (190) - which is valid in any picture:

$$
\begin{equation*}
\langle\alpha| \hat{A}|\beta\rangle=\left\langle\alpha\left(t_{0}\right)\right| \hat{u}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{s}} \hat{u}\left(t, t_{0}\right)\left|\beta\left(t_{0}\right)\right\rangle=\left\langle\alpha\left(t_{0}\right)\right| \hat{u}_{I}^{\dagger}\left(t, t_{0}\right) \hat{u}_{0}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{s}} \hat{u}_{0}\left(t, t_{0}\right) \hat{u}_{I}\left(t, t_{0}\right)\left|\beta\left(t_{0}\right)\right\rangle . \tag{4.211}
\end{equation*}
$$

This relation shows that all calculations of the observable expectation values and transition rates (i.e. all the results of quantum mechanics that may be experimentally verified) are expressed by the following formula, with the standard bra-ket structure (187),

$$
\begin{equation*}
\langle\alpha| \hat{A}|\beta\rangle=\left\langle\alpha_{I}(t)\right| \hat{A}_{I}(t)\left|\beta_{I}(t)\right\rangle \tag{4.212}
\end{equation*}
$$

if we assume that both the state vectors and operators evolve in time, with the vectors evolving due to the interaction operator $\hat{u}_{I}$,

$$
\begin{equation*}
\left\langle\alpha_{I}(t)\right| \equiv\left\langle\alpha\left(t_{0}\right)\right| \hat{u}_{I}^{\dagger}\left(t, t_{0}\right), \quad\left|\beta_{I}(t)\right\rangle \equiv \hat{u}_{I}\left(t, t_{0}\right)\left|\beta\left(t_{0}\right)\right\rangle \tag{4.213}
\end{equation*}
$$

while the operators' evolution being governed by the unperturbed operator $\hat{u}_{0}$ :

$$
\begin{equation*}
\hat{A}_{I}(t) \equiv \hat{u}_{0}^{\dagger}\left(t, t_{0}\right) \hat{A}_{\mathrm{s}} \hat{u}_{0}\left(t, t_{0}\right) \tag{4.214}
\end{equation*}
$$

These relations describe the interaction picture of quantum dynamics. Let me defer an example of its convenience until the perturbative analysis of open quantum systems in Sec. 7.6, and here end the discussion with a proof that the interaction evolution operator satisfies the Schrödinger equation,

$$
\begin{equation*}
i \hbar \dot{\hat{u}}_{I}=\hat{H}_{I} \hat{u}_{I} \tag{4.215}
\end{equation*}
$$

in which $\hat{H}_{I}$ is the interaction Hamiltonian transformed in accordance with rule (214):

$$
\begin{equation*}
\hat{H}_{I}(t) \equiv \hat{u}_{0}^{\dagger}\left(t, t_{0}\right) \hat{H}_{\mathrm{int}} \hat{u}_{0}\left(t, t_{0}\right) . \tag{4.216}
\end{equation*}
$$

The proof is very straightforward: first using definition (208), and then Eqs. (158) and the Hermitian conjugate of Eq. (207), we may write

$$
\begin{align*}
i \hbar \dot{\hat{u}}_{I} & =i \hbar \frac{d}{d t}\left(\hat{u}_{0}^{\dagger} \hat{u}\right)=i \hbar\left(\dot{\hat{u}}_{0}^{\dagger} \hat{u}+\hat{u}_{0}^{\dagger} \dot{\hat{u}}\right)=-\hat{H}_{0} \hat{u}_{0}^{\dagger} \hat{u}+\hat{u}_{0}^{\dagger} \hat{H} \hat{u}=-\hat{H}_{0} \hat{u}_{0}^{\dagger} \hat{u}+\hat{u}_{0}^{\dagger}\left(\hat{H}_{0}+\hat{H}_{\mathrm{int}}\right) \hat{u}  \tag{4.217}\\
& =-\hat{H}_{0} \hat{u}_{0}^{\dagger} \hat{u}+\hat{u}_{0}^{\dagger} \hat{H}_{0} \hat{u}+\hat{u}_{0}^{\dagger} \hat{H}_{\mathrm{int}} \hat{u}=\left(-\hat{H}_{0} \hat{u}_{0}^{\dagger}+\hat{u}_{0}^{\dagger} \hat{H}_{0}\right) \hat{u}+\hat{u}_{0}^{\dagger} \hat{H}_{\mathrm{int}} \hat{u} .
\end{align*}
$$

Since $\hat{u}_{0}^{\dagger}$ may be presented as an integral of $\hat{H}_{0}$ (similar to Eq. (181) relating $\hat{u}$ and $\hat{H}$ ), these operators commute, so that the parentheses in the last form of Eq. (217) vanish. Now plugging $\hat{u}$ from Eq. (209), we get the equation,

$$
\begin{equation*}
i \hbar \dot{\hat{u}}_{I}=\hat{u}_{0}^{\dagger} \hat{H}_{\mathrm{int}} \hat{u}_{0} u_{I}=\left(\hat{u}_{0}^{\dagger} \hat{H}_{\mathrm{int}} \hat{u}_{0}\right) \hat{u}_{I} \tag{4.218}
\end{equation*}
$$

that is equivalent to the combination of Eqs. (215) and (216).
Equation (215) shows that if the energy scale of interaction $H_{\text {int }}$ is much weaker than the background energy $H_{0}$, operators $\hat{u}_{I}$ and $\hat{u}_{I}^{\dagger}$, and hence the state vectors (213) evolve relatively slowly. Such an exclusion of fast background oscillations is especially convenient for the perturbative approaches to complex interacting systems, in particular to the open quantum systems that weakly interact with their environment - see Sec. 7.6.

### 4.7. Exercise problems

4.1. Let $\alpha$ and $\beta$ be two possible quantum states of the same system, and $\hat{A}$ be a linear operator. Which of the following expressions are legitimate (i. e. have a well-defined meaning) within the bra-ket formalism?

1. $\langle\alpha\rangle$
2. $\langle\alpha \mid \beta\rangle^{2}$
3. $|\alpha\rangle\langle\beta|$
4. $\hat{A}^{*}$
5. $\langle\hat{A}|$
6. $\langle\alpha| \hat{A}$
7. $\alpha|\hat{A}\rangle$
8. $|\alpha\rangle^{2}$
9. $\hat{A}^{2}$
10. $\left\langle\left.\alpha\right|^{\dagger}\right.$
4.2. Prove that if $\hat{A}$ and $\hat{B}$ are linear operators, then:
(i) $\left(\hat{A}^{\dagger}\right)^{\dagger}=\hat{A}$;
(ii) $(i \hat{A})^{\dagger}=-i \hat{A}^{\dagger}$;
(iii) $(\hat{A} \hat{B})^{\dagger}=\hat{B}^{\dagger} \hat{A}^{\dagger}$;
(iv) operators $\hat{A} \hat{A}^{\dagger}$ and $\hat{A}^{\dagger} \hat{A}$ are Hermitian.
4.3. Prove that for any linear operators $\hat{A}, \hat{B}, \hat{C}, \hat{D}$,

$$
[\hat{A} \hat{B}, \hat{C} \hat{D}]=\hat{A}\{\hat{B}, \hat{C}\} \hat{D}-\hat{A} \hat{C}\{\hat{B}, \hat{D}\}+\{\hat{A}, \hat{C}\} \hat{D} \hat{B}-\hat{C}\{\hat{A}, \hat{D}\} \hat{B}
$$

4.4. Calculate all possible binary products $\sigma_{j} \sigma_{j^{\prime}}$ (for $j, j^{\prime}=x, y, z$ ) of the Pauli matrices (105),

$$
\sigma_{x} \equiv\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right), \quad \sigma_{y} \equiv\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right), \quad \sigma_{z} \equiv\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right),
$$

and their commutators and anticommutators (defined similarly to those of the corresponding operators). Present the results using the Kronecker delta and Levi-Civita permutation symbols. ${ }^{47}$
4.5. Calculate the following expressions,
(i) $(\mathbf{c} \cdot \sigma)^{n}$, and then
(ii) $(\mathrm{bI}+\mathbf{c} \cdot \sigma)^{n}$,
for the scalar product $\mathbf{c} \cdot \sigma$ of the Pauli matrix vector $\sigma \equiv \mathbf{n}_{x} \sigma_{x}+\mathbf{n}_{y} \sigma_{y}+\mathbf{n}_{z} \sigma_{z}$ by an arbitrary $c$-number vector $\mathbf{c}$, where $n \geq 0$ is an integer, and $b$ is an arbitrary scalar $c$-number.

Hint: For task (ii), you may like to use the binomial theorem, ${ }^{48}$ and then transform the result in a way enabling you to use the same theorem backwards.
4.6. Use the results of the previous problem to derive Eqs. (2.165)-(2.166) for the transparency $T$ of a system of $N$ similar, equidistant, delta-functional tunnel barriers.
4.7. Use result of Problem 5 to spell out the following the following matrix: $\exp \{i \theta \mathbf{n} \cdot \sigma\}$, where $\sigma$ is the vector of Pauli matrices, $\mathbf{n}$ is a $c$-number vector of unit length, and $\theta$ is a $c$-number scalar.
4.8. Use the result of Problem 5(ii) to calculate $\exp \{A\}$, where $A$ is an arbitrary $2 \times 2$ matrix.
4.9. Express elements of matrix $B=\exp \{A\}$ explicitly via those of the $2 \times 2$ matrix $A$. Spell out your result for the following matrices:

$$
\mathrm{A}=\left(\begin{array}{ll}
a & a \\
a & a
\end{array}\right), \quad \mathrm{A}^{\prime}=\left(\begin{array}{ll}
i \varphi & i \varphi \\
i \varphi & i \varphi
\end{array}\right)
$$

with real $a$ and $\varphi$.
4.10. Prove that for arbitrary square matrices A and B ,

$$
\operatorname{Tr}(\mathrm{AB})=\operatorname{Tr}(\mathrm{BA}) .
$$

Is each diagonal element $(A B)_{j j}$ necessarily equal to $(B A)_{j j}$ ?

[^598]4.11. Prove that the matrix trace of an arbitrary operator does not change at an arbitrary unitary transformation.
4.12. Prove that for any two full and orthonormal bases $u_{j}, v_{j}$ of the same Hilbert space,
$$
\operatorname{Tr}\left(\left|u_{j}\right\rangle\left\langle v_{j^{\prime}}\right|\right)=\left\langle v_{j^{\prime}} \mid u_{j}\right\rangle .
$$
4.13. Is the 1D scattering matrix S, defined by Eq. (133), unitary? What about the 1D transfer matrix T defined by Eq. (134)?
4.14. Calculate the trace of the following matrix:
$$
\exp \{\mathbf{i} \cdot \boldsymbol{\sigma}\} \exp \{i \mathbf{b} \cdot \boldsymbol{\sigma}\}
$$
where $\boldsymbol{\sigma}$ is the Pauli matrix vector, while $\mathbf{a}$ and $\mathbf{b}$ are usual ( $c$-number) geometric vectors.
4.15. Let $A_{j}$ be eigenvalues of some operator $\hat{A}$. Express the following two sums,
$$
\Sigma_{1}=\sum_{j} A_{j}, \quad \Sigma_{2}=\sum_{j} A_{j}^{2}
$$
via the matrix elements $A_{j j}$, of this operator in an arbitrary basis.
4.16. Calculate $\left\langle\sigma_{z}\right\rangle$ of a two-level system in a quantum state with the following ket-vector:
$$
|\alpha\rangle=\operatorname{const} \times|\uparrow\rangle+|\downarrow\rangle+|\rightarrow\rangle+|\leftarrow\rangle),
$$
where $(\uparrow, \downarrow)$ and $(\rightarrow, \leftarrow)$ are eigenstates of the Pauli matrices $\sigma_{z}$ and $\sigma_{x}$, respectively.
Hint: Double-check whether the solution you are giving is general.
4.17. An electron is fully polarized in the positive $z$-direction. Calculate the probabilities of the alternative outcomes of a perfect Stern-Gerlach experiment with the magnetic field $\mathbf{B}$ oriented in the direction of some axis $\mathbf{n}$, performed on this electron.
4.18. A perfect Stern-Gerlach instrument makes a single-shot measurement of the following combination, $\left(S_{x}+S_{z}\right) / \sqrt{ } 2$, of two spin components of a $z$-polarized electron; after that, component $S_{z}$ of the same particle is measured. What are the possible outcomes of these measurements and their probabilities?
4.19. In a certain basis, the Hamiltonian of a spin- $1 / 2$ (two-level) system is described by matrix
\[

\mathrm{H}=\left($$
\begin{array}{cc}
E_{1} & 0 \\
0 & E_{2}
\end{array}
$$\right), \quad with E_{1} \neq E_{2},
\]

and the operator of some observable $A$, by matrix

$$
\mathrm{A}=\left(\begin{array}{ll}
1 & 1 \\
1 & 1
\end{array}\right)
$$

For the system's state with the energy equal exactly to $E_{1}$, find the possible results of measurements of observable $A$ and the probabilities of the corresponding measurement outcomes.
4.20. ${ }^{*}$ States $u_{1,2,3}$ form an orthonormal basis of a system with Hamiltonian

$$
\hat{H}=-\delta\left(\left|u_{1}\right\rangle\left\langle u_{2}\right|+\left|u_{2}\right\rangle\left\langle u_{3}\right|+\left|u_{3}\right\rangle\left\langle u_{1}\right|\right)+\text { h.c. }
$$

where $\delta$ is a real constant, and h.c. means the Hermitian conjugate of the previous expression. Calculate its stationary states and energy levels. Can you relate this system with any other(s) discussed earlier in the course?
4.21. Suggest a Hamiltonian describing particle's dynamics in an infinite 1D set of similar quantum wells in the tight-binding approximation, in the bra-ket formalism, and verify that is yields the correct dispersion relation (2.206).
4.22. Calculate eigenvectors and eigenvalues of the following matrices:

$$
A=\left(\begin{array}{lll}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{array}\right), \quad B=\left(\begin{array}{llll}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{array}\right)
$$

4.23. Find eigenvalues of the following matrix:

$$
\mathrm{A}=\mathbf{a} \cdot \boldsymbol{\sigma} \equiv a_{x} \sigma_{x}+a_{y} \sigma_{y}+a_{z} \sigma_{z},
$$

where $a_{x, y, z}$ are real $c$-numbers (scalars), and $\sigma_{x, y, z}$ are the Pauli matrices. Sketch the dependence of the eigenvalues on parameter $a_{z}$, with $a_{x}$ and $a_{y}$ fixed. Compare the result with Fig. 29.
4.24. Derive a differential equation for the time evolution of the expectation value of an observable, using both the Schrödinger picture and the Heisenberg picture of quantum mechanics.
4.25. At $t=0$, a spin $-1 / 2$ particle, whose interaction with an external field is described by Hamiltonian

$$
\hat{H}=\mathbf{a} \cdot \hat{\boldsymbol{\sigma}} \equiv a_{x} \hat{\sigma}_{x}+a_{y} \hat{\sigma}_{y}+a_{z} \hat{\sigma}_{z},
$$

(where $a_{x, y, z}$ are real and constant $c$-numbers, and $\hat{\sigma}_{x, y, z}$ are the operators that, in the $z$-basis, are represented by the Pauli matrices $\sigma_{x, y, z}$ ), was in state $\uparrow$, one of two eigenstates of operator $\hat{\sigma}_{z}$. Use the Schrödinger picture equations to calculate the time evolution of:
(i) the ket-vector $|\alpha\rangle$ of the system (in any stationary basis you like),
(ii) the probabilities to find the system in states $\uparrow$ and $\downarrow$, and
(iii) the expectation values of all 3 spatial components ( $\hat{S}_{x}$, etc.) of the spin vector operator $\hat{\mathbf{S}}=(\hbar / 2) \hat{\boldsymbol{\sigma}}$.

Analyze and interpret the results for the particular case $a_{y}=a_{z}=0$.
4.26. For the same system as in the previous problem, use the Heisenberg picture equations to calculate the time evolution of:
(i) all three spatial components ( $\hat{S}_{x}$, etc.) of the spin operator $\hat{\mathbf{S}}_{\mathrm{H}}(\mathrm{t})$,
(ii) the expectation values of the spin components.

Compare the latter results with those of the previous problem.
4.27. For the same system as in two last problems, calculate the matrix elements of operator $\hat{\sigma}_{z}$ in the basis of eigenstates $a_{1}, a_{2}$.

Hint: In contrast to the cited problems, the answer evidently does not depend on the initial conditions.
4.28. In the Schrödinger picture of quantum mechanics, three operators satisfy the following commutation relation:

$$
[\hat{A}, \hat{B}]=\hat{C}
$$

What is their relation in the Heisenberg picture (at the same time instant)?
4.29. A spin $-1 / 2$ particle is placed into a magnetic field $B(t)$, which is an arbitrary function of time. Derive the differential equations describing the time evolution of:
(i) the vector operator $\hat{\mathbf{S}}$ of particle's spin (in the Heisenberg picture), and
(ii) the expectation value $\langle\mathbf{S}\rangle$ of spin's vector.

Contemplate the relative merits of the latter equation for the description of a single spin and of a large collection of similar, non-interacting spins.
4.30.* Prove the Bloch theorem given by either Eq. (3.107) or Eq. (3.108).

Hint: Consider the translation operator $\hat{\tau}_{\mathrm{R}}$, defined by the following result of its action on an arbitrary function $f(\mathbf{r})$ :

$$
\hat{\tau}_{\mathbf{R}} f(\mathbf{r})=f(\mathbf{r}+\mathbf{R}),
$$

where $\mathbf{R}$ is an arbitrary vector of the Bravais lattice (3.106). In particular, analyze the commutation properties of the operator, and apply them to an eigenfunction $\psi(\mathbf{r})$ of the stationary Schrödinger equation for a particle in a 3D periodic potential described by Eq. (3.105).

## Chapter 5. Some Exactly Solvable Problems

This describes several simplest but important applications of the bra-ket formalism, notably including a few wave-mechanics problems we have already started to discuss in Chapters 2 and 3.

### 5.1. Two-level systems

In the course of discussion of the bra-ket formalism in the last chapter, we have already considered several examples of how it works for electron's spin. We have seen, in particular, that in magnetic field the electron has eigenenergies (4.167), i.e. two energy levels. As will be shown later in the course, such two-energy-level picture is valid not only for electrons and other spin- $1 / 2$ elementary particles (such as muons and neutrinos), but also may give a good approximation for other important quantum systems. For example, as was already mentioned in Chapter 2, two energy levels are sufficient for an approximate description of dynamics of two weakly coupled quantum wells (Sec. 2.6), and of level anticrossing in the weak-potential approximation of the band theory (Sec. 2.7). Such two-level systems (alternatively called "spin- $1 / 2$-like" systems) are nowadays the focus of additional attention in the view of prospects of their possible use for information processing and encryption. (In the last context, to be discussed in Sec. 8.5, a two-level system is usually called a qubit.)

This is why before proceeding to other problems, let us summarize in brief what we have already learned about properties and dynamics of two-level systems, in a more convenient language. According to the general Eq. (4.6), a ket- (or bra-) vector of an arbitrary pure (coherent) state $\alpha$ of such a system may be presented, at any instant, as a linear combination of two basis vectors, for example

$$
\begin{equation*}
|\alpha\rangle=\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle, \tag{5.1}
\end{equation*}
$$

and hence is completely described by two complex coefficients (c-numbers) - say, $\alpha \uparrow$ and $\alpha \downarrow$. These two numbers are not completely arbitrary; they are restricted by the normalization condition. If the basis vectors are normalized, then to have the system in some basis state with a $100 \%$ probability, we need

$$
\begin{equation*}
W_{\Sigma}=\langle\alpha \mid \alpha\rangle=\left(\langle\uparrow| \alpha_{\uparrow}^{*}+\langle\downarrow| \alpha_{\downarrow}^{*}\right)\left(\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle\right)=\alpha_{\uparrow}^{*} \alpha_{\uparrow}+\alpha_{\downarrow}^{*} \alpha_{\downarrow}=\left|\alpha_{\uparrow}\right|^{2}+\left|\alpha_{\downarrow}\right|^{2}=1 \tag{5.2}
\end{equation*}
$$

This requirement is automatically satisfied if we take the moduli of $\alpha \uparrow$ and $\alpha \downarrow$ equal to the sine and cosine of the same (real) angle. Thus we can write, for example,

$$
\begin{equation*}
\alpha_{\uparrow}=\cos \frac{\theta}{2} e^{i \gamma}, \quad \alpha_{\downarrow}=\sin \frac{\theta}{2} e^{i(\gamma+\varphi)} \tag{5.3}
\end{equation*}
$$

Moreover, according to the general Eq. (4.125), if we deal with just one system, ${ }^{1}$ the common phase factor $\exp \{i \gamma\}$ is unimportant for calculation of any expectation values, and we can take $\gamma=0$, so that Eq. (3) is reduced to

[^599]\[

$$
\begin{equation*}
\alpha_{\uparrow}=\cos \frac{\theta}{2}, \quad \alpha_{\downarrow}=\sin \frac{\theta}{2} e^{i \varphi} \tag{5.4}
\end{equation*}
$$

\]

Bloch sphere representation of state

The reason why the argument of sine and cosine functions is usually taken in the form $\theta / 2$, becomes clear from Fig. 1a: Eq. (4) conveniently maps each state $\alpha$ on a certain representation point of a unit-radius Bloch sphere, ${ }^{2}$ with polar angle $\theta$ and azimuthal angle $\varphi$. In particular, state $\uparrow$ (with $\alpha \uparrow=1$ and $\alpha \downarrow=0$ ) corresponds to the North Pole of the sphere $(\theta=0$ ), while state $\downarrow$ (with $\alpha \uparrow=0$ and $\alpha \downarrow=1$ ), to its South pole $(\theta=\pi) .{ }^{3}$ Similarly, states $\rightarrow$ and $\leftarrow$, described by Eqs. (4.122), i.e. having $\alpha \uparrow=1 / \sqrt{ } 2$ and $\alpha \downarrow= \pm 1 / \sqrt{2}$, correspond to points with $\theta=\pi / 2$ and to, respectively, $\varphi=0$ and $\varphi=\pi$. Two more special points (denoted in Fig. 1a as $\odot$ and $\otimes$ ) are also located on sphere's equator (at $\theta=\pi / 2$ and $\varphi=$ $\pm \pi / 2$ ); it is easy to check that they correspond to the eigenstates of matrix $\sigma_{y}$ (in the same $z$-basis).

In order to understand why such mutually perpendicular location of these three special point pairs on the Bloch sphere is not occasional, let us plug Eqs. (4) into Eqs. (4.131)-(4.133) for the expectation values of spin components. The result is

$$
\begin{equation*}
\left\langle S_{x}\right\rangle=\frac{\hbar}{2} \sin \theta \cos \varphi, \quad\left\langle S_{y}\right\rangle=\frac{\hbar}{2} \sin \theta \sin \varphi, \quad\left\langle S_{z}\right\rangle=\frac{\hbar}{2} \cos \theta \tag{5.5}
\end{equation*}
$$

showing that the radius-vector of the representation point on the sphere is (after multiplication by $\hbar / 2$ ) just the expectation value of the spin vector $\mathbf{S}$.


Fig. 5.1. Bloch sphere: (a) notation, and presentation of spin precession in magnetic fields directed along: (b) axis $z$, and (c) axis $x$.

Now let us see how does the representation point moves in various cases. First of all, according to Eqs. (4.157)-(4.158), in the absence of an external field (when the Hamiltonian operator is equal to zero and hence the time-evolution operator is constant) the point does not move at all. Now, if we apply to an electron a magnetic field directed along axis $z$, then, according to Eqs. (4.202), the Heisenberg operator of $S_{z}$ (and hence the expectation value $\left\langle S_{z}\right\rangle$ ) remains constant, while angle $\varphi$ in Eq. (5) evolves

[^600]in time as $\Omega t+$ const. This means that the torque-induced precession of the spin in a constant field $\boldsymbol{B}=$ $\mathbf{n}_{z} B$ is described by a circular rotation of the representation point about axis $z$ (in Fig. 1b, in the horizontal plane) with the classical precession frequency $\Omega$. This is essentially the classical picture of rotation of the angular momentum vector about the precession axis $z$, with both its length and the $z$ component conserved. ${ }^{4}$

It is straightforward to repeat all calculations of Sec. 4.6 for a field of a different orientation and prove the (virtually evident) result that the representation point performs a similar rotation about the field direction. (Fig. 1c shows such rotation for an $x$-directed field.) Finally, note that it is sufficient to turn off the field to stop the precession instantly. (Since Eq. (4.158) is the first-order differential equation, the representation point has no effective inertia. ${ }^{5}$ ) Hence changing the direction and magnitude of the external field, it is possible to move spin's representation point to any position on the Bloch sphere. (In Chapter 6 we will examine another method of manipulating the point position, that is based on external rf field and is more convenient for some two-level systems.)

In the context of quantum information, this means that in the absence of uncontrollable interaction with environment, it is possible to prepare a qubit in any pure quantum state, and then keep it unchanged. From here it is clear that a qubit is very much different from and a classical bistable system used to store single bits of information - such as the voltage state of a usual SRAM cell (a positivefeedback loop of two transistor-based inverters). As Eq. (4) shows, qubit's state is determined by two independent, continuous parameters $\theta$ and $\varphi$, so it may store much more information than one bit. (The difference is even more spectacular in qubit systems, to be discussed in Sec. 8.5.) However, classical bistable systems, due to their nonlinearity, are stable with respect to small perturbations, so that their operation is rather robust with respect to unintentional interaction with their environment. In contrast, qubit's state may be readily disturbed (i.e. its representation point on the Bloch sphere shifted) by even minor perturbations, and does not have an internal state stabilization mechanism. ${ }^{6}$ Due to this reason, qubit-based systems are rather vulnerable to environment-induced drifts, including dephasing and relaxation effects, which will be discussed in Chapter 7.

### 5.2. Revisiting wave mechanics

In order to use the bra-ket formalism for the description of the "orbital" motion of a particle as a whole, we have to either rewrite or even modify some of its formulas for the case of observables with continuous spectrum of eigenvalues. (One example we already know well are the momentum and kinetic energy of a free particle.) In that case, all the above expressions for states, their bra- and ket-vectors, and eigenvalues, should be stripped of discrete indices, like the index $j$ in the key equation (4.68), which determines eigenstates and eigenvalues of observable $A$. For that, Eq. (4.68) may be rewritten in the form

[^601]\[

$$
\begin{equation*}
\hat{A}\left|a_{A}\right\rangle=A\left|a_{A}\right\rangle . \tag{5.6}
\end{equation*}
$$

\]

More essentially, all sums over such continuous eigenstate sets should be replaced by integrals. For example, for a full and orthonormal set of eigenstates (6), the closure relation (4.44) should be replaced with

$$
\begin{equation*}
\int d A\left|a_{A}\right\rangle\left\langle a_{A}\right|=\hat{I} \tag{5.7}
\end{equation*}
$$

where the integral should be taken over the whole interval of possible values of observable $A$. Applying this relation to the ket-vector of an arbitrary state $\alpha$ (generally, not an eigenstate of operator $\hat{A}$ ), we get

$$
\begin{equation*}
|\alpha\rangle=\hat{I}|\alpha\rangle=\int d A\left|a_{A}\right\rangle\left\langle a_{A} \mid \alpha\right\rangle=\int d A\left\langle a_{A} \mid \alpha\right\rangle\left|a_{A}\right\rangle . \tag{5.8}
\end{equation*}
$$

This integral replaces sum (4.37) for the representation of an arbitrary ket-vector as an expansion over eigenstates of an operator. For the particular case when $|\alpha\rangle=\left|a_{A}{ }^{\prime}\right\rangle$, this relation requires ${ }^{7}$

$$
\begin{equation*}
\left\langle a_{A} \mid a_{A^{\prime}}\right\rangle=\delta\left(A-A^{\prime}\right) ; \tag{5.9}
\end{equation*}
$$

According to Eq. (8), in the continuous case the bra-ket $\left\langle a_{A} \mid \alpha\right\rangle$ still plays the role of the coefficient whose modulus squared determines state $a_{A}$ 's probability - see the last form of Eq. (4.120). However, in the continuous spectrum case the probability to find the system exactly in a particular state is infinitesimal. Instead we should speak about the probability density $w(A) \propto\left|\left\langle a_{A} \mid \alpha\right\rangle\right|^{2}$ to find the observable within a small interval $d A$ about a certain value $A$. The coefficient in that relation may be found by making the similar change from summation to integration (without any additional coefficients) in the normalization condition (4.121):

$$
\begin{equation*}
\int d A\left\langle\alpha \mid a_{A}\right\rangle\left\langle a_{A} \mid \alpha\right\rangle=1 \tag{5.10}
\end{equation*}
$$

Since the total probability of the system to be in some state should also equal $\int w(A) d A$, this means that

$$
\begin{equation*}
w(A)=\left\langle\alpha \mid a_{A}\right\rangle\left\langle a_{A} \mid \alpha\right\rangle=\left|\left\langle\alpha \mid a_{A}\right\rangle\right|^{2} \tag{5.11}
\end{equation*}
$$

Now let us see how we can calculate expectation values of continuous observables, i.e. their ensemble averages. If we speak about the same observable $A$ whose eigenstates are used as the basis (or any compatible observable), everything is simple. Inserting Eq. (11) into the general statistical relation

$$
\begin{equation*}
\langle A\rangle=\int w(A) A d A, \tag{5.12}
\end{equation*}
$$

which is just the evident continuous version of Eq. (1.37), we get

$$
\begin{equation*}
\langle A\rangle=\int\left\langle\alpha \mid a_{A}\right\rangle A\left\langle a_{A} \mid \alpha\right\rangle d A \tag{5.13}
\end{equation*}
$$

Presenting this expression as a double integral,

$$
\begin{equation*}
\langle A\rangle=\int d A \int d A^{\prime}\left\langle\alpha \mid a_{A}\right\rangle A \delta\left(A-A^{\prime}\right)\left\langle a_{A^{\prime}} \mid \alpha\right\rangle, \tag{5.14}
\end{equation*}
$$

[^602]and using the continuous-spectrum version of Eq. (4.98),
\[

$$
\begin{equation*}
\left\langle a_{A}\right| \hat{A}\left|a_{A^{\prime}}\right\rangle=A \delta\left(A-A^{\prime}\right), \tag{5.15}
\end{equation*}
$$

\]

we may write

$$
\begin{equation*}
\langle A\rangle=\int d A \int d A^{\prime}\left\langle\alpha \mid a_{A}\right\rangle\left\langle a_{A}\right| \hat{A}\left|a_{A^{\prime}}\right\rangle\left\langle a_{A^{\prime}} \mid \alpha\right\rangle=\langle\alpha| \hat{A}|\alpha\rangle, \tag{5.16}
\end{equation*}
$$

so that Eq. (4.125) remains valid in the continuous-spectrum case without any changes.
The situation is a bit more complicated for the expectation values of operators that do not commute with the base-creating operator, because the matrix of such an operators in that may not be diagonal. We will consider (and overcome :-) this technical difficulty very soon, but otherwise we are ready for the discussion of wave mechanics. (For the notation simplicity I will discuss its 1D version; the generalization to the 2D and 3D cases is straightforward.)

Let us consider what is called the coordinate representation, postulating the (intuitively almost evident) existence of a quantum state basis, whose with ket-vectors will be called $|x\rangle$, corresponding to a certain, exactly defined value $x$ of particle's coordinate. Writing the following evident identity:

$$
\begin{equation*}
x|x\rangle=x|x\rangle, \tag{5.17}
\end{equation*}
$$

and comparing this relation with Eq. (6), we see that they do not contradict each other if we assume that $x$ in the left-hand part of this equation is considered as the coordinate operator $\hat{x}$ whose action on a ket(or bra-) vector is just its multiplication by c-number $x$. (This looks like a proof, but is actually a separate, independent postulate, no matter how plausible.)

In this coordinate representation, the inner product $\left\langle a_{A} \mid \alpha(t)\right\rangle$ becomes $\langle x \mid \alpha(t)\rangle$, and Eq. (11) takes the form

$$
\begin{equation*}
w(x, t)=\langle\alpha(t) \mid x\rangle\langle x \mid \alpha(t)\rangle=\langle x \mid \alpha(t)\rangle^{*}\langle x \mid \alpha(t)\rangle . \tag{5.18}
\end{equation*}
$$

Comparing this formula with the basic postulate (1.22) of wave mechanics, we see that they coincide if the Schrödinger's wavefunction of time-evolving state $\alpha(t)$ is identified with that bra-ket: ${ }^{8}$

$$
\begin{equation*}
\Psi_{\alpha}(x, t)=\langle x \mid \alpha(t)\rangle \tag{5.19}
\end{equation*}
$$

This key formula provides the connection between the bra-ket formalism and wave mechanics, and should not be too surprising for the (thoughtful :-) reader. Indeed, Eqs. (4.45) shows that any inner product of vectors describing two states is a measure of their coincidence - just as the scalar product of two geometric vectors. (The orthonormality condition (4.38) is a particular manifestation of this fact.) In this language, value (19) of wavefunction $\Psi_{\alpha}$ at point $x$ and moment $t$ characterizes "how much of a particular coordinate $x$ " does the state $\alpha$ contain at that particular instance. (Of course this informal language is too crude to describe the fact that $\Psi_{\alpha}(x, t)$ is a complex function, which has not only a modulus, but also a phase.)

[^603]Let us rewrite the most important formulas of the bra-ket formalism (so far, in the Schrödinger picture) in the wave mechanics notation. In particular, let us use Eq. (19) to calculate the (partial) time derivative of the wavefunction, multiplied by the usual coefficient $i \hbar$ :

$$
\begin{equation*}
i \hbar \frac{\partial \Psi_{\alpha}}{\partial t}=i \hbar \frac{\partial}{\partial t}\langle x \mid \alpha(t)\rangle \tag{5.20}
\end{equation*}
$$

Since the coordinate operator $\hat{x}$ does not depend on time explicitly, its eigenstates $x$ are stationary, and we can swap the time derivative and the time-independent ket-vector and hence $\langle x|$. Making use of the Schrödinger-picture equations (4.157) and (4.158), and then inserting the identity operator in the continuous form (7) of the closure relation, written for the coordinate eigenstates,

$$
\begin{equation*}
\int d x^{\prime}\left|x^{\prime}\right\rangle\left\langle x^{\prime}\right|=\hat{I} \tag{5.21}
\end{equation*}
$$

we may continue to develop the right-hand part of Eq. (20) as

$$
\begin{align*}
\langle x| i \hbar \frac{\partial}{\partial t}|\alpha(t)\rangle & =\langle x| i \hbar \frac{\partial}{\partial t} \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\langle x| \hat{H} \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle=\langle x| \hat{H}|\alpha(t)\rangle  \tag{5.22}\\
& =\int d x^{\prime}\langle x| \hat{H}\left|x^{\prime}\right\rangle\left\langle x^{\prime} \mid \alpha(t)\right\rangle=\int d x^{\prime}\langle x| \hat{H}\left|x^{\prime}\right\rangle \Psi_{\alpha}\left(x^{\prime}, t\right) .
\end{align*}
$$

For a general Hamiltonian operator, we have to stop here, because if it does not commute with the coordinate operator, its matrix in the $x$-basis is not diagonal, and integral (22) cannot be worked out explicitly. However, there exists a broad set of space-local operators ${ }^{9}$ whose arguments include just one value of the spatial coordinate, for which we can move ket-vector $\langle x|$ to the right ${ }^{10}$

$$
\begin{equation*}
\langle x| \hat{A}\left|x^{\prime}\right\rangle \Psi\left(x^{\prime}, t\right)=\hat{A} \Psi\left(x^{\prime}, t\right)\left\langle x \mid x^{\prime}\right\rangle=\hat{A} \Psi(x, t) \delta\left(x-x^{\prime}\right) \tag{5.23}
\end{equation*}
$$

[^604]where operator $\hat{A}$ in the last two forms should be understood as its coordinate representation that is defined by Eq. (23) - if it is valid for a particular operator. For example, consider the 1 D version of operator (1.40),
\[

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}_{x}^{2}}{2 m}+U(\hat{x}, t), \tag{5.24}
\end{equation*}
$$

\]

which was the basis of all our discussions in Chapter 2. Its potential-energy part commutes with operator $\hat{x}$, so its matrix in the $x$-basis is diagonal, meaning that this part of Hamiltonian (24) is clearly local, with its coordinate representation given merely by the $c$-number function $U(x, t)$. The situation with the kinetic energy, which is a function of momentum operator $\hat{p}_{x}$, not commuting with $\hat{x}$, is less evident. Let me show that this operator is also local, and in the same shot derive (the 1D version of Eq. (1.26), if we postulate the commutation relation (2.14):

$$
\begin{equation*}
\hat{x} \hat{p}_{x}-\hat{p}_{x} \hat{x}=i \hbar \hat{I} \tag{5.25}
\end{equation*}
$$

[^605]For that, let us consider the following matrix element, $\langle x| \hat{x} \hat{p}_{x}-\hat{p}_{x} \hat{x}\left|x^{\prime}\right\rangle$. On one hand, we may use Eq. (25) to write

$$
\begin{equation*}
\langle x| \hat{x} \hat{p}_{x}-\hat{p}_{x} \hat{x}\left|x^{\prime}\right\rangle=\langle x| i \hbar \hat{I}\left|x^{\prime}\right\rangle=i \hbar\left\langle x \mid x^{\prime}\right\rangle=i \hbar \delta\left(x-x^{\prime}\right) . \tag{5.26}
\end{equation*}
$$

On the other hand, since $\hat{x}\left|x^{\prime}\right\rangle=x^{\prime}\left|x^{\prime}\right\rangle$ and $\langle x| \hat{x}=\langle x| x$, we can write

$$
\begin{equation*}
\langle x| \hat{x} \hat{p}_{x}-\hat{p}_{x} \hat{x}\left|x^{\prime}\right\rangle=\langle x| x \hat{p}_{x}-\hat{p}_{x} x^{\prime}\left|x^{\prime}\right\rangle=\left(x-x^{\prime}\right)\langle x| \hat{p}_{x}\left|x^{\prime}\right\rangle . \tag{5.27}
\end{equation*}
$$

Comparing Eqs. (26) and (27), we may write

$$
\begin{equation*}
\langle x| \hat{p}_{x}\left|x^{\prime}\right\rangle=i \hbar \frac{\delta\left(x-x^{\prime}\right)}{\left(x-x^{\prime}\right)} \tag{5.28a}
\end{equation*}
$$

Thus $\hat{p}_{x}$ is a local operator. Since Eq. (28a) may be rewritten as ${ }^{11}$

$$
\begin{equation*}
\langle x| \hat{p}_{x}\left|x^{\prime}\right\rangle=-i \hbar \frac{\partial}{\partial x} \delta\left(x-x^{\prime}\right) \tag{5.28b}
\end{equation*}
$$

its comparison with Eq. (23) shows that the formula used so much in Chapter 2,

$$
\begin{equation*}
\hat{p}_{x}=-i \hbar \frac{\partial}{\partial x} \tag{5.29}
\end{equation*}
$$

is indeed valid, but only for the coordinate representation of the momentum operator. (Later in this section we will see that in an alternative, momentum representation, this operator looks completely differently.)

It is straightforward to show (and virtually evident) that any operator $f(\hat{p})$ is local as well, with its coordinate representation being

$$
\begin{equation*}
f\left(-i \hbar \frac{\partial}{\partial x}\right) \tag{5.30}
\end{equation*}
$$

In particular, this pertains to the kinetic energy operator in Eq. (24), so that Eq. (20) is reduced to the Schrödinger equation in its familiar wave-mechanics form (1.28), if by $\hat{H}$ we mean its coordinate representation:

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m}\left(-i \hbar \frac{\partial}{\partial x}\right)^{2}+U(x, t)=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}}+U(x, t) \tag{5.31}
\end{equation*}
$$

Now let us return, as was promised, to operators that do not commute with operator $\hat{x}$, and hence do not have to share its continuous spectrum. Inner-multiplying both parts of the general Eq. (4.68) by ket-vector $\langle x|$, and inserting into the left-hand part the identity operator in form (21), we get

$$
\begin{equation*}
\int d x^{\prime}\langle x| \hat{A}\left|x^{\prime}\right\rangle\left\langle x^{\prime} \mid a_{j}\right\rangle=A_{j}\left\langle x \mid a_{j}\right\rangle, \tag{5.32}
\end{equation*}
$$

[^606]i.e., using the wavefunction definition (19),
\[

$$
\begin{equation*}
\int d x^{\prime}\langle x| \hat{A}\left|x^{\prime}\right\rangle \Psi_{j}\left(x^{\prime}, t\right)=A_{j} \Psi_{j}(x, t) . \tag{5.33}
\end{equation*}
$$

\]

If the operator $A$ is space-local, i.e. satisfies Eq. (23), then this result is immediately reduced to

$$
\begin{equation*}
\hat{A} \Psi_{j}(x, t)=A_{j} \Psi_{j}(x, t) \tag{5.34}
\end{equation*}
$$

Operator's eigenstates and eigenvalues
(where the left-hand part implies the coordinate representation of the operator), even if the operator does not commute with operator $\hat{x} .{ }^{12}$ The most important case of this coordinate-representation form of the eigenproblem (4.68) is the familiar Eq. (1.60) for eigenvalues $E_{n}$ of energy. Hence, the energy spectrum of a system (that, as we know very well from the first chapters of the course, may be discrete) is nothing more than the set of eigenvalues of its Hamiltonian operator - a very important conclusion indeed.

The operator locality also simplifies the expression for its expectation value. Indeed, plugging the completeness relation in the form (21) into the general Eq. (4.125) twice (written in the first case for $x$ and in the second case for $x$ '), we get

$$
\begin{equation*}
\langle A\rangle=\int d x \int d x^{\prime}\langle\alpha(t) \mid x\rangle\langle x| \hat{A}\left|x^{\prime}\right\rangle\left\langle x^{\prime} \mid \alpha(t)\right\rangle=\int d x \int d x^{\prime} \Psi_{\alpha}^{*}(x, t)\langle x| \hat{A}\left|x^{\prime}\right\rangle \Psi_{\alpha}\left(x^{\prime}, t\right) \tag{5.35}
\end{equation*}
$$

Now, Eq. (23) reduces this result to just

$$
\begin{equation*}
\langle A\rangle=\int d x \int d x \Psi_{\alpha}^{*}(x, t) \hat{A} \Psi_{\alpha}(x, t) \delta\left(x-x^{\prime}\right)=\int \Psi_{\alpha}^{*}(x, t) \hat{A} \Psi_{\alpha}(x, t) d x \tag{5.36}
\end{equation*}
$$

i.e. to Eq. (1.23), which we had to postulate in Chapter 1.

So, we have essentially derived all basic relations of wave mechanics from the bra-ket formalism, which will also allow us to get some important new results in that area. Before doing that, let us have a look at a pair of very interesting relations, together called the Ehrenfest theorem. In order to derive them, let us calculate the following commutator: ${ }^{13}$

$$
\begin{equation*}
\left[\hat{x}, \hat{p}_{x}^{2}\right] \equiv \hat{x} \hat{p}_{x} \hat{p}_{x}-\hat{p}_{x} \hat{p}_{x} \hat{x} . \tag{5.37}
\end{equation*}
$$

Rewriting Heisenberg's commutation relation (25) as

$$
\begin{equation*}
\hat{x} \hat{p}_{x}=\hat{p}_{x} \hat{x}+i \hbar \tag{5.38}
\end{equation*}
$$

we can use it twice in the first term of the right-hand part of Eq. (37) to sequentially move the momentum operators to the left:

$$
\begin{equation*}
\hat{x} \hat{p}_{x} \hat{p}_{x}=\left(\hat{p}_{x} \hat{x}+i \hbar\right) \hat{p}_{x}=\hat{p}_{x} \hat{x} \hat{p}_{x}+i \hbar \hat{p}_{x}=\hat{p}_{x}\left(\hat{p}_{x} \hat{x}+i \hbar\right)+i \hbar \hat{p}_{x}=\hat{p}_{x} \hat{p}_{x} \hat{x}+2 i \hbar \hat{p}_{x} . \tag{5.39}
\end{equation*}
$$

[^607]The first term of the result cancels with the second term of Eq. (37), so that the commutator is rather simple:

$$
\begin{equation*}
\left[\hat{x}, \hat{p}_{x}^{2}\right]=2 i \hbar \hat{p}_{x} \tag{5.40}
\end{equation*}
$$

Let us use this equality to calculate the Heisenberg-picture equation of motion for operator $\hat{x}$, applying the general Heisenberg equation (4.199) to the orbital motion, when the Hamiltonian has the form (31), with time-independent potential $U(x):^{14}$

$$
\begin{equation*}
\frac{d \hat{x}}{d t}=\frac{1}{i \hbar}[\hat{x}, \hat{H}]=\frac{1}{i \hbar}\left[\hat{x}, \frac{\hat{p}_{x}^{2}}{2 m}+U(\hat{x})\right] . \tag{5.41}
\end{equation*}
$$

The potential energy operator commutes with the coordinate operator. Thus, the right-hand part of Eq. (41) is proportional to commutator (40):

$$
\begin{equation*}
\frac{d \hat{x}}{d t}=\frac{\hat{p}_{x}}{m} \tag{5.42}
\end{equation*}
$$

In that operator equality, we readily recognize the classical relation between particle's momentum and is velocity.

Now let us see what does a similar procedure give for the momentum's derivative:

$$
\begin{equation*}
\frac{d \hat{p}_{x}}{d t}=\frac{1}{i \hbar}\left[\hat{p}_{x}, \hat{H}\right]=\frac{1}{i \hbar}\left[\hat{p}_{x}, \frac{\hat{p}_{x}^{2}}{2 m}+U(\hat{x})\right] . \tag{5.43}
\end{equation*}
$$

The kinetic energy operator commutes with the momentum operator, and hence may be dropped from the right-hand part of this equation. In order to calculate the remaining commutator of the momentum and potential energy, let us use the fact that any smooth potential profile may be represented by its Taylor expansion:

$$
\begin{equation*}
U(\hat{x})=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} U}{\partial \hat{x}^{k}} \hat{x}^{k}, \tag{5.44}
\end{equation*}
$$

where the derivatives of $U$ should be understood as $c$-numbers (evaluated at $x=0$ ), so that we may write

$$
\begin{equation*}
\left[\hat{p}_{x}, U(\hat{x})\right]=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} U}{\partial \hat{x}^{k}}\left[\hat{p}_{x}, \hat{x}^{k}\right]=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} U}{\partial \hat{x}^{k}}(\hat{p}_{x} \underbrace{\hat{x} \hat{x} . \hat{x}}_{k \text { times }}-\underbrace{\left.\hat{x} \hat{x} \ldots \hat{x} \hat{p}_{x}\right) . ~ . ~ . ~}_{k \text { times }} \tag{5.45}
\end{equation*}
$$

Applying Eq. (38) $k$ times to the last term in the parentheses, exactly as we did it in Eq. (39), we get

$$
\begin{equation*}
\left[\hat{p}_{x}, U(\hat{x})\right]=-\sum_{k=1}^{\infty} \frac{1}{k!} \frac{\partial^{k} U}{\partial \hat{x}^{k}} i k \hbar \hat{x}^{k-1}=-i \hbar \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k} U}{\partial \hat{x}^{k}} \hat{x}^{k-1} . \tag{5.46}
\end{equation*}
$$

But the last sum is just the Taylor expansion of the derivative $\partial U / \partial x$. Indeed,

$$
\begin{equation*}
\frac{\partial U}{\partial \hat{x}}=\sum_{k^{\prime}=0}^{\infty} \frac{1}{k^{\prime}!} \frac{\partial^{k^{\prime}}}{\partial \hat{x}^{k^{\prime}}}\left(\frac{\partial U}{\partial \hat{x}}\right) \hat{x}^{k^{\prime}}=\sum_{k^{\prime}=0}^{\infty} \frac{1}{k^{\prime}!} \frac{\partial^{k^{\prime}+1} U}{\partial \hat{x}^{k^{\prime}+1}} \hat{x}^{k^{\prime}}=\sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k} U}{\partial \hat{x}^{k}} \hat{x}^{k-1}, \tag{5.47}
\end{equation*}
$$

[^608]where at the last step I have replaced the notation of the summation index from $k$ ' to $k-1$. As a result, Eq. (43) yields:
\[

$$
\begin{equation*}
\frac{d \hat{p}_{x}}{d t}=-\frac{\partial}{\partial \hat{x}} U(\hat{x}) . \tag{5.48}
\end{equation*}
$$

\]

This equation again coincides with the classical equation of motion! Discussing spin dynamics in Sec. 4.6 and 5.1 , we have already seen that this is very typical of the Heisenberg picture. Moreover, averaging Eqs. (42) and (48) over the initial state (as Eq. (4.191) prescribes ${ }^{15}$ ), we get similar results for the expectation values: ${ }^{16}$

$$
\begin{equation*}
\frac{d\langle x\rangle}{d t}=\frac{\left\langle p_{x}\right\rangle}{m}, \quad \frac{d\left\langle p_{x}\right\rangle}{d t}=-\left\langle\frac{\partial U}{\partial x}\right\rangle . \tag{5.49}
\end{equation*}
$$

However, it is important to remember that the equivalence between these quantum-mechanical equations and similar equations of classical mechanics is superficial, and the degree of the similarity between the two mechanics very much depends on the problem. As one extreme, let us consider the case when a particle's state, at any moment between $t_{0}$ and $t$, may be accurately represented by one, relatively narrow wave packet. Then we may interpret Eqs. (49) as equations of essentially classical motion for the wave packet's center, in accordance with the correspondence principle. However, even in this case it is important to remember about the purely quantum mechanical effects of nonvanishing wave packet width and its spreading in time, which were discussed in Sec. 2.2.

In the opposite extreme, Eqs. (49), though valid, may tell almost nothing about system's dynamics. Maybe the most apparent example is the "leaky" quantum well that was discussed in Sec. 2.5 - see Fig. 2.18 and its discussion. Since both the potential $U(x)$ and the initial state are symmetric relative to point $x=0$, the right-hand parts of both Eqs. (49) identically equal zero. Of course, the result (that average values of both momentum and coordinate stay equal zero at all times) is correct, but it does not tell us too much about the rich dynamics of the system (the finite lifetime of the metastable state, the formation of two wave packets, their waveform and propagation speed), and about the important insight the solution gives for the quantum measurement theory. Another similar example is the band theory (Sec. 2.7), with its purely quantum effect of the allowed energy bands and forbidden gaps, of which Eq. (49) gives no clue.

To summarize, the Ehrenfest theorem is important as an illustration of the correspondence principle, but its predictive power should not be exaggerated.

Now we are ready to patch some holes left during our studies of wave mechanics in Chapters 13. First of all, I have promised you to develop a more balanced view at the monochromatic de Broglie waves (4.1), which would be more respectful to the evident $\mathbf{r} \leftrightarrow \mathbf{p}$ symmetry of the coordinate and momentum. Let us do this for the 1D case when the wave may be presented as ${ }^{17}$

[^609]\[

$$
\begin{equation*}
\psi_{p}(x)=a_{p} \exp \left\{i \frac{p x}{\hbar}\right\}, \quad \text { for all }-\infty<x<+\infty \tag{5.50}
\end{equation*}
$$

\]

Let us have a good look at this function. Since it satisfies equation (34) for the 1D momentum operator $\hat{p}=-i \hbar \partial / \partial x$,

$$
\begin{equation*}
\hat{p} \psi_{p}=p \psi_{p} \tag{5.51}
\end{equation*}
$$

$\psi_{p}$ is an eigenfunction of the momentum operator. But this means that we can also write Eq. (6) for the corresponding ket-vector:

$$
\begin{equation*}
\hat{p}|p\rangle=p|p\rangle, \tag{5.52}
\end{equation*}
$$

and according to Eq. (19) the wavefunction may be presented as

$$
\begin{equation*}
\psi_{p}(x)=\langle x \mid p\rangle . \tag{5.53}
\end{equation*}
$$

Expression (53) is quite remarkable in its $x \leftrightarrow p$ symmetry - which may be pursued further on. Before doing that, however, we have to discuss normalization of such functions. Indeed, in this case, the probability density $w(x)(18)$ is constant, so that its integral

$$
\begin{equation*}
\int_{-\infty}^{+\infty} w(x) d x=\int_{-\infty}^{+\infty} \psi_{p}(x) \psi_{p}^{*}(x) d x \tag{5.54}
\end{equation*}
$$

diverges if $a_{p} \neq 0$. Earlier in the course, we discussed two ways to avoid this divergence. One is to use a very large but finite integration volume - see Eq. (1.31). Another way to avoid the divergence is to form a wave packet of the type (2.20), possibly of a very large length and very narrow spread of momenta $p$. Then integral (54) may be required to equal 1 without any conceptual problem.

However, both these methods violate the $x \leftrightarrow p$ symmetry, and hence are inconvenient for our current purposes. Instead, let us continue to identify the bra- and ket-vectors $\left\langle a_{A}\right|$ and $\left|a_{A}\right\rangle$ of the general theory, developed in the beginning of this section, with eigenvectors $\langle p|$ and $|p\rangle$ of momentum - just as we have already done in Eq. (52). Then the normalization condition (9) becomes

$$
\begin{equation*}
\left\langle p \mid p^{\prime}\right\rangle=\delta\left(p-p^{\prime}\right) \tag{5.55}
\end{equation*}
$$

Inserting the identity operator in the form (21) (with the integration variable $x$ ' replaced by $x$ ) into the left-hand side of this equation, we can translate this normalization rule to the wavefunction language:

$$
\begin{equation*}
\int d x\langle p \mid x\rangle\left\langle x \mid p^{\prime}\right\rangle \equiv \int d x \psi_{p}^{*}(x) \psi_{p^{\prime}}(x)=\delta\left(p-p^{\prime}\right) \tag{5.56}
\end{equation*}
$$

Now using Eq. (50), this requirement turns into the following condition:

$$
\begin{equation*}
a_{p}^{*} a_{p^{\prime}}^{+\infty} \exp \left\{i \frac{\left(p-p^{\prime}\right) x}{\hbar}\right\} d x \equiv\left|a_{p}\right|^{2} 2 \pi \hbar \delta\left(p-p^{\prime}\right)=\delta\left(p-p^{\prime}\right) \tag{5.57}
\end{equation*}
$$

so that, finally, $a_{p}=\exp \{i \varphi\} /(2 \pi \hbar)^{1 / 2}$, where $\phi$ is an arbitrary (real) phase, and Eq. (50) becomes ${ }^{18}$

[^610]\[

$$
\begin{equation*}
\psi_{p}(x)=\frac{1}{(2 \pi \hbar)^{1 / 2}} \exp \left\{i\left(\frac{p x}{\hbar}+\phi\right)\right\}, \tag{5.58}
\end{equation*}
$$

\]

As was mentioned above, for finite-length wave packets such normalization is not really necessary. However, frequently it makes sense to keep the pre-exponential coefficient in Eq. (58) even for wave packets, because of the following reason. Let us form a wave packet of the type (2.20), based on wavefunctions (58) - taking $\phi=0$ for the notation brevity, because it may be incorporated into function $\varphi(p)$ :

$$
\begin{equation*}
\psi(x)=\frac{1}{(2 \pi \hbar)^{1 / 2}} \int \varphi(p) \exp \left\{i \frac{p x}{\hbar}\right\} d p \tag{5.59}
\end{equation*}
$$

From the mathematical point of view, this is just the equation of a 1D Fourier spatial transform, and its reciprocal is

$$
\begin{equation*}
\varphi(p) \equiv \frac{1}{(2 \pi \hbar)^{1 / 2}} \int \psi(x) \exp \left\{-i \frac{p x}{\hbar}\right\} d x \tag{5.60}
\end{equation*}
$$

These expressions are completely symmetrical, and present the same wave packet; this is why functions $\psi(x)$ and $\varphi(p)$ are frequently called, respectively, the coordinate ( $x-$ ) and momentum ( $p-$ ) representations of the (same) state of the particle. Using Eqs. (53) and (58), they may be presented in an even more manifestly symmetric form,

$$
\begin{equation*}
\psi(x)=\int \varphi(p)\langle x \mid p\rangle d p, \quad \varphi(p)=\int \psi(x)\langle p \mid x\rangle d x \tag{5.61}
\end{equation*}
$$

in which the scalar products satisfy the basic postulate (4.14) of the bra-ket formalism:

$$
\begin{equation*}
\langle p \mid x\rangle=\frac{1}{(2 \pi \hbar)^{1 / 2}} \exp \left\{-i \frac{p x}{\hbar}\right\}=\langle x \mid p\rangle^{*} \tag{5.62}
\end{equation*}
$$

We already know that in the $x$-representation, i.e. in the usual wave mechanics, the coordinate operator $\hat{x}$ is reduced to the multiplication by $x$, and the momentum operator is proportional to a derivative over $x$ :

$$
\begin{equation*}
\left.\hat{x}\right|_{\operatorname{in} x}=x,\left.\quad \hat{p}\right|_{\operatorname{in} x}=-i \hbar \frac{\partial}{\partial x} . \tag{5.63}
\end{equation*}
$$

It is natural to guess that in the $p$-representation, the expressions for operators would be reciprocal:

$$
\begin{equation*}
\left.\hat{x}\right|_{\text {in } p}=i \hbar \frac{\partial}{\partial p},\left.\quad \hat{p}\right|_{\text {in } p}=p \tag{5.64}
\end{equation*}
$$

with the difference in one sign only, due to the opposite signs of the Fourier exponents in Eqs. (59) and (60). The proof of Eqs. (64) is straightforward; for example, acting by the momentum operator to wavefunction (59), we get

$$
\begin{align*}
\hat{p} \psi(x) & =-i \hbar \frac{\partial}{\partial x} \psi(x)=\frac{1}{(2 \pi \hbar)^{1 / 2}} \int \varphi(p)\left(-i \hbar \frac{\partial}{\partial x} \exp \left\{i \frac{p x}{\hbar}\right\}\right) d p  \tag{5.65}\\
& =\frac{1}{(2 \pi \hbar)^{1 / 2}} \int p \varphi(p) \exp \left\{i \frac{p x}{\hbar}\right\} d p,
\end{align*}
$$

and similarly for operator $\hat{x}$ acting on function $\varphi(p)$. Hence, the action of the operators (63) on wavefunction $\psi$ (i.e. state's $x$-representation) gives the same results as the action of operators (64) on function $\varphi$ (i.e. its $p$-representation).

It is interesting to have one more, different look at this coordinate-to-momentum duality. For that, notice that according to Eqs. (4.82)-(4.84), we may consider the bra-ket $\langle x \mid p\rangle$ as an element of the (infinite-size) matrix $U_{x p}$ of the unitary transform from the $x$-basis to $p$-basis. Now let us derive the operator transform rule that would be a continuous version of Eq. (4.92). Say, we want to calculate a matrix element of some operator in the $p$-representation:

$$
\begin{equation*}
\langle p| \hat{A}\left|p^{\prime}\right\rangle \tag{5.66}
\end{equation*}
$$

Inserting two identity operators (21) into this bra-ket, and then using Eq. (53) and its complex conjugate, and also Eq. (23) (again, valid only for space-local operators!), we get

$$
\begin{align*}
& \langle p| \hat{A}\left|p^{\prime}\right\rangle=\int d x \int d x^{\prime}\langle p \mid x\rangle\langle x| \hat{A}\left|x^{\prime}\right\rangle\left\langle x^{\prime} \mid p^{\prime}\right\rangle=\int d x \int d x^{\prime} \psi_{p}^{*}(x)\langle x| \hat{A}\left|x^{\prime}\right\rangle \psi_{p^{\prime}}\left(x^{\prime}\right) \\
& =\frac{1}{2 \pi \hbar} \int d x \int d x^{\prime} \exp \left\{-i \frac{p x}{\hbar}\right\} \delta\left(x-x^{\prime}\right) \hat{A} \exp \left\{i \frac{p^{\prime} x^{\prime}}{\hbar}\right\}=\frac{1}{2 \pi \hbar} \int d x \exp \left\{-i \frac{p x}{\hbar}\right\} \hat{A} \exp \left\{i \frac{p^{\prime} x}{\hbar}\right\} . \tag{5.67}
\end{align*}
$$

For example, for the momentum operator itself, this relation yields:

$$
\begin{equation*}
\langle p| \hat{p}\left|p^{\prime}\right\rangle=\frac{1}{2 \pi \hbar} \int d x \exp \left\{-i \frac{p x}{\hbar}\right\}\left(-i \hbar \frac{\partial}{\partial x}\right) \exp \left\{i \frac{p^{\prime} x}{\hbar}\right\}=\frac{p^{\prime}}{2 \pi \hbar} \int_{-\infty}^{+\infty} \exp \left\{i \frac{\left(p^{\prime}-p\right) x}{\hbar}\right\} d x=p^{\prime} \delta\left(p^{\prime}-p\right) \tag{5.68}
\end{equation*}
$$

Due to Eq. (52), this result is equivalent to the second of Eqs. (64).
A natural question arises: why is the momentum representation used much less frequently than the coordinate representation - i.e., the wave mechanics? The answer is purely practical: besides the special case of the harmonic oscillator (to be revisited in Sec. 4 below), the orbital motion Hamiltonian (31) is not $x \leftrightarrow p$ symmetric, with the potential energy $U(x)$ being typically a more complex function than the kinetic energy, which is quadratic in momentum. Because of that, it is easier for problem solution to keep the potential energy operator just a wavefunction multiplier, as it is in the coordinate representation.

The most significant exception of this rule is the motion in a periodic potential, especially in the presence of additional external force $F(t)$, which may result in the effects discussed in Secs. 2.8 and 2.9 (the Bloch oscillations, Landau-Zener tunneling etc.). Indeed, in this case the dispersion relation $E_{n}(q)$, typically rather involved, plays the role of the effective kinetic energy, while the effective potential energy $U_{\mathrm{ef}}=-F(t) x$ in the field of the additional force is a simple function of $x$. This is why discussions of the listed and more complex issues of the band theory (such as quasiparticle scattering, mobility, diffusion, etc.) in solid state physics theory are most typically based on the momentum representation.

### 5.3. Feynman's path integrals

As has been already mentioned, even within the realm of wave mechanics, the bra-ket language allows to streamline some calculations that would be very bulky using the notation used in Chapters 1-3. Probably the best example in the famous alternative, path integral formulation of quantum mechanics,
developed in 1948 by R. Feynman. ${ }^{19}$ I will review this important concept - admittedly cutting one math corner for brevity. ${ }^{20}$ (This shortcut will be clearly marked.)

Let us inner-multiply both parts of Eq. (4.157), which is essentially the definition of the timeevolution operator, by the bra-vector of state $x$,

$$
\begin{equation*}
\langle x \mid \alpha(t)\rangle=\langle x| \hat{u}\left(t, t_{0}\right)\left|\alpha\left(t_{0}\right)\right\rangle, \tag{5.69}
\end{equation*}
$$

insert the identity operator before the ket-vector in the right-hand part, and then use the closure condition in the form of Eq. (21), with $x$ ' replaced with $x_{0}$ :

$$
\begin{equation*}
\langle x \mid \alpha(t)\rangle=\int d x_{0}\langle x| \hat{u}\left(t, t_{0}\right)\left|x_{0}\right\rangle\left\langle x_{0} \mid \alpha\left(t_{0}\right)\right\rangle . \tag{5.70}
\end{equation*}
$$

According to Eq. (19), this equality may be presented as

$$
\begin{equation*}
\Psi_{\alpha}(x, t)=\int d x_{0}\langle x| \hat{u}\left(t, t_{0}\right)\left|x_{0}\right\rangle \Psi_{\alpha}\left(x_{0}, t_{0}\right) . \tag{5.71}
\end{equation*}
$$

Comparing this expression with Eq. (2.44), we see that the bra-ket in this relation is nothing else than the 1D propagator, which was discussed in Sec. 2.2:

$$
\begin{equation*}
\langle x| \hat{u}\left(t, t_{0}\right)\left|x_{0}\right\rangle=G\left(x, t ; x_{0}, t_{0}\right) . \tag{5.72}
\end{equation*}
$$

As a reminder, we have already calculated the propagator for a free particle - see Eq. (2.49).
Now let us break the time segment $\left[t_{0}, t\right]$ into $N$ (for the time being, not necessarily equal) parts by inserting ( $N-1$ ) intermediate points (Fig. 2)

$$
\begin{equation*}
t_{0}<t_{1}<\ldots<t_{k}<\ldots<t_{N-1}<t \tag{5.73}
\end{equation*}
$$

and rewrite the time evolution operator in the form

$$
\begin{equation*}
\hat{u}\left(t, t_{0}\right)=\hat{u}\left(t, t_{N-1}\right) \hat{u}\left(t_{N-1}, t_{N-2}\right) \ldots \hat{u}\left(t_{2}, t_{1}\right) \hat{u}\left(t_{1}, t_{0}\right), \tag{5.74}
\end{equation*}
$$

whose correctness is evident from the very definition (4.157) of the operator. Plugging Eq. (74) into Eq. (72), let us insert the identity operator, again in the form (21) but written for $x_{k}$ rather than $x^{\prime}$, between each two partial evolution operators including time argument $t_{k}$. The result is

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\int d x_{N-1} \int d x_{N-2} \ldots \int d x_{1}\langle x| \hat{u}\left(t, t_{N-1}\right)\left|x_{N-1}\right\rangle\left\langle x_{N-1}\right| \hat{u}\left(t_{N-1}, t_{N-2}\right)\left|x_{N-2}\right\rangle \ldots\left\langle x_{1}\right| \hat{u}\left(t_{1}, t_{0}\right)\left|x_{0}\right\rangle . \tag{5.75}
\end{equation*}
$$



Fig. 5.2. Time partition and coordinate notation at the initial stage of the Feynman's path integral derivation.

[^611]The physical sense of each integration variable $x_{k}$ is the wavefunction's argument at time $t_{k}$ - see Fig. 2. The key Feynman's breakthrough was the realization that if all intervals are similar and sufficiently small, $t_{k}-t_{k-1}=d \tau \rightarrow 0$, all the partial bra-kets participating in Eq. (75) may be readily expressed via Eq. (2.49), even if the particle is not free, but moves in a stationary potential profile $U(x)$. To show that, let us use either Eq. (4.175) or Eq. (4.181), which, for a small time interval $d \tau$, give the same result:

$$
\begin{equation*}
\hat{u}(\tau+d \tau, \tau)=\exp \left\{-\frac{i}{\hbar} \hat{H} d \tau\right\}=\exp \left\{-\frac{i}{\hbar}\left(\frac{\hat{p}^{2}}{2 m} d \tau+U(\hat{x}) d \tau\right)\right\} . \tag{5.76}
\end{equation*}
$$

Generally, an exponent of a sum of two operators may be treated as that of $c$-number arguments, and in particular factored into a product of two exponents, only if the operators commute. (Indeed, in this case we can use all the standard algebra for exponents of $c$-number arguments.) In our case, this is not so, because operator $\hat{p}$ does not commute with $\hat{x}$, and hence with $U(\hat{x})$. However, it may be shown ${ }^{21}$ that for an infinitesimal time interval $d \tau$, the nonvanishing commutator

$$
\begin{equation*}
\left[\frac{\hat{p}^{2}}{2 m} d \tau, U(\hat{x}) d \tau\right] \neq 0 \tag{5.77}
\end{equation*}
$$

proportional to $(d \tau)^{2}$, is so small that in the first approximation in $d \tau$ its effects may be ignored. As a result, we may factor the right-hand part in Eq. (76) by writing

$$
\begin{equation*}
\hat{u}(\tau+d \tau, \tau)_{d \tau \rightarrow 0} \rightarrow \exp \left\{-\frac{i}{\hbar} \frac{\hat{p}^{2}}{2 m} d \tau\right\} \exp \left\{-\frac{i}{\hbar} U(\hat{x}) d \tau\right\} \tag{5.78}
\end{equation*}
$$

(This approximation is very much similar in spirit to the rectangle-formula approximation for a usual 1D integral, which in also asymptotically impeachable.)

Since the second exponential function in the right-hand part of Eq. (78) commutes with the coordinate operator, we can move it out of each partial bra-ket participating in Eq. (75), with $U(x)$ turning into a $c$-number function:

$$
\begin{equation*}
\left\langle x_{\tau+d \tau}\right| \hat{u}(\tau+d \tau, \tau)\left|x_{\tau}\right\rangle=\left\langle x_{\tau+d \tau}\right| \exp \left\{-\frac{i}{\hbar} \frac{\hat{p}^{2}}{2 m} d \tau\right\}\left|x_{\tau}\right\rangle \exp \left\{-\frac{i}{\hbar} U(x) d \tau\right\} . \tag{5.79}
\end{equation*}
$$

But the remaining bra-ket is just the propagator of a free particle, and we can use Eq. (2.49) for it:

$$
\begin{equation*}
\left\langle x_{\tau+d \tau}\right| \exp \left\{-\frac{i}{\hbar} \frac{\hat{p}^{2}}{2 m} d \tau\right\}\left|x_{\tau}\right\rangle=\left(\frac{m}{2 \pi i \hbar d \tau}\right)^{1 / 2} \exp \left\{i \frac{m(d x)^{2}}{2 \hbar d \tau}\right\} \tag{5.80}
\end{equation*}
$$

As the result, the full propagator (75) takes the form

$$
\begin{equation*}
G\left(x, t ; x_{0} t_{0}\right)=\lim _{\substack{d \tau \rightarrow 0 \\ N \rightarrow \infty}} \int d x_{N-1} \int d x_{N-2} . . \int d x_{1}\left(\frac{m}{2 \pi i \hbar d \tau}\right)^{N / 2} \exp \left\{\sum_{k=1}^{N}\left[i \frac{m(d x)^{2}}{2 \hbar d \tau}-i \frac{U(x)}{\hbar} d \tau\right]\right\} . \tag{5.81}
\end{equation*}
$$

[^612]At $N \rightarrow \infty$ and hence $d \tau \equiv\left(t-t_{0}\right) / N \rightarrow 0$, the sum under the exponent in this expression tends to an integral:

$$
\begin{equation*}
\sum_{k=1}^{N} \frac{i}{\hbar}\left[\frac{m}{2}\left(\frac{d x}{d \tau}\right)^{2}-U(x)\right]_{\tau=t_{k}} d \tau \rightarrow \frac{i}{\hbar} \int_{t_{0}}^{t}\left[\frac{m}{2}\left(\frac{d x}{d \tau}\right)^{2}-U(x)\right] d \tau \tag{5.82}
\end{equation*}
$$

and the expression in square brackets is just the particle's Lagrangian function $L .{ }^{22}$ The integral of the function over time is the classical action $S$ calculated along a particular "path" $x(\tau) .{ }^{23}$ As a result, defining the (1D) path integral as

$$
\begin{equation*}
\int(\ldots) D[x(\tau)] \equiv \lim _{\substack{d \tau \rightarrow 0 \\ N \rightarrow \infty}}\left(\frac{m}{2 \pi i \hbar d \tau}\right)^{N / 2} \int d x_{N-1} \int d x_{N-2} . . \int d x_{1}(\ldots) \tag{5.83a}
\end{equation*}
$$

we can bring our result to a superficially simple form

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\int \exp \left\{\frac{i}{\hbar} \varsigma[x(\tau)]\right\} D[x(\tau)] \tag{5.83b}
\end{equation*}
$$

1D path
integral: definition

The name "path integral" for the mathematical construct (83a) may be readily explained if we keep the number $N$ of time intervals large but finite, and also approximate each of the enclosed integrals by a sum over $M \gg 1$ discrete points along the coordinate axis (Fig. 3a).



Fig. 5.3. Several 1D classical paths in (a) the discrete approximation and (b) the continuous limit.

Then the path integral is a product of $(N-1)$ sums corresponding to different values of time $\tau$, each of them with $M$ terms, each of the terms representing the function under the integral at a particular spatial point. Multiplying those $(N-1)$ sums, we get a sum of $(N-1) M$ terms, each evaluating the function at a specific spatial-temporal point $[x, \tau]$. These terms may be now grouped to represent all possible different continuous classical paths $x[\tau]$ from the initial point $\left[x_{0}, t_{0}\right]$ to the finite point $[x, t]$. It is evident that the last interpretation remains true even in the continuous limit $N, M \rightarrow \infty-$ see Fig. 3b.

Why does such representation of the sum has sense? This is because in the classical limit the particle follows just a certain path, corresponding to the minimum of action $S^{22}$ Hence, for all close trajectories, the difference $\left(S-S_{\mathrm{cl}}\right)$ is proportional to the square of the deviation from the classical trajectory. Hence, for a quasiclassical motion, with $S_{\mathrm{cl}} \gg \hbar$, there is a substantial bunch of close trajectories, with $\left(S-S_{\mathrm{cl}}\right) \ll \hbar$, that give similar contributions to the path integral. On the other hand,

[^613]strongly non-classical trajectories, with $\left(S-S_{\mathrm{cl}}\right) \gg \hbar$, give phases $S \hbar$ rapidly oscillating from one trajectory to the next one, and their contributions to the path integral are averaged out. ${ }^{24}$ As a result, for the quasiclassical motion, the propagator's exponent may be evaluated on the classical path:
\[

$$
\begin{equation*}
G_{\mathrm{cl}} \propto \exp \left\{\frac{i}{\hbar} S_{\mathrm{cl}}\right\}=\exp \left\{\frac{i}{\hbar} \int_{t_{0}}^{t}\left[\frac{m}{2}\left(\frac{d x}{d \tau}\right)^{2}-U(x)\right] d \tau\right\} . \tag{5.84}
\end{equation*}
$$

\]

The sum of the kinetic and potential energies is the full energy $E$ of the particle, that remains constant for motion in a stationary potential $U(x)$, so that we may rewrite the expression under the integral as ${ }^{25}$

$$
\begin{equation*}
\left[\frac{m}{2}\left(\frac{d x}{d \tau}\right)^{2}-U(x)\right] d \tau=\left[m\left(\frac{d x}{d \tau}\right)^{2}-E\right] d \tau=m \frac{d x}{d \tau} d x-E d \tau \tag{5.85}
\end{equation*}
$$

With that replacement, Eq. (83b) yields

$$
\begin{equation*}
G_{\mathrm{cl}} \propto \exp \left\{\frac{i}{\hbar} \int_{x_{0}}^{x} m \frac{d x}{d \tau} d x\right\} \exp \left\{-\frac{i}{\hbar} E\left(t-t_{0}\right)\right\}=\exp \left\{\frac{i}{\hbar} \int_{x_{0}}^{x} p(x) d x\right\} \exp \left\{-\frac{i}{\hbar} E\left(t-t_{0}\right)\right\}, \tag{5.86}
\end{equation*}
$$

where $p$ is the classical momentum of the particle. But (at least, leaving the pre-exponential factor alone) this is exactly the WKB approximation result that was derived and studied in detail in Chapter 2!

One may question the value of a calculation that yields the results that could be readily obtained from Schrödinger's wave mechanics. The Feynman's approach, is indeed not used too often, but it has its merits. First, it has an important philosophical (and hence heuristic) value. Indeed, Eq. (83) may be interpreted by saying that the essence of quantum mechanics is the exploration, by the system, of all possible paths $x(\tau)$, each of them classical-like in the sense that the particle's coordinate $x$ and velocity $d x / d \tau$ (and hence its momentum) are exactly defined simultaneously at each point. The resulting contributions to the path integral are added up coherently to form the final propagator $G$, and via it, the final probability $W \propto|G|^{2}$ of the particle propagation from $\left[x_{0}, t_{0}\right]$ to $[x, t]$. Of course, as the scale of action (i.e. of the energy-by-time product) of the motion decreases and becomes comparable to $\hbar$, more and more paths produce substantial contribution to this sum, and hence to $W$, ensuring a larger and larger difference between the quantum and classical properties of the system.

Second, the path integral provides a justification for some simple explanations of quantum phenomena. A typical example is the quantum interference effects discussed in Sec. 3.1 - see, e.g., Fig. 3.1 and the corresponding text. At that discussion, we used the Huygens principle to argue that at the two-slit interference, the WKB approximation might be restricted of effects by two paths that pass through different slits, but otherwise consisting of straight-line segments. To have another look at that assumption, let us generalize the path integral to multi-dimensional geometries. Fortunately, the simple structure of Eq. (83b) makes such generalization virtually evident:

[^614]\[

$$
\begin{gather*}
G\left(\mathbf{r}, t ; \mathbf{r}_{0}, t_{0}\right)=\int \exp \left\{\frac{i}{\hbar} S[\mathbf{r}(\tau)]\right\} D[\mathbf{r}(\tau)] \\
S \equiv \int_{t_{0}}^{t} L\left(\mathbf{r}, \frac{d \mathbf{r}}{d \tau}\right) d \tau=\int_{t_{0}}^{t}\left[\frac{m}{2}\left(\frac{d \mathbf{r}}{d \tau}\right)^{2}-U(\mathbf{r})\right] d \tau \tag{5.87}
\end{gather*}
$$
\]

SD propagator via the path integral
where definition (83a) of the path integral should be also modified correspondingly. (I will not go into these technical details.) For the Young-type experiment (Fig. 3.1), where a classical particle could reach the detector only after passing through one of the slits, the classical paths are the straight-line segments shown in Fig. 3.1, and if they are much longer than the de Broglie wavelength, the propagator may be well approximated by the sum of two integrals of $L d \tau=i \mathbf{p}(\mathbf{r}) \cdot d \mathbf{r} / \hbar$ - as it was done in Sec. 3.1.

Last but not least, the path integral allows simple solutions of some problems that would be hard to get by other methods. As the simplest example, let us consider the problem of tunneling in multidimensional space, sketched in Fig. 4 for the 2D case - just for graphics' simplicity. Here, potential $U(x$, $y$ ) has the "saddle" shape. (Another helpful image is a mountain path between two summits, in Fig. 4 located on the top and at the bottom of the drawing.) A particle of energy $E$ may move classically in the left and right regions with $U(x, y)<E$, but can pass from one of these regions to another one only via the quantum-mechanical tunneling under the pass. Let us calculate the transparency of this tunnel barrier in the WKB approximation, ignoring the possible pre-exponential factor.


Fig. 5.4. Saddle-type 2D potential profile and the instanton trajectory of a particle of energy $E$ (dashed line, schematically).

According to the evident multi-dimensional generalization Eq. (86), for the classically forbidden region, where $E<U(x, y)$, the contributions to propagator (87) are proportional to

$$
\begin{equation*}
\exp \left\{-\int_{\mathrm{r}_{0}}^{\mathbf{r}} \boldsymbol{\kappa}(\mathbf{r}) \cdot d \mathbf{r}\right\} \exp \left\{-\frac{i}{\hbar} E\left(t-t_{0}\right)\right\}, \tag{5.88}
\end{equation*}
$$

where the magnitude of vector $\kappa$ at each point may be calculated just in the 1 D case - see, egg., Eq. (2.97),

$$
\begin{equation*}
\frac{\hbar^{2} \kappa^{2}(\mathbf{r})}{2 m}=U(\mathbf{r})-E, \tag{5.89}
\end{equation*}
$$

while its direction should be tangential to the path trajectory in space. Now the path integral is actually much simpler than in the classically-allowed region, because the spatial exponents are purely real and there is no complex interference between them. Because of the minus sign in the exponent, the largest
contribution to $G$ evidently comes from the trajectory (or rather a narrow bundle of trajectories) for which the functional

$$
\begin{equation*}
\int_{\mathbf{r}_{0}}^{\mathbf{r}} \boldsymbol{\kappa}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime} \tag{5.90}
\end{equation*}
$$

has the smallest value, and the barrier transmission coefficient may be calculated as

$$
\begin{equation*}
T \approx|G|^{2} \approx \exp \left\{-2 \int_{\mathbf{r}_{0}}^{\mathbf{r}} \boldsymbol{\kappa}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime}\right\} \tag{5.91}
\end{equation*}
$$

where $\mathbf{r}$ and $\mathbf{r}_{0}$ are certain points on the opposite classical turning-point surfaces: $U(\mathbf{r})=U\left(\mathbf{r}_{0}\right)=E .{ }^{26}$
Thus the tunneling problem is reduced to finding the trajectory (including points $\mathbf{r}$ and $\mathbf{r}_{0}$ ) that connects the two surfaces and minimizes functional (90). This is of course a well-known problem of the calculus of variations, ${ }^{27}$ but it is interesting that the path integral provides a simple alternative way of solving it. Let us consider an auxiliary problem of particle's motion in a potential profile $U_{\mathrm{inv}}(\mathbf{r})$ that is inverted relative to particle's energy $E$, i.e. is defined by the following equality:

$$
\begin{equation*}
U_{\mathrm{inv}}(\mathbf{r})-E \equiv E-U(\mathbf{r}) \tag{5.92}
\end{equation*}
$$

As was discussed above, at fixed energy $E$, the path integral for the WKB motion in the classically allowed region of potential $U_{\mathrm{inv}}(x, y)$ (that coincides with the classically forbidden region of the original problem) is dominated by the classical trajectory corresponding to the minimum of

$$
\begin{equation*}
\boldsymbol{S}_{\text {inv }}=\int_{\mathbf{r}_{0}}^{\mathbf{r}} \mathbf{p}_{\text {inv }}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}^{\prime}=\hbar \int_{\mathbf{r}_{0}}^{\mathbf{r}} \mathbf{k}_{\text {inv }}\left(\mathbf{r}^{\prime}\right) \cdot d \mathbf{r}, \tag{5.93}
\end{equation*}
$$

where $\mathbf{k}_{\text {inv }}$ should be determined from the relation

$$
\begin{equation*}
\frac{\hbar^{2} k_{\mathrm{inv}}^{2}(\mathbf{r})}{2 m} \equiv E-U_{\mathrm{inv}}(\mathbf{r}) \tag{5.94}
\end{equation*}
$$

But comparing Eqs. (89), (92), and (94), we see that $\mathbf{k}_{\text {inv }}=\boldsymbol{\kappa}$ at each point of space! This means that the tunneling path (in the WKB limit) corresponds to the classical (so-called instanton) ${ }^{28}$ trajectory of the same particle in the inverted potential $U_{\text {inv }}(\mathbf{r})$. If the initial point $\mathbf{r}_{0}$ is fixed, this trajectory may be readily found by the means of classical mechanics. (Note that the initial velocity of the instanton launched from point $\mathbf{r}_{0}$ should be zero, because by the classical turning point definition: $U_{\mathrm{inv}}\left(\mathbf{r}_{0}\right)=U\left(\mathbf{r}_{0}\right)$ $=E$.) Thus the problem is reduced to a simpler task of maximizing the transparency (91) over the position of $\mathbf{r}_{0}$ on the equipotential surface $U\left(\mathbf{r}_{0}\right)=E$. Moreover, for many symmetric potentials, the position of this point may be readily guessed without calculations.

[^615]Note that besides the calculation of barrier transparency, the instanton trajectory has one more important implication: the so-called traversal time $\tau_{t}$ of the classical motion along it, in the inverted potential, defined by Eq. (94), plays the role of the most important (though not the only one) time scale of particle's tunneling under the potential barrier. ${ }^{29}$

### 5.4. Revisiting harmonic oscillator

Let us return to the 1D harmonic oscillator, i.e. any system described by Hamiltonian (2.50) with potential energy (2.111):

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}+\frac{m \omega_{0}^{2} \hat{x}^{2}}{2} \tag{5.95}
\end{equation*}
$$

In Sec. 2.10 we have used the "brute-force" (wave-mechanics) approach to analyze the eigenfunctions $\psi_{n}(x)$ and eigenvalues $E_{n}$ of this Hamiltonian, and found that, unfortunately, that approach required relatively complex math that obscures the physics of these stationary ("Fock") states. Now let us use the bra-ket formalism to make the properties of these states much more transparent, using very simple calculations.

First, introducing normalized (dimensionless) operators of coordinates and momentum: ${ }^{30}$

$$
\begin{equation*}
\hat{\xi} \equiv \frac{\hat{x}}{x_{0}}, \quad \hat{\zeta} \equiv \frac{\hat{p}}{m \omega_{0} x_{0}}, \tag{5.96}
\end{equation*}
$$

where $x_{0} \equiv\left(\hbar / m \omega_{0}\right)^{1 / 2}$ is the natural coordinate scale ( $\sqrt{ } 2$ the r.m.s. spread of ground-state wavefunction) which was discussed in detail in Sec. 2.10, we can present Hamiltonian (95) in a very simple and $x \leftrightarrow p$ symmetric form:

$$
\begin{equation*}
\hat{H}=\frac{\hbar \omega_{0}}{2}\left(\hat{\xi}^{2}+\hat{\zeta}^{2}\right) . \tag{5.97}
\end{equation*}
$$

Now, let us introduce a new operator

$$
\begin{equation*}
\hat{a} \equiv \frac{1}{\sqrt{2}}(\hat{\xi}+i \hat{\zeta})=\left(\frac{m \omega_{0}}{2 \hbar}\right)^{1 / 2}\left(\hat{x}+i \frac{\hat{p}}{m \omega_{0}}\right) . \tag{5.98a}
\end{equation*}
$$

Since both operators $\hat{\xi}$ and $\hat{\zeta}$ correspond to real observables, i.e. have real eigenvalues and hence are Hermitian (self-adjoint), the Hermitian conjugate of operator $\hat{a}$ is simply its complex conjugate:

$$
\begin{equation*}
\hat{a}^{\dagger}=\frac{1}{\sqrt{2}}(\hat{\xi}-i \hat{\zeta})=\left(\frac{m \omega_{0}}{2 \hbar}\right)^{1 / 2}\left(\hat{x}-i \frac{\hat{p}}{m \omega_{0}}\right) \tag{5.98b}
\end{equation*}
$$

Solving the system of two equations (98) for $\hat{\xi}$ and $\hat{\zeta}$, we may readily get reciprocal relations

[^616]\[

$$
\begin{equation*}
\hat{\xi}=\frac{1}{\sqrt{2}}\left(\hat{a}+\hat{a}^{\dagger}\right), \quad \hat{\zeta}=\frac{1}{\sqrt{2} i}\left(\hat{a}-\hat{a}^{\dagger}\right) . \tag{5.99}
\end{equation*}
$$

\]

Our Hamiltonian (97) includes squares of these operators. Calculating them, we have to be careful to avoid swapping the new operators, because they do not commute. Indeed, for the normalized operators (96), Eq. (2.14) gives

$$
\begin{equation*}
[\hat{\xi}, \hat{\zeta}]=\frac{1}{x_{0}^{2} m \omega_{0}}[\hat{x}, \hat{p}]=i \hat{I}, \tag{5.100}
\end{equation*}
$$

Creationannihilation operators: commutation relation
so that Eqs. (98) yield

$$
\begin{equation*}
\left[\hat{a}, \hat{a}^{\dagger}\right]=\frac{1}{2}[(\hat{\xi}+i \hat{\zeta}),(\hat{\xi}-i \hat{\zeta})]=-\frac{i}{2}([\hat{\xi}, \hat{\zeta}]-[\hat{\zeta}, \hat{\xi})=\hat{I} . \tag{5.101}
\end{equation*}
$$

With such due caution, Eq. (99) gives

$$
\begin{equation*}
\hat{\xi}^{2}=\frac{1}{2}\left(\hat{a}^{2}+\hat{a}^{\dagger^{2}}+\hat{a} \hat{a}^{\dagger}+\hat{a}^{\dagger} \hat{a}\right), \quad \hat{\zeta}^{2}=-\frac{1}{2}\left(\hat{a}^{2}+\hat{a}^{\dagger^{2}}-\hat{a} \hat{a}^{\dagger}-\hat{a}^{\dagger} \hat{a}\right) . \tag{5.102}
\end{equation*}
$$

Plugging these expressions back into Eq. (97), we get

$$
\begin{equation*}
\hat{H}=\frac{\hbar \omega_{0}}{2}\left(\hat{a} \hat{a}^{\dagger}+\hat{a}^{\dagger} \hat{a}\right) \tag{5.103}
\end{equation*}
$$

This expression is elegant enough, but may be recast into an even more convenient form. For that, let us rewrite the commutation relation (100) as

$$
\begin{equation*}
\hat{a} \hat{a}^{\dagger}=\hat{a}^{\dagger} \hat{a}+\hat{I} \tag{5.104}
\end{equation*}
$$

and plug it into Eq. (103). The result is

$$
\begin{equation*}
\hat{H}=\frac{\hbar \omega_{0}}{2}\left(2 \hat{a}^{\dagger} \hat{a}+\hat{I}\right)=\hbar \omega_{0}\left(\hat{N}+\frac{1}{2} \hat{I}\right) \tag{5.105}
\end{equation*}
$$

where, in the last form, one more (evidently, Hermitian) operator,

$$
\begin{equation*}
\hat{N} \equiv \hat{a}^{\dagger} \hat{a} \tag{5.106}
\end{equation*}
$$

has been introduced. Since, according to Eq. (105), operators $\hat{H}$ and $\hat{N}$ differ only by the addition of an identity operator and the multiplication by a $c$-number, these operators commute. Hence, according to the general arguments of Sec. 4.5, they share the set of stationary (Fock) eigenstates $n$, and we can write the eigenproblem for the new operator as

$$
\begin{equation*}
\hat{N}|n\rangle=N_{n}|n\rangle \tag{5.107}
\end{equation*}
$$

where $N_{n}$ are some eigenvalues that, according to Eq. (105), determine also the energy spectrum of the oscillator:

$$
\begin{equation*}
E_{n}=\hbar \omega_{0}\left(N_{n}+\frac{1}{2}\right) \tag{5.108}
\end{equation*}
$$

So far, we know only that all eigenvalues $N_{n}$ are real, but not much more. In order to calculate them, let us carry out the following calculation - splendid in its simplicity and efficiency. Consider the result of action of operator $\hat{N}$ on the ket-vector $\hat{a}^{\dagger}|n\rangle$. Using the definition (106) and the associative rule, we may write

$$
\begin{equation*}
\hat{N}\left(\hat{a}^{\dagger}|n\rangle\right)=\left(\hat{a}^{\dagger} \hat{a}\right)\left(\hat{a}^{\dagger}|n\rangle\right)=\hat{a}^{\dagger}\left(\hat{a} \hat{a}^{\dagger}\right)|n\rangle . \tag{5.109}
\end{equation*}
$$

Now using the commutation relation (104), and then Eq. (107), we may continue as

$$
\begin{equation*}
\hat{a}^{\dagger}\left(\hat{a} \hat{a}^{\dagger}\right)|n\rangle=\hat{a}^{\dagger}\left(\hat{a}^{\dagger} \hat{a}+\hat{I}\right)|n\rangle=\hat{a}^{\dagger}(\hat{N}+\hat{I})|n\rangle=\hat{a}^{\dagger}\left(N_{n}+1\right)|n\rangle=\left(N_{n}+1\right)\left(\hat{a}^{\dagger}|n\rangle\right) . \tag{5.110}
\end{equation*}
$$

Let us summarize the result of this calculation:

$$
\begin{equation*}
\hat{N}\left(\hat{a}^{\dagger}|n\rangle\right)=\left(N_{n}+1\right)\left(\hat{a}^{\dagger}|n\rangle\right) . \tag{5.111}
\end{equation*}
$$

Performing an absolutely similar calculation with operator $\hat{a}$, we can also get another formula:

$$
\begin{equation*}
\hat{N}(\hat{a}|n\rangle)=\left(N_{n}-1\right)(\hat{a}|n\rangle) . \tag{5.112}
\end{equation*}
$$

It is time to stop calculations and translate these results into plain English: if $|n\rangle$ is an eigenket of operator $\hat{N}$ with eigenvalue $N_{n}$, then $\hat{a}^{\dagger}|n\rangle$ and $\hat{a}|n\rangle$ are also eigenkets of that operator, with eigenvalues $\left(N_{n}+1\right)$, and $\left(N_{n}-1\right)$, respectively. This statement may be presented with the ladder diagram shown in Fig. 5.


Fig. 5.5. Hierarchy (the "ladder diagram") of eigenstates of a 1D harmonic oscillator. Arrows show the actions of the creation and annihilation operators on the eigenstates.

Operator $\hat{a}^{\dagger}$ moves the system a step up the ladder, while operator $\hat{a}$ brings it one step down. In other words, the former operator creates a new excitation of the system, ${ }^{31}$ while the latter operator kills ("annihilates") such excitation. This is why $\hat{a}^{\dagger}$ is called the creation operator, and $\hat{a}$, the annihilation operator. In its turn, according to Eq. (107), operator $\hat{N}$ does not change the state of the system, but "counts" its position on the ladder:

$$
\begin{equation*}
\langle n| \hat{N}|n\rangle=\langle n| N_{n}|n\rangle=N_{n} . \tag{5.113}
\end{equation*}
$$

[^617]This is why $\hat{N}$ is called the number operator, in our current context meaning the number of the elementary excitations of the oscillator.

This calculation still needs a completion. Indeed, we still do not know whether the ladder shown in Fig. 5 shows all eigenstates of the oscillator, and what exactly the numbers $N_{n}$ are. Fascinating enough, both questions may be answered by exploring a single paradox. Let us start with some state (step of the ladder), and keep going down it, applying operator $\hat{a}$ again and again. Each time, eigenvalue $N_{n}$ is decreased by one, so that eventually it should become negative. However, this cannot happen, because any real eigenstate, including the states presented by kets $|d\rangle \equiv \hat{a}|n\rangle$ and $|n\rangle$, should have a positive norm - see Eq. (4.16). Comparing the norms,

$$
\begin{equation*}
\|n\|^{2}=\langle n \mid n\rangle, \quad\|d\|^{2}=\langle n| \hat{a}^{\dagger} a|n\rangle=\langle n| \hat{N}|n\rangle=N_{n}\langle n \mid n\rangle, \tag{5.114}
\end{equation*}
$$

we see that the both of them cannot be positive simultaneously if $N_{n}$ is negative.
The way toward the resolution of this paradox is to notice that the action of the creation and annihilation operators on the stationary states may consist in not only their promotion to the next step of the ladder diagram, but also by their multiplication by some $c$-numbers:

$$
\begin{equation*}
\hat{a}|n\rangle=A_{n}|n-1\rangle, \quad \hat{a}^{\dagger}|n\rangle=A_{n}^{\prime}|n+1\rangle . \tag{5.115}
\end{equation*}
$$

(Linear relations (111) and (112) clearly allow that.) Let us calculate coefficients $A_{n}$ assuming, for convenience, that all eigenstates, including states $n$ and ( $n-1$ ), are normalized:

$$
\begin{equation*}
\langle n \mid n\rangle=1, \quad\langle n-1 \mid n-1\rangle=\langle n| \frac{\hat{a}^{\dagger}}{A_{n}^{*}} \frac{\hat{a}}{A_{n}}|n\rangle=\frac{1}{A_{n}^{*} A_{n}}\langle n| \hat{N}|n\rangle=\frac{N_{n}}{A_{n}^{*} A_{n}}\langle n \mid n\rangle=1 . \tag{5.116}
\end{equation*}
$$

From here, we get $\left|A_{n}\right|=\left(N_{n}\right)^{1 / 2}$, i.e.

$$
\begin{equation*}
\hat{a}|n\rangle=N_{n}^{1 / 2} e^{i \varphi_{n}}|n-1\rangle, \tag{5.117}
\end{equation*}
$$

where $\varphi_{n}$ is an arbitrary real phase. Now let us consider what happens if all numbers $N_{n}$ are integers. (Because of the definition of $N_{n}$, given by Eq. (107), it is convenient to call these integers $n$, i.e. by the same letter as the corresponding eigenstate.) Then when we have come down to state with $n=0$, an attempt to make one more step down gives

$$
\begin{equation*}
\hat{a}|0\rangle=0|-1\rangle . \tag{5.118}
\end{equation*}
$$

But in accordance with Eq. (4.9), the state in the right-hand part of this equation is the "null-state", i.e. does not exist. ${ }^{32}$ This gives the (only known :-) resolution of the state ladder paradox: the ladder has the lowest step with $N_{n}=n=0$.

As a by-product of our discussion, we have obtained a very important relation $N_{n}=n$, which means, in particular, that the state ladder includes all eigenstates of the oscillator. Plugging this relation into Eq. (108), we see that the full spectrum of eigenenergies of the harmonic oscillator is described by the simple formula

[^618]\[

$$
\begin{equation*}
E_{n}=\hbar \omega_{0}\left(n+\frac{1}{2}\right), \quad n=0,1,2 \ldots \tag{5.119}
\end{equation*}
$$

\]

which was already discussed in Sec. 2.10. It is rather remarkable that the bra-ket formalism has allowed us to derive it without calculation of the corresponding (rather cumbersome) wavefunctions $\psi_{n}(x)$ - see Eqs. (2.279).

Moreover, the formalism may be also used to calculate virtually any bra-ket pertaining to the oscillator, without using $\psi_{n}(x)$. In order to illustrate that, let us first calculate $A_{n}{ }_{n}$ participating in the latter of relations (115). This can be done absolutely similarly to the above calculation of $A_{n}$; otherwise, since we already know that $\left|A_{n}\right|=\left(N_{n}\right)^{1 / 2}=n^{1 / 2}$, we may notice that according to Eqs. (106) and (115), the eigenproblem (107), that in our new notation for $N_{n}$ becomes

$$
\begin{equation*}
\hat{N}|n\rangle=n|n\rangle \tag{5.120}
\end{equation*}
$$

may be rewritten as

$$
\begin{equation*}
n|n\rangle=\hat{a}^{\dagger} \hat{a}|n\rangle=\hat{a}^{\dagger} A_{n}|n-1\rangle=A_{n} A_{n-1}^{\prime}|n\rangle . \tag{5.121}
\end{equation*}
$$

Comparing the first and the last form of this equality, we see that $\left|A_{n-1}^{\prime}\right|=n /\left|A_{n}\right|=n^{1 / 2}$, i.e. $A^{\prime}{ }_{n}=(n+$ $1)^{1 / 2} \exp \left(i \varphi_{n}{ }^{\prime}\right)$. Taking all phases $\varphi_{n}$ and $\varphi_{n}{ }^{\prime}$ equal to zero for simplicity, we may reduce Eqs. (115) to their final, standard form ${ }^{33}$

$$
\begin{equation*}
\hat{a}^{\dagger}|n\rangle=(n+1)^{1 / 2}|n+1\rangle, \quad \hat{a}|n\rangle=n^{1 / 2}|n-1\rangle . \tag{5.122}
\end{equation*}
$$

Now we can use these formulas to calculate, for example, the matrix elements of operator $\hat{x}$ in the Fock state basis:

$$
\begin{equation*}
\left\langle n^{\prime}\right| \hat{x}|n\rangle=x_{0}\left\langle n^{\prime}\right| \hat{\xi}|n\rangle=\frac{x_{0}}{\sqrt{2}}\left\langle n^{\prime}\right|\left(\hat{a}+\hat{a}^{\dagger}\right)|n\rangle=\frac{x_{0}}{\sqrt{2}}\left(\left\langle n^{\prime}\right| \hat{a}|n\rangle+\left\langle n^{\prime}\right| \hat{a}^{\dagger}|n\rangle\right) . \tag{5.123}
\end{equation*}
$$

To complete the calculation, we may now use Eqs. (122) and the Fock state orthonormality:

$$
\begin{equation*}
\left\langle n^{\prime} \mid n\right\rangle=\delta_{n^{\prime} n} . \tag{5.124}
\end{equation*}
$$

The result is

$$
\begin{equation*}
\left\langle n^{\prime}\right| \hat{x}|n\rangle=\frac{x_{0}}{\sqrt{2}}\left(n^{1 / 2} \delta_{n^{\prime}, n-1}+(n+1)^{1 / 2} \delta_{n^{\prime}, n+1}\right)=\left(\frac{\hbar}{2 m \omega_{0}}\right)^{1 / 2}\left(n^{1 / 2} \delta_{n^{\prime}, n-1}+(n+1)^{1 / 2} \delta_{n^{\prime}, n+1}\right) \tag{5.125}
\end{equation*}
$$

Acting absolutely similarly, for the momentum bra-kets we get a similar expression:

$$
\begin{equation*}
\left\langle n^{\prime}\right| \hat{p}|n\rangle=i\left(\frac{\hbar m \omega_{0}}{2}\right)^{1 / 2}\left(-n^{1 / 2} \delta_{n^{\prime}, n-1}+(n+1)^{1 / 2} \delta_{n^{\prime}, n+1}\right) \tag{5.126}
\end{equation*}
$$

Hence the matrices of both operators in the Fock-state basis have only two diagonals, adjacent to the main diagonal; all other elements (including the diagonal ones) are zeros.

[^619]Matrix elements of higher powers of these operators, as well as their products, may be handled similarly, though the higher is the power, the bulkier is the result. For example, ${ }^{34}$

$$
\begin{align*}
\left\langle n^{\prime}\right| \hat{x}^{2}|n\rangle & =\left\langle n^{\prime}\right| \hat{x} \hat{x}|n\rangle=\sum_{n^{\prime \prime}=0}^{\infty}\left\langle n^{\prime}\right| \hat{x}\left|n^{\prime \prime}\right\rangle\left\langle n^{\prime \prime}\right| \hat{x}|n\rangle \\
& =\frac{x_{0}^{2}}{2} \sum_{n^{\prime \prime}=0}^{\infty}\left(\left(n^{\prime \prime}\right)^{1 / 2} \delta_{n^{\prime}, n^{\prime \prime}-1}+\left(n^{\prime \prime}+1\right)^{1 / 2} \delta_{n^{\prime}, n^{\prime \prime}+1}\right)\left(n^{1 / 2} \delta_{n^{\prime \prime}, n-1}+(n+1)^{1 / 2} \delta_{n^{\prime \prime}, n+1}\right)  \tag{5.127}\\
& =\frac{x_{0}^{2}}{2}\left\{[n(n-1)]^{1 / 2} \delta_{n^{\prime}, n-2}+[(n+1)(n+2)]^{1 / 2} \delta_{n^{\prime}, n+2}+(2 n+1) \delta_{n^{\prime}, n}\right\} .
\end{align*}
$$

For applications, the most important of these matrix elements are those on its main diagonal:

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=\langle n| \hat{x}^{2}|n\rangle=\frac{x_{0}^{2}}{2}(2 n+1) \tag{5.128}
\end{equation*}
$$

This expression shows, in particular, that the expectation value of oscillator's potential energy in $n$-th Fock state is

$$
\begin{equation*}
\langle U\rangle=\frac{m \omega_{0}^{2}}{2}\left\langle x^{2}\right\rangle=\frac{\hbar \omega_{0}}{2}\left(n+\frac{1}{2}\right) . \tag{5.129}
\end{equation*}
$$

This is exactly $1 / 2$ of the total energy (119) of the oscillator. As a sanity check, an absolutely similar calculation of the kinetic energy shows that

$$
\begin{equation*}
\left\langle\frac{p^{2}}{2 m}\right\rangle=\frac{1}{2 m}\langle n| \hat{p}^{2}|n\rangle=\frac{\hbar \omega_{0}}{2}\left(n+\frac{1}{2}\right), \tag{5.130}
\end{equation*}
$$

i.e. both partial energies equal $E_{n} / 2$, just as in a classical oscillator. ${ }^{35}$

### 5.5. The Glauber and squeezed states

There is evidently a huge difference between a quantum stationary (Fock) state of the oscillator and its classical state. Indeed, let us write the classical Hamilton equations of motion of the oscillator (using capital letters to distinguish the classical variables from arguments of quantum wavefunctions):

$$
\begin{equation*}
\dot{X}=\frac{P}{m}, \quad \dot{P}=-\frac{\partial U}{\partial x}=-m \omega_{0}^{2} X \tag{5.131}
\end{equation*}
$$

On the "phase plane" with Cartesian coordinates $x$ and $p$ (Fig. 6), these equations describe clockwise rotation of the representation point $\{X(t), P(t)\}$ along an elliptic trajectory starting from the initial point $\{X(0), P(0)\}$. (The normalization of momentum by $m \omega_{0}$, similar to the one performed by the second of Eqs. (96), makes the trajectory pleasingly circular, with a constant radius equal to oscillation's amplitude $A$, reflecting the constant full energy

[^620]\[

$$
\begin{equation*}
E_{c}=\frac{m \omega_{0}^{2}}{2} A^{2}, \quad A^{2}=[X(t)]^{2}+\left[\frac{P(t)}{m \omega_{0}}\right]^{2}=\mathrm{const}=[X(0)]^{2}+\left[\frac{P(0)}{m \omega_{0}}\right]^{2}, \tag{5.132}
\end{equation*}
$$

\]

determined by the initial conditions.)
For the forthcoming comparison with quantum states, it is convenient to describe this classical solution by the following dimensionless complex variable

$$
\begin{equation*}
\alpha(t) \equiv \frac{1}{\sqrt{2} x_{0}}\left(X(t)+i \frac{P(t)}{m \omega_{0}}\right), \tag{5.133}
\end{equation*}
$$

which is essentially the standard complex-number representation of system's position on the 2D phase plane, with $|\alpha| \equiv A / \sqrt{ } 2 x_{0}$. With this definition, Eqs. (131) are conveniently merged into one equation,

$$
\begin{equation*}
\dot{\alpha}=-i \omega_{0} \alpha, \tag{5.134}
\end{equation*}
$$

with an evident, very simple solution

$$
\begin{equation*}
\alpha(t)=\alpha(0) e^{-i \omega_{0} t} \tag{5.135}
\end{equation*}
$$

where the constant $\alpha(0)$ may be complex, and is just the (normalized) classical complex amplitude of oscillations. ${ }^{36}$ This equation describes sinusoidal oscillations of both $X(t) \propto \operatorname{Re}[\alpha(t)]$ and $P \propto \operatorname{Im}[\alpha(t)]$, with a phase shift of $\pi / 2$ between them.


Fig. 5.6. Schematic representation of various states of a harmonic oscillator on the phase plane. The bold black point represents a classical state, with the dashed line showing its trajectory. (Very imperfect) classical images of the Fock states with $n=0,1$, and 2 are shown in blue, while the blurred red spot is the (equally schematic) Glauber state's image. Finally, the magenta elliptical spot is a classical image of a squeezed ground state. Arrows show the direction of states' evolution in time.

On the other hand, according to the basic Eqs. (4.157)-(4.158), the time dependence of a Fock state, as of a stationary state of the oscillator, is limited to the phase factor $\exp \left\{-i E_{n} t / \hbar\right\}$ not in observables, but rather in the wavefunction, and a result, gives time-independent expectation values of $x$, $p$, or of any function thereof. (Moreover, as Eqs. (125) and (126) show, $\langle x\rangle=\langle p\rangle=0$.) Taking into

[^621]account Eqs. (129) and (130), the closest (though very imperfect) geometric image ${ }^{37}$ for such a state on the phase plane is a blurred circle of radius $A_{n}=x_{0}(2 n+1)^{1 / 2}$, along which the wavefunction is uniformly spread as a wave - see the blue rings in Fig. 6. For the ground state $(n=0)$, with wavefunction (2.269), a better image is a blurred round spot, of radius $\sim x_{0}$, at the origin.

However, the Fock states $n$ are not the only possible quantum states of the oscillator: according to the basic Eq. (4.6), a state described by ket-vector

$$
\begin{equation*}
|\alpha\rangle=\sum_{n=0}^{\infty} \alpha_{n}|n\rangle \tag{5.136}
\end{equation*}
$$

with any set of (complex) $c$-numbers $\alpha_{n}$, is also its legitimate state, subject only to the normalization condition $\langle\alpha \mid \alpha\rangle=1$, giving

$$
\begin{equation*}
\sum_{n=0}^{\infty}\left|\alpha_{n}\right|^{2}=1 \tag{5.137}
\end{equation*}
$$

It is natural to ask: can we select coefficients $\alpha_{n}$ in such a special way that the state properties would be closer to the classical ones; in particular the expectation values $\langle x\rangle$ and $\langle p\rangle$ of coordinate and momentum would evolve in time just as the classical values $X(t)$ and $P(t)$, while the uncertainties of these observables would be time-independent and the same as in the ground state:

$$
\begin{equation*}
\delta x=\frac{x_{0}}{\sqrt{2}}=\left(\frac{\hbar}{2 m \omega_{0}}\right)^{1 / 2}, \quad \delta p=\frac{m \omega_{0} x_{0}}{\sqrt{2}}=\left(\frac{\hbar m \omega_{0}}{2}\right)^{1 / 2} \tag{5.138}
\end{equation*}
$$

with the smallest possible value of the uncertainty product, $\delta x \delta p=\hbar / 2 .{ }^{38}$ Let me show that such a Glauber state, ${ }^{39}$ which is schematically represented in Fig. 6 by a blurred red spot around the classical point $\{X(t), P(t)\}$, is indeed possible.

Conceptually the simplest way to find the corresponding coefficients $\alpha_{n}$ would be to calculate $\langle x\rangle,\langle p\rangle, \delta x$ and $\delta p$ for an arbitrary set of $\alpha_{n}$, and then try to optimize these coefficients to reach our goal. However, this problem may be solved much easier using wave mechanics. Indeed, let us consider the following wavefunction

$$
\begin{equation*}
\Psi_{\alpha}(x, t)=C_{0} \exp \left\{-\frac{m \omega_{0}}{2 \hbar}[x-X(t)]^{2}+i \frac{P(t) x}{\hbar}\right\} \tag{5.139}
\end{equation*}
$$

Its comparison with Eqs. (2.16) and (2.269) shows that this is just a Gaussian wave packet with the average momentum $P$ and the coordinate width $\delta x$ given by Eq. (138), but shifted along axis $x$ by $X$.

[^622]Hence, this wavefunction satisfies all the above requirements, and a straightforward (though a bit bulky) differentiation over $x$ and $t$ shows it also satisfies oscillator's Schrödinger equation, provided that that functions $X(t)$ and $P(t)$ satisfy classical Eqs. (131).

This fact is true even for a more general situation when the oscillator, initially in its ground state ${ }^{40}$ comes under effect of a classical force $F(t)$. (Evidently, for its description its is sufficient to add this function to the right-hand part of the second of Eqs. (131).) Moreover, the electromagnetic radiation formed in "good" (single-mode) lasers is also in the Glauber state. (As will be discussed in Chapter 9, the experimental formation of Fock states $n$, with the only exception of $n=0$, i.e. the ground state, is much harder.) This is why the Glauber states are so important.

Though Eq. (139) gives the full wave-mechanics description of a Glauber state, there is a substantial place for the bra-ket formalism here too. For example, in order to calculate the corresponding coefficients in expansion (136),

$$
\begin{equation*}
\alpha_{n}=\langle n \mid \alpha\rangle=\int d x\langle n \mid x\rangle\langle x \mid \alpha\rangle=\int \psi_{n}^{*}(x) \psi_{\alpha}(x) d x \tag{5.140}
\end{equation*}
$$

we would need to use not only the simple Eq. (139), but also the Fock state wavefunctions $\psi_{n}(x)$, which are not very appealing - see Eq. (2.279). Instead, this calculation may be readily done in the bra-ket formalism, giving us one important byproduct result.

Let us start from expressing the double shift of the ground state (by $X$ and $P$ ), that has led us to Eq. (139), in the operator language. Forgetting about the $P$ for a minute, let us find a translation operator $\hat{\tau}_{X}$ that produces the desirable shift of coordinate by $X$ of an arbitrary wavefunction $\psi(x)$ - say represented as the standard wave packet (59). Evidently, the result of its action, in the coordinate representation, is

$$
\begin{equation*}
\hat{\tau}_{X} \psi(x)=\psi(x-X)=\frac{1}{(2 \pi \hbar)^{1 / 2}} \int \varphi(p) \exp \left\{i \frac{p(x-X)}{\hbar}\right\} d p \tag{5.141}
\end{equation*}
$$

Hence, the shift may be achieved by the multiplication of each Fourier component of the packet, with momentum $p$, by $\exp \{-i p X / \hbar\}$. This gives us a hint that the general form of the translation operator, valid in any representation, should be

$$
\begin{equation*}
\hat{\tau}_{X}=\exp \left\{-i \frac{\hat{p} X}{\hbar}\right\} \tag{5.142}
\end{equation*}
$$

The proof of this formula is provided by the fact that any operator is uniquely determined by the set of its matrix elements in any full and orthogonal basis, in particular the basis of momentum states $p$. According to Eq. (141), the analog of Eq. (23) for the $p$-representation, applied to the translation operator (which is evidently local), is

$$
\begin{equation*}
\langle p| \hat{\boldsymbol{T}}_{X}\left|p^{\prime}\right\rangle \varphi\left(p^{\prime}\right)=\delta\left(p-p^{\prime}\right) \exp \left\{-i \frac{p X}{\hbar}\right\} \varphi(p) \tag{5.143}
\end{equation*}
$$

so that operator (142) does exactly the job we need it to.

[^623]The operator that provides the shift of momentum by $P$ is absolutely similar - with the opposite sign under the exponent, due to the opposite sign of the exponent in the reciprocal Fourier transform, so that the simultaneous shift by both $X$ and $P$ may be achieved by the following translation operator:
$\alpha$-translation operator

$$
\begin{equation*}
\hat{\tau}_{\alpha}=\exp \left\{i \frac{P \hat{x}-\hat{p} X}{\hbar}\right\} \tag{5.144}
\end{equation*}
$$

As we already know, for a harmonic oscillator the creation-annihilation operators are more natural, so that we may use Eqs. (96) and (99) to recast Eq. (144) as

$$
\begin{equation*}
\hat{\tau}_{\alpha}=\exp \left\{\alpha \hat{a}^{\dagger}-\alpha^{*} \hat{a}\right\}, \text { with } \hat{\tau}_{\alpha}^{\dagger}=\exp \left\{\alpha^{*} \hat{a}-\alpha \hat{a}^{\dagger}\right\} \tag{5.145}
\end{equation*}
$$

where the $c$-number $\alpha$ (generally, a function of time) is defined by Eq. (133). Now, according to Eq.

Glauber state as ground state's translation (139), we may form the Glauber state's ket-vector just as

$$
\begin{equation*}
|\alpha\rangle=\hat{\tau}_{\alpha}|0\rangle \tag{5.146}
\end{equation*}
$$

This formula looks nice and simple, but making practical calculations (say, calculating expectation values of variables) with the translation operator (144) is not too easy because of its exponent-of-operators form. Fortunately, it turns out that a much simpler representation for the Glauber state is possible. To show than, let us start with the following general (and very useful) property of exponential functions of operators: if

$$
\begin{equation*}
[\hat{A}, \hat{B}]=\mu \hat{I} \tag{5.147}
\end{equation*}
$$

(where $\hat{A}$ and $\hat{B}$ are arbitrary operators, and $\mu$ is a $c$-number), then ${ }^{41}$

$$
\begin{equation*}
\exp \{+\hat{A}\} \hat{B} \exp \{-\hat{A}\}=\hat{B}+\mu \hat{I} \tag{5.148}
\end{equation*}
$$

Let us apply Eqs. (147)-(148) to two cases, both with

$$
\begin{equation*}
\hat{A}=\alpha^{*} \hat{a}-\alpha \hat{a}^{\dagger}, \quad \text { so that } \exp \{+\hat{A}\}=\hat{\tau}_{\alpha}^{\dagger}, \quad \exp \{-\hat{A}\}=\hat{\tau}_{\alpha} . \tag{5.149}
\end{equation*}
$$

First, let us take $\hat{B}=\hat{I}$, then Eq. (147) is valid with $\mu=0$, and Eq. (148) yields

$$
\begin{equation*}
\hat{\tau}_{\alpha}^{\dagger} \hat{\tau}_{\alpha}=\hat{I} \tag{5.150}
\end{equation*}
$$

This equality means that the translation operator is unitary - not a big surprise, because if we shift a classical point on the complex phase plane by $(+\alpha)$ and then by $(-\alpha)$, we certainly must come back to the initial position. Relation (150) means merely that this fact is also true for any quantum state as well.

Second, let us take $\hat{B}=\hat{a}$; in order to verify Eq. (147) and find the corresponding $\mu$, let us calculate the commutator. Using, at the due stage of calculation, Eq. (104), we get

$$
\begin{equation*}
[\hat{A}, \hat{B}]=\left[\alpha^{*} \hat{a}-\alpha \hat{a}^{\dagger}, \hat{a}\right]=-\alpha\left[\hat{a}^{\dagger}, \hat{a}\right]=\alpha \hat{I} \tag{5.151}
\end{equation*}
$$

[^624]so that in this case $\mu=\alpha$, and Eq. (148) yields
\[

$$
\begin{equation*}
\hat{\tau}_{\alpha}^{\dagger} \hat{a} \hat{\gamma}_{\alpha}=\hat{a}+\alpha \hat{I} \tag{5.152}
\end{equation*}
$$

\]

We have approached the summit of this beautiful calculation. Let us consider operator

$$
\begin{equation*}
\hat{\tau}_{\alpha} \hat{\sigma}_{\alpha}^{\dagger} \hat{a} \hat{\tau}_{\alpha} . \tag{5.153}
\end{equation*}
$$

Using Eq. (150), we may reduce this expression to $\hat{a} \hat{\gamma}_{\alpha}$, while the application of Eq. (151) to the same expression yields $\hat{\gamma}_{\alpha} \hat{a}+\alpha \hat{\gamma}_{\alpha}$. Hence, we get the following operator equality

$$
\begin{equation*}
\hat{a} \hat{\tau}_{\alpha}=\hat{\tau}_{\alpha} \hat{a}+\alpha \hat{\tau}_{\alpha}, \tag{5.154}
\end{equation*}
$$

which may be applied to any state. Now acting by these two operators on the ground state $|0\rangle$ and using the facts that $\hat{a}|0\rangle$ is the null-state, while $\hat{T}_{\alpha}|0\rangle \equiv|\alpha\rangle$, we finally get a very simple and elegant result: ${ }^{42}$

$$
\begin{equation*}
\hat{a}|\alpha\rangle=\alpha|\alpha\rangle \tag{5.155}
\end{equation*}
$$

Thus any Glauber state is just one of eigenstates of the annihilation operator, namely the one with the eigenvalue equal to parameter $\alpha$, i.e. to the complex representation (133) of the classical state which is the center of the Glauber state's distribution. ${ }^{43}$ This fact makes the calculations of the Glauber state properties much simpler. As the simplest example, let us use Eq. (155) to find $\langle x\rangle$ in the Glauber state:

$$
\begin{equation*}
\langle x\rangle=\langle\alpha| \hat{x}|\alpha\rangle=\frac{x_{0}}{\sqrt{2}}\langle\alpha|\left(\hat{a}+\hat{a}^{\dagger}\right)|\alpha\rangle=\frac{x_{0}}{\sqrt{2}}\left(\langle\alpha| \hat{a}|\alpha\rangle+\langle\alpha| \hat{a}^{\dagger}|\alpha\rangle\right) . \tag{5.156}
\end{equation*}
$$

In the first term in the parentheses, we can apply Eq. (155) directly, while in the second term, we can use the bra-counterpart of that relation, $\langle\alpha| \hat{a}^{\dagger}=\langle\alpha| \alpha^{*}$. Now assuming that the Glauber state is normalized, $\langle\alpha \mid \alpha\rangle=1$, and using Eq. (133), we get

$$
\begin{equation*}
\langle x\rangle=\frac{x_{0}}{\sqrt{2}}\left(\langle\alpha| \alpha|\alpha\rangle+\langle\alpha| \alpha^{*}|\alpha\rangle\right)=\frac{x_{0}}{\sqrt{2}}\left(\alpha+\alpha^{*}\right)=X, \tag{5.157}
\end{equation*}
$$

Acting absolutely similarly, we may readily extend this sanity check to verify that $\langle p\rangle=P$, and that $\delta x$ and $\delta p$ indeed obey Eq. (138).

As a more thorough sanity check, let us use Eq. (155) to re-calculate Glauber state's wavefunction (139). Inner-multiplying both sides of that relation by bra-vector $\langle x|$, and using definition (98a) of the annihilation operator, we get

[^625]\[

$$
\begin{equation*}
\frac{1}{\sqrt{2} x_{0}}\left\langle\left. x\left(\hat{x}+i \frac{\hat{p}}{m \omega_{0}}\right) \right\rvert\, \alpha\right\rangle=\alpha\langle x \mid \alpha\rangle . \tag{5.158}
\end{equation*}
$$

\]

Since $\langle x|$ is the bra-vector of the eigenstate of the Hermitian operator $\hat{x}$, they may be swapped, with the operator giving its eigenvalue $x$; acting on that bra-vector by the (local!) operator of momentum, we have to use it in the coordinate representation (63). As a result, we get

$$
\begin{equation*}
\frac{1}{\sqrt{2} x_{0}}\left(x\langle x \mid \alpha\rangle+\frac{\hbar}{m \omega_{0}} \frac{\partial}{\partial x}\langle x \mid \alpha\rangle\right)=\alpha\langle x \mid \alpha\rangle . \tag{5.159}
\end{equation*}
$$

But $\langle x \mid \alpha\rangle$ is nothing else than the Glauber state's wavefunction $\Psi_{\alpha}$, so that Eq. (153) gives for it a firstorder differential equation

$$
\begin{equation*}
\frac{1}{\sqrt{2} x_{0}}\left(x \Psi_{\alpha}+\frac{\hbar}{m \omega_{0}} \frac{\partial}{\partial x} \Psi_{\alpha}\right)=\alpha \Psi_{\alpha} \tag{5.160}
\end{equation*}
$$

Chasing $\Psi_{\alpha}$ and $x$ to the opposite sides of the equation, and using definition (133) of parameter $\alpha$, we may bring this equation to a form

$$
\begin{equation*}
\frac{\partial \Psi_{\alpha}}{\Psi_{\alpha}}=\frac{m \omega_{0}}{\hbar}\left[-x+\left(X+i \frac{P}{m \omega_{0}}\right)\right] \partial x . \tag{5.161}
\end{equation*}
$$

Integrating both parts, we return to Eq. (139) that had been derived by wave-mechanics means.
Now that we can use Eq. (155) for finding coefficients $\alpha_{n}$ in the expansion (136) of the Glauber state $\alpha$ in series over the Fock states $n$. Plugging Eq. (136) into each side of Eq. (155), using the first of Eq. (122) in the left-hand part, and requiring the coefficients at each ket-vector $|n\rangle$ in both parts to be equal, we get the following recurrence relation for the coefficients:

$$
\begin{equation*}
\alpha_{n+1}=\frac{\alpha}{(n+1)^{1 / 2}} \alpha_{n} \tag{5.162}
\end{equation*}
$$

Assuming some value of $\alpha_{0}$, and applying the relation sequentially for $n=1,2$, etc., we get

$$
\begin{equation*}
\alpha_{n}=\frac{\alpha^{n}}{(n!)^{1 / 2}} \alpha_{0} \tag{5.163}
\end{equation*}
$$

Now we can find $\alpha_{0}$ from the normalization requirement (137), getting

$$
\begin{equation*}
\left|\alpha_{0}\right|^{2} \sum_{n=0}^{\infty} \frac{|\alpha|^{2 n}}{n!}=1 \tag{5.164}
\end{equation*}
$$

In this sum, we may readily recognize the Taylor expansion of function $\exp \left\{|\alpha|^{2}\right\}$, so that the final result (besides an arbitrary common phase multiplier) is

Glauber
state as Fock states' superposition

$$
\begin{equation*}
|\alpha\rangle=\exp \left\{-\frac{|\alpha|^{2}}{2}\right\} \sum_{n=0}^{\infty} \frac{\alpha^{n}}{(n!)^{1 / 2}}|n\rangle . \tag{5.165}
\end{equation*}
$$

It means in particular that the probability $W_{n} \equiv \alpha_{n} \alpha_{n}{ }^{*}$ of finding the system energy on $n$-th energy level (119) obeys the well-known Poisson distribution (Fig. 7):


Fig. 5.7. The Poisson distribution for several values of $\langle n\rangle$. Note that $W_{n}$ are defined only for integer values of $n$; lines are only guides for the eye.

$$
\begin{equation*}
W_{n}=\frac{\langle n\rangle^{n}}{n!} e^{-\langle n\rangle} \tag{5.166}
\end{equation*}
$$

Poisson distribution
where in our particular case

$$
\begin{equation*}
\langle n\rangle=|\alpha|^{2} \tag{5.167}
\end{equation*}
$$

For applications, perhaps the most important mathematical property of this distribution is

$$
\begin{equation*}
\delta n=\langle n\rangle^{1 / 2} \tag{5.168}
\end{equation*}
$$

note also that at $\langle n\rangle \gg 1$, and hence $\delta n \ll\langle n\rangle$, the Poisson distribution approaches the Gaussian ("normal") one.

Now let us discuss the evolution of the Glauber state in time. In the Schrödinger language, it is completely described by dynamics (131) of the $c$-number shifts $X(t)$ and $P(t)$ participating in wavefunction (139). Note again that, in contrast to the spread of the wave packet of a free particle, discussed in Sec. 2.2, in the harmonic oscillator the Gaussian packet of special width (138) does not spread at all!

An alternative and equivalent way of dynamics description is to use the Heisenberg equation of motion. As Eqs. (42) and (48) tell us, such equations for Heisenberg operators of coordinate and momentum they have to be similar to the classical equation (131):

$$
\begin{equation*}
\dot{\hat{x}}_{\mathrm{H}}=\frac{\hat{p}_{\mathrm{H}}}{m}, \quad \dot{\hat{p}}_{\mathrm{H}}=-m \omega_{0}^{2} \hat{x}_{\mathrm{H}} . \tag{5.169}
\end{equation*}
$$

Now using Eqs. (98), for the Heisenberg-picture creation and annihilation operators we get equations

$$
\begin{equation*}
\dot{\hat{a}}_{\mathrm{H}}=-i \omega_{0} \hat{a}_{\mathrm{H}}, \quad \dot{\hat{a}}_{\mathrm{H}}^{\dagger}=+i \omega_{0} \hat{a}_{\mathrm{H}}^{\dagger}, \tag{5.170}
\end{equation*}
$$

that are completely similar for the classical equation (134) for the $c$-number parameter $\alpha$ and its complex conjugate, and hence have the solutions identical to Eq. (135):

$$
\begin{equation*}
\hat{a}_{\mathrm{H}}(t)=\hat{a}_{\mathrm{H}}(0) e^{-i \omega_{0} t}, \quad \hat{a}_{\mathrm{H}}^{\dagger}(t)=\hat{a}_{\mathrm{H}}^{\dagger}(0) e^{i \omega_{0} t} . \tag{5.171}
\end{equation*}
$$

As was discussed in Sec. 4.6, such equations are very convenient because they enable simple calculation of time evolution of observables for any initial state of the oscillator (Fock, Glauber, or any other) using Eq. (4.191). Applied to a Glauber state $\alpha(0)$, such calculation gives the same results as have already been derived earlier in this section, in particular confirms that the Gaussian wave packet of the special width (138) does not spread in time.

Now let us consider what happens if the initial wave packet is still Gaussian, but has a different width, say $\delta x<x_{0} / \sqrt{ } 2$. As we already know from Sec. 2.2, the momentum spread $\delta p$ will be correspondingly larger, still with the smallest uncertainty product: $\delta x \delta p=\hbar / 2$. Such squeezed ground state $\Sigma$, with zero expectation values of $x$ and $p$, may be generated from the Fock/Glauber ground state:

Squeezed ground state

$$
\begin{equation*}
|\nu\rangle=\hat{S}_{1}|0\rangle, \tag{5.172a}
\end{equation*}
$$

using the so-called squeezing operator,

Squeezing operator

$$
\begin{equation*}
\hat{S}_{\imath}=\exp \left\{\frac{1}{2}\left(s^{*} \hat{a} \hat{a}-s \hat{a}^{\dagger} \hat{a}^{\dagger}\right)\right\} \tag{5.172b}
\end{equation*}
$$

which depends on a complex $c$-number parameter $ュ=r e^{i \theta}$. Parameter's modulus $r$ determines the squeezing degree; it is straightforward to use Eq. (172) for checking that if $\lrcorner$ is real $(\theta=0, \xi=r)$, then

$$
\begin{equation*}
\delta x=\frac{x_{0}}{\sqrt{2}} e^{-r}=\left(\frac{\hbar}{2 m \omega_{0}}\right)^{1 / 2} e^{-r}, \quad \delta p=\frac{m \omega_{0} x_{0}}{\sqrt{2}} e^{r}=\left(\frac{\hbar m \omega_{0}}{2}\right)^{1 / 2} e^{r}, \quad \text { so that } \quad \delta x \delta p=\frac{\hbar}{2} . \tag{5.173}
\end{equation*}
$$

On the phase plane (Fig. 6), this state, with $r>0$, may be represented by an oval spot squeezed along axis $x$ (hence the state's name) and stretched along axis $p$; the same formulas but with $r<0$ describe the opposite squeezing. On the other hand, phase $\theta$ of the squeeze parameter $ュ$ determines the angle $\theta / 2$ of oval's turn about the phase plane origin - see the magenta ellipse in Fig. 6; if $\theta \neq 0$, Eqs. (173) are valid for variables $\left\{x^{\prime}, p^{\prime}\right\}$ obtained from $\{x, p\}$ via clockwise rotation by that angle. For any of such origin-centered squeezed states, time evolution is reduced to an increase of the angle with rate $\omega_{0}$, i.e. to the clockwise rotation of the ellipse, without its deformation, with angular velocity $\omega_{0}$ - see the magenta arrows in Fig. 6. As a result, uncertainties $\delta x$ and $\delta p$ oscillate in time with double frequency $2 \omega_{0}$, while their product is constant at its minimal possible value $\hbar / 2$.

Such squeezed ground states have important implications for quantum measurements (see Sec. 7.7 below) and may be formed, for example, by parametric excitation of the oscillator, ${ }^{44}$ with a parameter modulation depth close to, but still below the threshold of parametric oscillations excitation. Unfortunately, I do have time for a further discussion of this interesting topic, ${ }^{45}$ but still need to mention

[^626]a more general class of squeezed states, centered to an arbitrary point $\{X, P\}$ rather than the origin, that may be formed by an additional action of the displacement operator (144) on the squeezed ground state (172). Calculations similar to those that led us from Eq. (145) to Eq. (155), but now for the product operator $\hat{\gamma}_{\alpha} \hat{\mathcal{S}}_{s}$ rater than bare $\hat{\gamma}_{\alpha}$, show that such a general squeezed state is an eigenstate of the following mixed operator
\[

$$
\begin{equation*}
\hat{b} \equiv \hat{a} \cosh r+\hat{a}^{\dagger} e^{i \theta} \sinh r \tag{5.174a}
\end{equation*}
$$

\]

with eigenvalue

$$
\begin{equation*}
\beta=\alpha \cosh r+\alpha^{*} e^{i \theta} \sinh r \tag{5.174b}
\end{equation*}
$$

For the particular case $\alpha=0$, Eq. (174b) yields $\beta=0$, i.e. the action of operator (174a) on the squeezed ground state $=$ with the same $r$ and $\theta$ yields the null-state, thus generalizing Eq. (118), which is valid for the "usual" (non-squeezed) ground state.

### 5.6. Revisiting spherically-symmetric problems

One more blank spot to fill has been left in our study of wave mechanics of spherically-3D symmetric systems in Sec. 3.6. Indeed, while the eigenfunctions describing axially-symmetric 2D systems, and the azimuthal components of those in spherically-symmetric 3D systems, are very simple,

$$
\begin{equation*}
\psi_{m}=\frac{1}{(2 \pi)^{1 / 2}} e^{i m \varphi}, \quad m=0, \pm 1, \pm 2, \ldots \tag{5.175}
\end{equation*}
$$

the polar components of the eigenfunctions in the latter case (i.e., of spherical harmonics) include the associate Legendre functions $P_{l}^{m}(\cos \theta)$ that may be expressed via elementary functions only indirectly - see Eqs. (3.165) and (3.168). This makes all the calculations less than transparent and, in particular, does not allow a clear insight into the origin of the very simple eigenvalue spectrum - see, e.g., Eq. (3.163). The bra-ket formalism, applied to the angular momentum operator, allows one to get such insight, and also produces a very convenient tool for many calculations involving spherically-symmetric potentials.

Let us start from using the correspondence principle to spell out the quantum-mechanical operator of the orbital angular momentum $\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}$ of a point particle:

$$
\hat{\mathbf{L}} \equiv \hat{\mathbf{r}} \times \hat{\mathbf{p}}=\left|\begin{array}{rrr}
\mathbf{n}_{x} & \mathbf{n}_{y} & \mathbf{n}_{z}  \tag{5.176}\\
\hat{x} & \hat{y} & \hat{z} \\
\hat{p}_{x} & \hat{p}_{y} & \hat{p}_{z}
\end{array}\right|, \quad \text { i.e. } \hat{L}_{x} \equiv \hat{y} \hat{p}_{z}-\hat{z} \hat{p}_{y}, \text { etc. }
$$

From this definition, we can readily calculate the commutation relations for all Cartesian components of operators $\hat{\mathbf{L}}, \hat{\mathbf{r}}$, and $\hat{\mathbf{p}}$; for example,

$$
\begin{equation*}
\left[\hat{L}_{x}, \hat{y}\right]=\left[\hat{y} \hat{p}_{z}-\hat{z} \hat{p}_{y}, \hat{y}\right]=-\hat{z}\left[\hat{p}_{y}, \hat{y}\right]=i \hbar \hat{z} \tag{5.177}
\end{equation*}
$$

etc. Using the sequential numbering of coordinate axes ( $x=r_{1}$, etc.), the summary of these calculations may be presented in similar, compact (and beautiful!) forms:
relations

$$
\begin{equation*}
\left[\hat{L}_{j}, \hat{r}_{j^{\prime}}\right]=i \hbar \hat{r}_{j^{\prime}} \varepsilon_{i j j^{\prime \prime}}, \quad\left[\hat{L}_{j}, \hat{p}_{j^{\prime}}\right]=i \hbar \hat{p}_{j^{\prime \prime}} \varepsilon_{i j j^{\prime \prime}}, \quad\left[\hat{L}_{j}, \hat{L}_{j^{\prime}}\right]=i \hbar \hat{L}_{j^{\prime \prime}} \varepsilon_{i j j^{\prime \prime}} \tag{5.178}
\end{equation*}
$$

where each of indices $j$ and $j$ ' and $j$ " may take any of values 1,2 , and $3, j$ " is the complementary index of the same set (not equal to either $j$ or $j$ '), and $\varepsilon_{j j} j^{\prime \prime}$ " is the Levi-Civita symbol (or "permutation symbol"). ${ }^{46}$ Also introducing in the natural way a (scalar!) operator of the observable $L^{2}=|\mathbf{L}|^{2}$,

$$
\begin{equation*}
\hat{L}^{2} \equiv \hat{L}_{x}^{2}+\hat{L}_{y}^{2}+\hat{L}_{z}^{2} \tag{5.179}
\end{equation*}
$$

it is straightforward to check that this operator commutes with each of the Cartesian components:

$$
\begin{equation*}
\left[\hat{L}^{2}, \hat{L}_{j}\right]=0 \tag{5.180}
\end{equation*}
$$

This result, at the first sight, may seem to contradict the last of Eqs. (178). Indeed, haven't we learned in Sec. 4.5 that commuting operators (e.g., $\hat{L}^{2}$ and any of $\hat{L}_{j}$ ) share their eigenstate sets? If yes, shouldn't that mean that this set has to be common for all 4 operators? ${ }^{47}$ The resolution in this paradox may be found in the condition that was mentioned just after Eq. (4.138), but (sorry!) not sufficiently emphasized there. According to that relation, if an operator has degenerate eigenstates (i.e. if $A_{j}=A_{j}$, even for $j \neq j^{\prime}$ ), they should not be necessarily shared by another compatible operator. This is exactly the situation with the orbital angular momentum operators, that may be schematically shown at a Venn diagram (Fig. 8):48 the set of eigenstates of operator $\hat{L}^{2}$ is highly degenerate, ${ }^{49}$ and is broader than those of the component operators $\hat{L}_{j}$ (that, as will be shown below, are non-degenerate until we consider particle's spin).


Fig. 5.8. Venn diagram showing (schematically) the partitioning of the set of eigenstates of operator $\hat{L}^{2}$. Each inner sector corresponds to the states shared with one of Cartesian component operators $\hat{L}_{j}$, while the outer (shaded) ring presents the eigenstates of $\hat{L}^{2}$ that are not shared with either of $\hat{L}_{j}$ - e.g., all linear combinations of eigenstates of different component operators.

[^627]Let us focus on just one of these 3 joint sets of eigenstates - by tradition, of operators $\hat{L}^{2}$ and $\hat{L}_{z}$. (This tradition is due to the canonical form of spherical coordinates, in which the polar angle is measured from axis $z$. Indeed, using Eqs. (63), in the coordinate representation we get the following expression,

$$
\begin{equation*}
\hat{L}_{z} \equiv \hat{x} p_{y}-\hat{y} p_{x}=x\left(-i \hbar \frac{\partial}{\partial y}\right)-y\left(-i \hbar \frac{\partial}{\partial x}\right)=-i \hbar \frac{\partial}{\partial \varphi} . \tag{5.181}
\end{equation*}
$$

Writing the standard eigenproblem for the operator in this representation, $\hat{L}_{z} \psi_{m}=L_{z} \psi_{m}$, we see that it is satisfied by eigenfunctions (175), with eigenvalues $L_{z}=\hbar m$ - at was already conjectured in Sec. 3.5.) More specifically, let us consider a set of eigenstates $\{l, m\}$ corresponding to a certain degenerate eigenvalue of operator $\hat{L}^{2}$ but all possible eigenvalues of operator $\hat{L}_{z}$, i.e. all possible quantum numbers $m$. (At this point, $l$ is just some parameter that determines the eigenvalue of $\hat{L}^{2}$; it will be defined more explicitly in a minute.) In order to analyze this set, it is instrumental to introduce the so-called ladder (also called, respectively, "raising" and "lowering") operators

$$
\begin{equation*}
\hat{L}_{ \pm} \equiv \hat{L}_{x} \pm i \hat{L}_{y} \tag{5.182}
\end{equation*}
$$

- note a substantial similarity between this definition and Eqs. (98). It is straightforward to use this definition and the last of Eqs. (178) to calculate the following commutators:

$$
\begin{equation*}
\left[\hat{L}_{+}, \hat{L}_{-}\right]=2 \hbar \hat{L}_{z}, \quad \text { and }\left[\hat{L}_{z}, \hat{L}_{ \pm}\right]= \pm \hbar \hat{L}_{ \pm}, \tag{5.183}
\end{equation*}
$$

and use Eq. (179) to prove another important relation:

$$
\begin{equation*}
\hat{L}^{2}=\hbar \hat{L}_{z}+\hat{L}_{z}^{2}+\hat{L}_{-} \hat{L}_{+} . \tag{5.184}
\end{equation*}
$$

Now let us rewrite the last of Eqs. (183) as

$$
\begin{equation*}
\hat{L}_{z} \hat{L}_{ \pm}=\hat{L}_{ \pm} \hat{L}_{z} \pm \hbar \hat{L}_{ \pm}, \tag{5.185}
\end{equation*}
$$

and act by its both parts on the ket-vector $|l, m\rangle$ of the set specified above:

$$
\begin{equation*}
\hat{L}_{z} \hat{L}_{ \pm}|l, m\rangle=\hat{L}_{ \pm} \hat{L}_{z}|l, m\rangle \pm \hbar \hat{L}_{ \pm}|l, m\rangle . \tag{5.186}
\end{equation*}
$$

Since eigenvalues of operator $\hat{L}_{z}$ are equal to $\hbar m$, in the first term of the right-hand part we may write

$$
\begin{equation*}
\hat{L}_{z}|l, m\rangle=\hbar m|l, m\rangle . \tag{5.187}
\end{equation*}
$$

With that, Eq. (186) may be recast as

$$
\begin{equation*}
\hat{L}_{z}\left(\hat{L}_{ \pm}|l, m\rangle\right)=\hbar(m \pm 1)\left(\hat{L}_{ \pm}|l, m\rangle\right) . \tag{5.188}
\end{equation*}
$$

In a spectacular similarity with Eqs. (111)-(112) for the harmonic oscillator, Eq. (188) means that states $\hat{L}_{ \pm}|l, m\rangle$ are also the eigenstates of operator $\hat{L}_{z}$, corresponding to eigenvalues ( $m \pm 1$ ). Thus the ladder operators act exactly as the creation and annihilation operators in the oscillator, moving the system up or down a ladder of eigenstates (Fig. 9). The most significant difference is that now the state
ladder must end in both directions, because an infinite increase of $|m|$, with whatever sign, would cause the expectation values of operator

$$
\begin{equation*}
\hat{L}_{x}^{2}+\hat{L}_{y}^{2}=\hat{L}^{2}-\hat{L}_{z}^{2}, \tag{5.189}
\end{equation*}
$$

which corresponds to a non-negative observable, to become negative. Hence there should be two states on both ends of the ladder, $\left|l, m_{\max }\right\rangle$ and $\left|l, m_{\min }\right\rangle$, for whom

$$
\begin{equation*}
\hat{L}_{+}\left|l, m_{\max }\right\rangle=0, \quad \hat{L}_{-}\left|l, m_{\min }\right\rangle=0 . \tag{5.190}
\end{equation*}
$$

Due to the symmetry of the whole problem with respect to the replacement $m \rightarrow-m$, we should have $m_{\min }=-m_{\max }$. This $m_{\max }$ is exactly the quantum number that is traditionally called $l$, so that


Fig. 5.9. Hierarchy (ladder diagram) of the common eigenstates of operators $\hat{L}^{2}$ and $\hat{L}_{z}$.

Evidently, this relation of quantum numbers $m$ and $l$ is compatible with the almost-classical image of various orientations of the angular momentum vector of the same length in various directions, with its $z$-component taking several $(2 l+1)$ possible values $\hbar m$. In this simple picture, however, $L^{2}$ would be equal to square of $\left(L_{z}\right)_{\max }$, i.e. to $(\hbar l)^{2}$; however, this is not so. Indeed, applying the operator equality (184) to the top state $\left|l, m_{\max }\right\rangle \equiv|l, l\rangle$, we get

$$
\begin{align*}
\hat{L}^{2}|l, l\rangle & =\hbar \hat{L}_{z}|l, l\rangle+\hat{L}_{z}^{2}|l, l\rangle+\hat{L}_{-} \hat{L}_{+}|l, l\rangle=\hbar^{2} l|l, l\rangle+\hbar^{2} l^{2}|l, l\rangle+0  \tag{5.192}\\
& =\hbar^{2} l(l+1)|l, l\rangle .
\end{align*}
$$

Since by our initial assumption, all eigenvectors $|l, m\rangle$ correspond to the same eigenvalue of operator $\hat{L}^{2}$, this result means that all these eigenvalues are equal to $\hbar^{2} l(l+1)$. Just as in case of the spin- $1 / 2$ vector operators, the deviation of this result from $\hbar^{2} l^{2}$ may be interpreted as the result of unavoidable uncertainties ("fluctuations") of the $x$ - and $y$-components of the angular momentum, that give a finite positive contribution to $L^{2}$ even if the angular momentum vector is aligned in the best possible way with the $z$-axis.

Now let us compare our results with those of Sec. 3.6. Using the expression of Cartesian coordinates via the spherical ones exactly as was done in Eq. (181), we get the following expressions for the ladder operators (182) in the coordinate representation:

$$
\begin{equation*}
\hat{L}_{ \pm}=\hbar e^{ \pm i \varphi}\left( \pm \frac{\partial}{\partial \theta}+i \cot \operatorname{an} \theta \frac{\partial}{\partial \varphi}\right) \tag{5.193}
\end{equation*}
$$

Now plugging this equation, together with Eq. (181), into Eq. (184), we get

$$
\begin{equation*}
\hat{L}^{2}=-\hbar^{2}\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial}{\partial \theta}\right)+\frac{1}{\sin ^{2} \theta} \frac{\partial^{2}}{\partial \varphi^{2}}\right] . \tag{5.194}
\end{equation*}
$$

But this is exactly the operator (besides its division by constant parameter $2 m R^{2}$ ) that stands in the lefthand part of Eq. (3.156). Hence that equation, which was explored by the "brute-force" (wavemechanical) approach in Sec. 3.6, may be understood as the eigenproblem for operator $\hat{L}^{2}$ in the coordinate representation, with eigenfunctions $Y_{l}^{m}(\theta, \varphi)$ corresponding to eigenkets $\{l, m\}$, and eigenvalues $L^{2}=2 m R^{2} E$. As a reminder, the main result of that, rather involved analysis was expressed by Eq. (3.163), which now may be rewritten as

$$
\begin{equation*}
L_{l}^{2}=2 m R^{2} E_{l}=\hbar^{2} l(l+1), \tag{5.195}
\end{equation*}
$$

in a full agreement with what was obtained in this section by much more efficient means based on the bra-ket formalism. In particular, it is fascinating to see how easy are now many operations with eigenvectors $|l, m\rangle$, albeit wavefunctions of these states, spherical harmonics $Y_{l}^{m}(\theta, \varphi)$, have rather complex spatial behavior - please have one more look at Eq. (3.171) and Fig. 3.19. ${ }^{50}$

### 5.7. Spin and its addition to orbital angular momentum

Surprisingly, the theory described in the last section is useful for much more than orbital motion analysis. In particular, it helps to generalize the spin $-1 / 2$ results discussed in Chapter 4 to other values of spin $s$ - the parameter still has to be defined. For that, let us notice that the commutation relations that were derived, for $s=1 / 2$, from the Pauli matrix properties, may be rewritten in exactly the same form as Eqs. (178) and (180) for the orbital momentum:

$$
\begin{equation*}
\left[\hat{S}_{j}, \hat{S}_{j^{\prime}}\right]=i \hbar \hat{S}_{j^{\prime \prime}} \varepsilon_{j j^{\prime \prime \prime} j^{\prime \prime}}, \quad\left[\hat{S}^{2}, \hat{S}_{j}\right]=0 \tag{5.196}
\end{equation*}
$$

[^628]It has been postulated (and confirmed by numerous experiments) that these relations hold true for any quantum particle. Now note that all the calculations of the last section have been based almost exclusively on such relations - the exception will be discussed imminently. Hence, we may repeat them for spin operators, and get the relations similar to Eq. (187) and (192):

[^629]Spin operators: eigenstates eigenvalues

$$
\begin{equation*}
\hat{S}_{z}\left|s, m_{s}\right\rangle=\hbar m_{s}\left|s, m_{s}\right\rangle, \quad \hat{S}^{2}\left|s, m_{s}\right\rangle=\hbar^{2} s(s+1)\left|s, m_{s}\right\rangle, \quad 0 \leq s, \quad-s \leq m_{s} \leq+s \tag{5.197}
\end{equation*}
$$

where $m_{s}$ is a quantum number similar to the orbital number $m$, and the non-negative constant $s$ is defined as the maximum value of $\left|m_{s}\right|$. This parameter is exactly what is called particle's spin - in the narrow sense of the word.

Now let us return to the only part of our orbital moment calculations that has not been derived from the commutation relations. This was the fact, based on solution (175) of the orbital motion problems, that quantum numbers $m$ (the analog of $m_{s}$ ) are integer. For spin, we do not have such a solution, so that the spectrum of numbers $m_{s}$ (and hence its limits $\pm s$ ) should be found from the more loose requirement that the eigenstate ladder, extending from $-s$ to $+s$, has an integer number of steps. Hence, $2 s$ has to be integer, i.e. spin $s$ of a quantum particle may be either integer (as it is, for example, for photons and gluons), or half-integer (e.g., for all quarks and leptons including electrons). ${ }^{51}$

For $s=1 / 2$, this picture yields all spin properties of electron that were derived in Chapter 4 from postulate (4.117). In particular, operators $\hat{S}^{2}$ and $\hat{S}_{z}$ have only 2 common eigenstates, with $S_{z}=\hbar m_{s}=$ $\pm \hbar / 2$, and both with $S^{2}=s(s+1) \hbar^{2}=(3 / 4) \hbar^{2}$. Note that this analogy with the angular momentum sheds a new light on the symmetry properties of electrons. Indeed, the fact that $m$ in Eq. (175) is integer was derived in Sec. 3.5 from the requirement that making a full circle around axis $z$, we should find a similar value of wavefunction $\psi_{m}$, which differs from the initial one by an inconsequential factor $\exp \{2 \pi i m\}$. With the replacement $m \rightarrow m_{s}= \pm 1 / 2$, such operation would multiply the wavefunction by $\exp \{ \pm \pi i\}$, i.e. reverse its sign. On course, spin cannot be described by a usual wavefunction, but this odd parity of electrons (and all other spin- $1 / 2$ particles) is clearly revealed in multiparticle systems - see Chapter 8.

Now we are sufficiently equipped to analyze particles that have both the orbital momentum and the spin. In classical mechanics, such a particle would be characterized by the total angular momentum vector $\mathbf{J}=\mathbf{L}+\mathbf{S}$. Following the correspondence principle, we may make an assumption that quantummechanical properties of this observable may be analyzed using the similarly defined vector operator:

$$
\begin{equation*}
\hat{\mathbf{J}} \equiv \hat{\mathbf{L}}+\hat{\mathbf{S}}, \tag{5.198}
\end{equation*}
$$

with Cartesian components

$$
\begin{equation*}
\hat{J}_{z} \equiv \hat{L}_{z}+\hat{S}_{z} \tag{5.199}
\end{equation*}
$$

etc, and the magnitude squared equal to

$$
\begin{equation*}
\hat{J}^{2} \equiv \hat{J}_{x}^{2}+\hat{J}_{y}^{2}+\hat{J}_{z}^{2} \tag{5.200}
\end{equation*}
$$

Let us examine the properties of this vector operator. Since its two components describe different degrees of freedom of the particle (again, you may say "belong to different Hilbert spaces"), they may be considered as completely commuting:

$$
\begin{equation*}
\left[\hat{L}_{j}, \hat{S}_{j^{\prime}}\right]=0, \quad\left[\hat{L}^{2}, \hat{S}^{2}\right]=0 \tag{5.201}
\end{equation*}
$$

[^630]These above equalities are sufficient to derive the commutation rules of the total angular momentum, and, not surprisingly, they turn out to be absolutely similar to those of its components:

$$
\begin{equation*}
\left[\hat{J}_{j}, \hat{J}_{j^{\prime}}\right]=i \hbar \hat{J}_{j^{\prime \prime}} \varepsilon_{i j j^{\prime \prime}}, \quad\left[\hat{J}^{2}, \hat{J}_{j}\right]=0 \tag{5.202}
\end{equation*}
$$

Now repeating all arguments of the last section, we may derive the following expressions for the common eigenstates of operators $\hat{J}^{2}$ and $\hat{J}_{z}$ :

$$
\begin{equation*}
J_{z}\left|j, m_{j}\right\rangle=\hbar m_{j}\left|j, m_{j}\right\rangle, \quad \hat{J}^{2}\left|j, m_{j}\right\rangle=\hbar^{2} j(j+1)\left|j, m_{j}\right\rangle, \quad 0 \leq j, \quad-j \leq m_{j} \leq+j \tag{5.203}
\end{equation*}
$$

Total momentum: eigenstates, and eigenvalues
where $j$ and $m_{j}$ are new quantum numbers. Repeating the arguments made for $m_{s}$, we may conclude that $j$ and $m_{j}$ may be either integer or half-integer.

Before we proceed, one remark on notation: it is very convenient to use the same letter $m$ for numbering eigenstates of all momentum components participating in Eq. (199), with corresponding indices $(j, l$, and $s)$, in particular, to replace what we called $m$ with $m_{l}$. With this replacement, the main results of the last section may be summarized in the form similar to Eqs. (197) and (203):

$$
\begin{equation*}
\hat{L}_{z}\left|l, m_{l}\right\rangle=\hbar m_{l}\left|l, m_{l}\right\rangle, \quad \hat{L}^{2}\left|l, m_{l}\right\rangle=\hbar^{2} l(l+1)\left|l, m_{l}\right\rangle, \quad 0 \leq l, \quad-l \leq m_{l} \leq+l . \tag{5.204}
\end{equation*}
$$

In order to understand which eigenstates used is Eqs. (197), (203), and (204) are compatible with each other, let us use Eqs. (198)-(202) to calculate the mutual commutators of the operators squared and their $z$-components. The result is

$$
\begin{array}{ll}
{\left[\hat{J}^{2}, \hat{L}^{2}\right]=0,} & {\left[\hat{J}^{2}, \hat{S}^{2}\right]=0} \\
{\left[\hat{J}^{2}, \hat{L}_{z}\right] \neq 0,} & {\left[\hat{J}^{2}, \hat{S}_{z}\right] \neq 0} \tag{5.206}
\end{array}
$$

This result may be presented schematically on the following Venn diagram (Fig. 10), in which the crossed arrows indicate the only non-commuting pairs of operators.

operators diagonal in
the coupled
representation

Fig. 5.10. Venn diagram for angular momentum operators, and their mutually-commuting groups.

This means that just as for each component angular momentum ( $\mathbf{J}, \mathbf{L}$, and $\mathbf{S}$ ) considered separately we could select a group of common eigenstates for its magnitude squared and the $z$ component, we also may find eigenstates shared by two broader groups of operators, encircled with colored lines in Fig. 10. The first group (within the red circle), consists of all operators but $\hat{J}^{2}$. This means that there are eigenstates shared by 5 remaining operators, and they may be characterized by certain values of the corresponding quantum numbers: $l, m_{l}, s, m_{s}$, and $m_{j}$. Actually, only 4 of these
numbers are independent, because due to Eq. (199) for these compatible operators, for each eigenstate of the group, their "magnetic" quantum numbers $m$ have to satisfy the following relation:

$$
\begin{equation*}
m_{j}=m_{l}+m_{s} . \tag{5.207}
\end{equation*}
$$

Hence the common eigenstates of the operators of this group are fully defined by just 4 quantum numbers, for example, $l, m_{l}, s$, and $m_{s}$. For some calculations, especially those for systems whose Hamiltonians include only operators of this group, it is convenient to the use this set of eigenstates as the basis; frequently this is called the uncoupled representation.

However, in some situations we cannot ignore interactions between the orbital and spin degrees of freedom (in the common jargon, the spin-orbit coupling), which leads in particular to splitting (called the fine structure) of atomic energy levels even in the absence of external magnetic field. I will discuss these effects in detail in the next chapter, and now will only note that they may be described by a separate term, proportional to product $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$, in the system's Hamiltonian. If this term is not negligible, the uncoupled representation becomes inconvenient. Indeed, writing

$$
\begin{equation*}
\hat{J}^{2}=(\hat{\mathbf{L}}+\hat{\mathbf{S}})^{2}=\hat{L}^{2}+\hat{S}^{2}+2 \hat{\mathbf{L}} \cdot \hat{\mathbf{S}} \tag{5.208}
\end{equation*}
$$

and looking at Fig. 10 again, we see that the operator $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$, describing the spin-orbit coupling, does not commute with operators $\hat{L}_{z}$ and $\hat{S}_{z}$. This means that stationary states of the system with such term in the Hamiltonian do not belong to the uncoupled representation basis. On the other hand, Eq. (208) shows that operator $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ does commute with all 4 operators of another group, encircled with the blue line in Fig. 10. According to Eqs. (201), (202), and (205), all operators of that group also commute to each other, so that they have common eigenstates that may be marked by the corresponding quantum numbers, $l, s, j$, and $m_{j}$. This group is the basis for the coupled representation of particle's state.

Excluding the quantum numbers $l$ and $s$, common for both groups, from notation, it is convenient to denote the common ket-vectors of each group as, respectively,

Coupled and uncoupled bases

$$
\begin{array}{ll}
\left|m_{l}, m_{s}\right\rangle, & \text { for the uncolpled representation's basis, } \\
\left|j, m_{j}\right\rangle, & \text { for the coupled representation's basis. } \tag{5.209}
\end{array}
$$

As we will see in the next chapter, for solution of some important problems (e.g., the fine structure of atomic spectra and the Zeeman effect), we will need the relation between the kets $\left|j, m_{j}\right\rangle$ and the kets $\mid m_{l}$, $\left.m_{s}\right\rangle$. This relation may be represented as the usual linear superposition,

$$
\begin{equation*}
\left|j, m_{j}\right\rangle=\sum_{m_{l}, m_{s}}\left|m_{l}, m_{s}\right\rangle\left\langle m_{l}, m_{s} \mid j, m_{j}\right\rangle, \tag{5.210}
\end{equation*}
$$

whose bra-kets (c-numbers), essentially the elements of the unitary matrix of the transformation between two eigenstate bases (209), are called the Clebsch-Gordan coefficients.

The best (though imperfect) classical interpretation of Eq. (210) I can offer is as follows. If the lengths of vectors $\mathbf{L}$ and $\mathbf{S}$ (in quantum mechanics associated with numbers $l$ and $s$, respectively), and also their scalar product $\mathbf{L} \cdot \mathbf{S}$, are all fixed, then so is the length of vector $\mathbf{J}=\mathbf{L}+\mathbf{S}$ (whose length in quantum mechanics is described by quantum number $j$ ). Hence, the classical image of a specific eigenket $\left|j, m_{j}\right\rangle$, in which $l, s, j$, and $m_{j}$ are all fixed, is a state in which $L^{2}, S^{2}, J^{2}$, and $J_{z}$ are fixed.

However, this fixation still allows for an arbitrary rotation of the pair of vectors $\mathbf{L}$ and $\mathbf{S}$ (with a fixed angle between them, and hence fixed $\mathbf{L} \cdot \mathbf{S}$ and $J^{2}$ ) about the direction of vector $\mathbf{J}$ - see Fig. 11.



Fig. 5.11. Classical image of two quantum states with the same $l, s, j$, and $m_{j}$, but different $m_{l}$ and $m_{s}$.

Hence the components $L_{z}$ and $S_{z}$ in these conditions are not fixed, and in classical mechanics may take a continuum of values, two of which (with the largest and smallest possible values of $S_{z}$ ) are shown in Fig. 11. In quantum mechanics, these components are quantized, with their states represented by eigenkets $\left|m_{l}, m_{s}\right\rangle$, so that a linear combination of such kets is necessary to represent ket $\left|j, m_{j}\right\rangle$. This is exactly what Eq. (210) does.

Some of properties of the Clebsch-Gordan coefficients $\left\langle m_{l}, m_{s} \mid j, m_{j}\right\rangle$ may be readily established. For example, the coefficients do not vanish only if the involved magnetic quantum numbers satisfy Eq. (207); let us prove this fact. ${ }^{52}$ All matrix elements of the null-operator

$$
\begin{equation*}
\hat{J}_{z}-\left(\hat{L}_{z}+\hat{S}_{z}\right)=\hat{0} \tag{5.211}
\end{equation*}
$$

should equal zero in any basis; in particular

$$
\begin{equation*}
\left\langle j, m_{j}\right| \hat{J}_{z}-\left(\hat{L}_{z}+\hat{S}_{z}\right)\left|m_{l}, m_{s}\right\rangle=0 \tag{5.212}
\end{equation*}
$$

Acting by operator $\hat{J}_{z}$ on the bra-vector, and by the sum $\left(\hat{L}_{z}+\hat{S}_{z}\right)$ on the ket-vector, we get

$$
\begin{equation*}
\left[m_{j}-\left(m_{l}+m_{s}\right)\right]\left\langle j, m_{j} \mid m_{l}, m_{s}\right\rangle=0 \tag{5.213}
\end{equation*}
$$

thus proving that $\left\langle m_{l}, m_{s} \mid j, m_{j}\right\rangle \equiv\left\langle j, m_{j} \mid m_{l}, m_{s}\right\rangle^{*}=0$, if $m_{j}-\left(m_{l}+m_{s}\right) \neq 0$.
For the most important case of spin- $1 / 2$ particles ( $s=1 / 2$, and hence $m_{s}= \pm 1 / 2$ ), whose uncoupled representation basis includes $2 \times(2 l+1)$ states, restriction (207) enables the representation of all nonvanishing Clebsch-Gordan coefficients on the simple diagram shown in Fig. 12. Indeed, each coupled-representation eigenket $\left|j, m_{j}\right\rangle$, with $m_{j}=m_{l}+m_{s}=m_{l} \pm 1 / 2$, may be related with non-zero Clebsch-Gordan coefficients to at most two uncoupled-representation eigenstates $\left|m_{l}, m_{s}\right\rangle$. Since $m_{l}$ may only take integer values from $-l$ to $+l, m_{j}$ may only take semi-integer values on the interval $[-l-1 / 2, l+$ $1 / 2]$. Hence, by the definition of $j$ as $\left(m_{j}\right)_{\max }$, its maximum value has to be $l+1 / 2$, and for $m_{j}=l+1 / 2$, this is the only possible value. This means that the uncoupled state with $m_{l}=l$ and $m_{s}=1 / 2$ should be identical to the coupled-representation state with $j=l+1 / 2$ and $m_{j}=l+1 / 2$ :

$$
\begin{equation*}
\left|j=l+\frac{1}{2}, m_{j}=l+\frac{1}{2}\right\rangle=\left|m_{l}=m_{j}-\frac{1}{2}, m_{s}=+\frac{1}{2}\right\rangle . \tag{5.214}
\end{equation*}
$$

[^631]

Fig. 5.12. All possible sets of eigenvalues $m_{l}, m_{s}$ for a particle with fixed $l$, and $s=1 / 2$. Each uncoupled-representation state is represented by a dot, while each the coupled-representation state, by a single sloped line connecting the dots.

However, already for the next value, $m_{j}=l-1 / 2$, we need to have two values of $j$, so that two $\mid m_{l}$, $\left.m_{s}\right\rangle$ kets is to be related to two $\left|j, m_{j}\right\rangle$ kets by two Clebsch-Gordan coefficients. Since $l$ changes in unit steps, these values of $j$ have to be $l \pm 1 / 2$. This choice,

$$
\begin{equation*}
j=l \pm 1 / 2 \tag{5.215}
\end{equation*}
$$

evidently satisfies all lower values of $m_{j}$ (again, with only one value, $j=l+1 / 2$, necessary for the lowest $\left.m_{j}=-l-1 / 2\right)-$ see Fig. 12. Note that the total number of the coupled-representation states is $1+2 \times 2 l+1$ $=2(2 l+1)$, i.e. the same as in the uncoupled representation. So, each sum (210), for fixed $j, m_{j}$ (and fixed common parameter $l$ ), has at most 2 terms, i.e. involves at most 2 Clebsch-Gordan coefficients.

These coefficients may be calculated in a few steps, all but the last one rather simple even for arbitrary spin $s$. First, the matrix elements of ladder operators $\hat{L}_{ \pm}$in the standard $z$-basis (i.e. in the basis of kets $\left|m_{l}\right\rangle$ ) may be calculated from Eq. (184). Next, the similarity of vector operators $\hat{\mathbf{J}}$ and $\hat{\mathbf{S}}$ to operators $\hat{\mathbf{L}}$, expressed by Eqs. (197), (203), and (204), may be used to argue that the matrix elements of operators $\hat{S}_{ \pm}$and $\hat{J}_{ \pm}$, defined absolutely similarly to $\hat{L}_{ \pm}$, have similar matrix elements in the bases of kets $\left|m_{s}\right\rangle$ and $\left|m_{j}\right\rangle$, respectively. After that, acting by operator $\hat{J}_{ \pm}=\hat{L}_{ \pm}+\hat{S}_{ \pm}$upon both parts of Eq. (210), and then inner-multiplying the result by the bra vector $\left\langle m_{l}, m_{s}\right|$ and using the above matrix elements, we get recurrence relations for the Clebsch-Gordan coefficients. Finally, these relations may be recurrently applied to the adjacent states in both representations, starting from any of the two states common for them - for example, from state with ket-vectors (214), corresponding to the top right point in Fig. 12. Let me leave these straightforward but a bit tedious calculations for reader's exercise and just cite the final result of this procedure for $s=1 / 2: 53$

Clebsch Gordan coefficients for $s=1 / 2$

$$
\begin{align*}
& \left\langle m_{l}=m_{j}-\frac{1}{2}, \left.m_{s}=+\frac{1}{2} \right\rvert\, j=l \pm \frac{1}{2}, m_{j}\right\rangle= \pm\left(\frac{l \pm m_{j}+1 / 2}{2 l+1}\right)^{1 / 2},  \tag{5.216a}\\
& \left\langle m_{l}=m_{j}+\frac{1}{2}, \left.m_{s}=-\frac{1}{2} \right\rvert\, j=l \pm \frac{1}{2}, m_{j}\right\rangle=+\left(\frac{l \mp m_{j}+1 / 2}{2 l+1}\right)^{1 / 2}
\end{align*}
$$

[^632]For applications, it may be more convenient to use this result in the following equivalent form:

$$
\begin{align*}
& \left|j=l \pm \frac{1}{2}, m_{j}\right\rangle \\
& = \pm\left(\frac{l \pm m_{j}+1 / 2}{2 l+1}\right)^{1 / 2}\left|m_{l}=m_{j}-\frac{1}{2}, m_{s}=+\frac{1}{2}\right\rangle+\left(\frac{l \mp m_{j}+1 / 2}{2 l+1}\right)^{1 / 2}\left|m_{l}=m_{j}+\frac{1}{2}, m_{s}=-\frac{1}{2}\right\rangle \tag{5.216b}
\end{align*}
$$

We will use this relation in Sec. 6.4 for an analysis of the anomalous Zeeman effect, based on the perturbation theory. Moreover, most of the angular momentum addition theory described above is immediately applicable to the addition of angular momenta in multiparticle systems, so we will revisit it in Chapter 8.

To conclude this section, I have to note that the Clebsch-Gordan coefficients (for arbitrary $s$ ) participate also in the so-called Wigner-Eckart theorem that expresses matrix elements of certain spherical tensors, in the coupled-representation basis $\left|j, m_{j}\right\rangle$, via a reduced set of matrix elements. Unfortunately, a discussion of this theorem and its applications would require a higher mathematical background than I can expect from my readers, and more time/space than I can afford. ${ }^{54}$

### 5.8. Exercise problems

5.1. Use the discussion of Sec. 1 to find an alternative solution of Problem 4.17.
5.2. A two-level system is in a quantum state $\alpha$, described by ket-vector $|\alpha\rangle=\alpha_{\uparrow}|\uparrow\rangle+\alpha_{\downarrow}|\downarrow\rangle$, with given (generally, complex) c-number coefficients $\alpha \uparrow \downarrow$. Prove that we can always select a 3-component vector $\mathbf{a}=\left\{a_{x}, a_{y}, a_{z}\right\}$ of real $c$-numbers, such that $\alpha$ is an eigenstate of operator $\mathbf{a} \cdot \hat{\boldsymbol{\sigma}}$, where $\hat{\boldsymbol{\sigma}}$ is the operator described, in $z$-basis, by the Pauli matrix vector. Find all possible values of a satisfying this condition, and the second eigenstate of operator $\mathbf{a} \cdot \hat{\boldsymbol{\sigma}}$, orthogonal to the given $\alpha$. Give a Bloch-sphere interpretation of your result.
5.3. A spin $-1 / 2$ particle is in a constant vertical field, so that its Hamiltonian

$$
\hat{H}=\frac{\hbar \Omega}{2} \hat{\sigma}_{z}
$$

but its spin's initial state is an eigenstate of a different Hamiltonian: ${ }^{55}$

$$
\hat{H}_{i n i}=\mathbf{a} \cdot \hat{\boldsymbol{\sigma}} \equiv a_{x} \hat{\sigma}_{x}+a_{y} \hat{\sigma}_{y}+a_{z} \hat{\sigma}_{z} .
$$

Use any approach you like to calculate the time evolution of the expectation values of the spin components. Interpret the results.
5.4. For any periodic motion of a single particle in a confining potential $U(\mathbf{r})$, the virial theorem of non-relativistic classical mechanics ${ }^{56}$ is reduced to the following equality:

[^633]$$
\bar{T}=\frac{1}{2} \overline{\mathbf{r} \cdot \nabla U},
$$
where $T$ is particle's kinetic energy, and the top bar means averaging over the period of motion. Prove the quantum-mechanical version of the theorem for an arbitrary stationary quantum state, in the absence of spin effects:
$$
\langle T\rangle=\frac{1}{2}\langle\mathbf{r} \cdot \nabla U\rangle,
$$
where the angular brackets mean, as everywhere in these notes, the expectation value of the variable inside them.

Hint: Mimicking the proof of the classical virial theorem, consider the time evolution of operator

$$
\hat{G} \equiv \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} .
$$

5.5. A constant force $F$ is applied to an (otherwise free) 1D particle of mass $m$. Calculate the eigenfunctions of the problem, using
(i) the coordinate representation, and
(ii) the momentum representation.

Discuss the relation between the results.
5.6. The momentum representation of an operator, defined in the Hilbert space of 1D orbital states of a particle, equals $p^{-1}$. Find its coordinate representation.
5.7.* For a particle moving in a 3D periodic potential, develop the bra-ket formalism for the $\mathbf{q}$ representation, in which a complex amplitude similar to $a_{q}$ in Eq. (2.234) (but generalized to 3D and all energy bands) plays the role of the wavefunction. In particular, calculate operators $\mathbf{r}$ and $\mathbf{v}$ in this representation, and use the result to prove Eq. (2.237) for 1D motion in the low-field limit.

Hint: Try to generalize the analysis of the momentum representation in Sec. 5.2.
5.8. In the Heisenberg picture of quantum dynamics, find the operator of velocity and acceleration,

$$
\hat{\mathbf{v}} \equiv \frac{d \hat{\mathbf{r}}}{d t} \quad \text { and } \hat{\mathbf{a}} \equiv \frac{d \hat{\mathbf{v}}}{d t},
$$

of an electron moving in an arbitrary electromagnetic field. Compare the results with the corresponding classical expressions.
5.9. Calculate, in the WKB approximation, the transmission coefficient $T$ for tunneling of a 2D particle with energy $E<U_{0}$ through a saddle-shaped potential "pass"

$$
U(x, y)=U_{0}\left(1+\frac{x y}{a^{2}}\right),
$$

where $U_{0}$ and $a$ are real constants.
5.10. Calculate the so-called Gamow factor ${ }^{57}$ for the alpha decay of atomic nuclei, i.e. the exponential factor in the transparency of the tunnel barrier, resulting from the following simple model of the particle's potential energy as a function of its distance from the nuclear center:

$$
U(r)= \begin{cases}U_{0}<0, & \text { for } r<R \\ \frac{Z Z^{\prime} e^{2}}{4 \pi \varepsilon_{0} r}, & \text { for } R<r,\end{cases}
$$

(where $Z e=2 e>0$ is the charge of the alpha-particle, $Z^{\prime} e>0$ is that of the nucleus after the decay, and $R$ is the nucleus' radius), in the WKB approximation.
5.11. For a 1D harmonic oscillator with mass $m$ and frequency $\omega_{0}$, calculate:
(i) all matrix elements $\langle n| \hat{x}^{3}\left|n^{\prime}\right\rangle$, and
(ii) diagonal matrix elements $\langle n| \hat{x}^{4}|n\rangle$,
where $n$ are the Fock states.
5.12. Calculate the sum (over all $n>0$ ) of the so-called oscillator strengths,

$$
\left.f_{n} \equiv \frac{2 m}{\hbar^{2}}\left(E_{n}-E_{0}\right)|\langle n| \hat{x}| 0\right\rangle\left.\right|^{2},
$$

of quantum transitions between the $n^{\text {th }}$ energy level and the ground state, for
(i) a 1 D harmonic oscillator, and
(ii) a 1D particle confined in an arbitrary stationary potential.
5.13.* Prove the so-called the Bethe sum rule,

$$
\left.\sum_{n^{\prime}}\left(E_{n^{\prime}}-E_{n}\right)\left|\langle n| e^{i k x}\right| n^{\prime}\right\rangle\left.\right|^{2}=\frac{\hbar^{2} k^{2}}{2 m}
$$

(where $k$ is a $c$-number), valid for a 1D particle moving in an arbitrary time-independent potential $U(x)$, and discuss its relation with the Thomas-Reiche-Kuhn sum rule, whose derivation was the subject of the previous problem.

Hint: Calculate the expectation value, in a stationary state $n$, of the following double commutator,

$$
\left.\hat{D} \equiv\left[\hat{H}, e^{i k x}\right], e^{-i k x}\right],
$$

in two ways - first, just spelling out both commutators, and, second, using the commutation relations between operators $\hat{p}$ and $e^{ \pm i k x}$, and compare the results.
5.14. Simplify the following operators:
(i) $\exp \{+i a \hat{x}\} \hat{p}_{x} \exp \{-i a \hat{x}\}$, and

[^634](ii) $\exp \left\{+i a \hat{p}_{x}\right\} \hat{x} \exp \left\{-i a \hat{p}_{x}\right\}$,
where $a$ is a $c$-number.
5.15. Use the Heisenberg equation of motion for a direct derivation of time evolution law (5.171) of the creation and annihilation operators of a harmonic oscillator.

### 5.16. Calculate:

(i) the expectation value of energy, and
(ii) the laws of time evolution of expectation values of the coordinate and momentum for a 1D harmonic oscillator, provided that in the initial moment $(t=0)$ it was in state

$$
|\alpha\rangle=\frac{1}{\sqrt{2}}(|15\rangle+|16\rangle),
$$

where $|n\rangle$ are ket-vectors of the stationary (Fock) states of the oscillator.
5.17.* Re-derive the London dispersion force potential between two 3D harmonic oscillators (already calculated in Problem 3.19), using the language of mutually-induced polarization.
5.18. The discussion of the Glauber state properties in Sec. 5 has used the following general statement: if

$$
[\hat{A}, \hat{B}]=\mu \hat{I}
$$

where $\hat{A}$ and $\hat{B}$ are arbitrary operators, and $\mu$ is an arbitrary $c$-number, then

$$
\exp \{+\hat{A}\} \hat{B} \exp \{-\hat{A}\}=\hat{B}+\mu \hat{I}
$$

Prove the statement.
Hint: One (of several) ways to prove the statement is to expand operator $\hat{f}(\lambda)=\exp \{\lambda \hat{A}\} \hat{B} \exp \{-\lambda \hat{A}\}$ into the Taylor series in c-number $\lambda$, and then evaluate it at $\lambda=1$.
5.19. An external force pulse $F(t)$, of a finite time duration $T$, is exerted on a 1D harmonic oscillator, initially in its ground state. Use the Heisenberg-picture equations of motion to calculate the expectation value of oscillator's energy at the end of the pulse.
5.20. Calculate the energy of the squeezed ground state $\perp$ of a harmonic oscillator, defined by Eq. (172).
5.21. Use Eqs. (5.178) of the lecture notes to prove that operators $\hat{L}_{j}$ and $\hat{L}^{2}$ commute with the Hamiltonian of a spinless particle placed in any central potential field.
5.22. Prove the following relations for the operators of the angular momentum:

$$
\hat{L}^{2}=\hat{L}_{z}^{2}+\hat{L}_{+} \hat{L}_{-}-\hbar \hat{L}_{z}=\hat{L}_{z}^{2}+\hat{L}_{-} \hat{L}_{+}+\hbar \hat{L}_{z} .
$$

(One of them, Eq. (184), was already used in Sec. 6.)
5.23. According to Eqs. (188) and their discussion, action of the ladder operators on the common eigenkets $|l, m\rangle$ of operators $\hat{L}^{2}$ and $\hat{L}_{z}$ may be described as

$$
\hat{L}_{ \pm}|l, m\rangle=L_{ \pm}^{(m)}|l, m \pm 1\rangle .
$$

Calculate coefficients $L_{ \pm}{ }^{(m)}$, assuming that the eigenstates are normalized: $\langle l, m \mid l, m\rangle=1$.
5.24. In the basis of common eigenstates of operators $\hat{L}_{z}$ and $\hat{L}^{2}$, described by eigenkets $|l, m\rangle$ :
(i) calculate matrix elements $\left\langle l, m_{1}\right| \hat{L}_{x}\left|l, m_{2}\right\rangle$ and $\left\langle l, m_{1}\right| \hat{L}_{x}^{2}\left|l, m_{2}\right\rangle$;
(ii) spell out your results for diagonal matrix elements (with $m_{1}=m_{2}$ ) and their $y$-axis counterparts; and
(iii) calculate diagonal matrix elements $\langle l, m| \hat{L}_{x} \hat{L}_{y}|l, m\rangle$ and $\langle l, m| \hat{L}_{y} \hat{L}_{x}|l, m\rangle$.
5.25. For the state described by the common eigenket $|l, m\rangle$ of operators $\hat{L}_{z}$ and $\hat{L}^{2}$ in a reference frame $\{x, y, z\}$, calculate the expectation values $\left\langle L_{z^{\prime}}\right\rangle$ and $\left\langle L_{z^{\prime}}{ }^{2}\right\rangle$ in the reference frame whose axis $z^{\prime}$ forms angle $\theta$ with axis $z$.
5.26. Write down the matrices of the following angular momentum operators: $\hat{L}_{x}, \hat{L}_{y}, \hat{L}_{z}$, and $\hat{L}_{ \pm}$, in the $z$-basis of states with $l=1$.
5.27. Find the angular part of the orbital wavefunction of a particle with a definite value of $L^{2}$, equal to $6 \hbar^{2}$, and the largest possible value of $L_{x}$. What is this value?
5.28. ${ }^{*}$ A charged 2D particle is trapped in a soft in-plane potential well $U(x, y)=m \omega_{0}^{2}\left(x^{2}+y^{2}\right) / 2$. Calculate its energy spectrum in the presence of an additional uniform magnetic field $\mathcal{B}$, normal to the plane.
5.29. Calculate the spectrum of rotational energies of an axially-symmetric, rigid molecule.
5.30. For the state with wavefunction $\psi=C x y e^{-\lambda r}$, with a real, positive $\lambda$, calculate:
(i) the expectation values of observables $L_{x}, L_{y}, L_{z}$ and $L^{2}$, and
(ii) the normalization constant $C$.
5.31. An angular state of a spinless particle is described by the following ket-vector:

$$
\left.|\alpha\rangle=\frac{1}{\sqrt{2}}(l=3, m=0\rangle+|l=3, m=1\rangle\right) .
$$

Find the expectation values of the $x$ - and $y$-components of its angular momentum. Is it sensitive to a possible phase shift between two component eigenkets?
5.32. ${ }^{*}$ Simplify the following double commutator: $\hat{A}_{i j^{\prime}} \equiv\left[\hat{r}_{j},\left[\hat{L}^{2}, \hat{r}_{j^{\prime}}\right]\right.$.
5.33. Express the commutators listed in Eq. (206), $\left[\hat{J}^{2}, \hat{L}_{z}\right]$ and $\left[\hat{J}^{2}, \hat{S}_{z}\right]$, via $\hat{L}_{j}$ and $\hat{S}_{j}$.
5.34. Find the operator $\hat{\tau}_{\phi}$ describing the state rotation by angle $\phi$ about a certain axis, using the similarity of this operation with the shift of a Cartesian coordinate, discussed in Sec. 5. Then use it to calculate the probabilities of measurements of a beam of particles with $z$-polarized spin- $1 / 2$, by a SternGerlach instrument turned by angle $\theta$ within the $[z, x]$ plane (where $y$ is the axis of particle propagation - see Fig. 4.1). ${ }^{58}$
5.35. The rotation ("angle translation") operators $\hat{\tau}_{\phi}$, analyzed in the previous problem, and the coordinate translation operator $\hat{\tau}_{X}$, discussed in Sec. 5.5 of the lecture notes, have a similar structure:

$$
\hat{\tau}_{\lambda}=\exp \left\{-i \frac{\hat{C} \lambda}{\hbar}\right\}
$$

where $\lambda$ is a real $c$-number, characterizing shift's magnitude, and $\hat{C}$ is a Hermitian operator that does not explicitly depend on time.
(i) Prove that all such operators $\hat{\tau}_{\lambda}$ are unitary.
(ii) Prove that if the shift by $\lambda$, induced by operator $\hat{\tau}_{\lambda}$, leaves the Hamiltonian of some system unchanged for any $\lambda$, then the variable $C$, corresponding to the operator $\hat{C}$, is a constant of motion.
(iii) Discuss what does the last conclusion give for the particular operators $\hat{\gamma}_{X}$ and $\hat{\tau}_{\phi}$.
5.36. A particle is in a state $\alpha$ with the orbital wavefunction proportional to the spherical harmonic $Y_{1}^{1}(\theta, \varphi)$. Find the angular dependence of the wavefunctions corresponding to the following ket-vectors:
(i) $\hat{L}_{x}|\alpha\rangle$,
(ii) $\hat{L}_{y}|\alpha\rangle$,
(iii) $\hat{L}_{z}|\alpha\rangle$,
(iv) $\hat{L}_{+} \hat{L}_{-}|\alpha\rangle$, and (v) $\hat{L}^{2}|\alpha\rangle$.
5.37. For a state with definite quantum numbers $l$ and $j$, prove that observable $\mathbf{L} \cdot \mathbf{S}$ also has a definite value, and calculate this value.
5.38.* Derive the general recurrence relations for the Clebsh-Gordan coefficients.

Hint: Using the similarity of commutation relations, discussed in Sec. 7, generalize the solution of Problem 19 to all angular momentum operators, and apply them to Eq. (198).
5.39. The byproduct of the solution of the previous problem is the general relation for the spin operators (valid for any spin $s$ ), which may be rewritten as

[^635]$$
\left\langle m_{s} \pm 1\right| \hat{S}_{ \pm}\left|m_{s}\right\rangle=\hbar\left[\left(s \pm m_{s}+1\right)\left(s \mp m_{s}\right)\right]^{1 / 2}
$$
provided that all other quantum numbers are fixed. Use this result to spell out the matrices $\mathrm{S}_{x}, \mathrm{~S}_{y}, \mathrm{~S}_{z}$, and $\mathrm{S}^{2}$ of a particle with $s=1$, in the $z$-basis - defined as the basis in which the matrix $\mathrm{S}_{z}$ is diagonal.
5.40.* For a particle with spin $s$, moving in a spherically-symmetric field, find the ranges of possible values of quantum numbers $m_{j}$ and $j$, necessary to describe, in the coupled representation basis:
(i) all states with a definite quantum number $l$, and
(ii) a state with definite value of not only $l$, but also $m_{l}$ and $m_{s}$.

Give an interpretation of your results in terms of the classical geometric vector diagram (see Fig. 11).
5.41. A spin- $1 / 2$ particle moves in a centrally-symmetric potential $U(r)$. Using Eqs. (216) for the Clebsch-Gordan coefficients,
(i) write explicit expressions for the ket vectors for states that would be simultaneously the eigenstates of operators $\hat{L}^{2}, \hat{J}^{2}$, and $\hat{J}_{z}$, via spin eigenkets $|\uparrow\rangle$ and $|\downarrow\rangle$;
(ii) for each such state, find all the possible values of observables $L^{2}, L_{z}, S^{2}$, and $S_{z}$, the probability of each listed value, and the expectation value for each of the observables.
5.42. Taking into account electron's spin, find the energy spectrum of an electron, free to move within a plane, besides being placed into a uniform magnetic field $\mathbf{B}$, normal to the plane. Compare the result with the Landau level picture discussed in Sec. 3.2.

## Chapter 6. Perturbation Theories

This chapter discusses several perturbative approaches to problems of quantum mechanics, and their simplest applications including the Stark effect, the fine structure of atomic levels, and the Zeeman effect. Moreover, the discussion of the perturbation theory of transitions to continuous spectrum and the Golden Rule of quantum mechanics in the end of this chapter will naturally bring us to the issue of open quantum systems - to be discussed in more detail in the next chapter.

### 6.1. Eigenvalue/eigenstate problems

Unfortunately, only a few problems of quantum mechanics may be solved exactly in the analytical form. Actually, in the previous chapters we have solved a substantial fraction of such problems for a single particle, and for multi-particle problems the exactly solvable cases are even more rare. However, most practical problems of physics feature a certain small parameter, and this smallness may be exploited by various approximate analytical methods. Earlier in the course, we have explored one of them, the WKB approximation, which is adequate for a particle moving through a slowly changing potential profile. Now I will discuss alternative approaches that are more suitable for other cases. The historic name for these approaches is the perturbation theory, but it is more fair to speak about several such theories, because they differ depending on the type of the problem.

The simplest perturbation theories address eigenproblems for systems described by timeindependent Hamiltonians of the type

$$
\begin{equation*}
\hat{H}=\hat{H}^{(0)}+\hat{H}^{(1)}, \tag{6.1a}
\end{equation*}
$$

where the perturbation operator $\hat{H}^{(1)}$ is "small" - in the sense its addition to the unperturbed operator $\hat{H}^{(0)}$ results in a relatively small change of eigenvalues $E_{n}$ of the system. A typical problem of this type is the 1D weakly anharmonic oscillator (Fig. 1) described by Hamiltonian (1a) with

Weakly
anharmonic oscillator

$$
\begin{equation*}
\hat{H}^{(0)}=\frac{\hat{p}^{2}}{2 m}+\frac{m \omega_{0}^{2}}{2} \hat{x}^{2}, \quad \hat{H}^{(1)}=\alpha \hat{x}^{3}+\beta \hat{x}^{4}+\ldots \tag{6.1b}
\end{equation*}
$$

with small coefficients $\alpha, \beta, \ldots$
I will use the anharmonic oscillator as our first particular example, but let me start from describing the perturbative approach to the general time-independent Hamiltonian (1a). In the bra-ket formalism, the eigenproblem for the perturbed system is

$$
\begin{equation*}
\left(\hat{H}^{(0)}+\hat{H}^{(1)}\right)|n\rangle=E_{n}|n\rangle . \tag{6.2}
\end{equation*}
$$

Let the eigenstates and eigenvalues of the unperturbed Hamiltonian, which satisfy equation

$$
\begin{equation*}
\hat{H}^{(0)}\left|n^{(0)}\right\rangle=E_{n}^{(0)}\left|n^{(0)}\right\rangle \tag{6.3}
\end{equation*}
$$

be known. In this case, to solve problem (2) means to find, first, its perturbed eigenvalues $E_{n}$ and, second, coefficients $\left\langle n^{,(0)} \mid n\right\rangle$ of the expansion of perturbed state vectors $|n\rangle$ in series over the unperturbed ones, $\left|n^{,(0)}\right\rangle$ :


Fig. 6.1. The simplest problem for the perturbation theory application: a 1D weakly anharmonic oscillator. (Dashed lines characterize the unperturbed, harmonic oscillator.)

Let us plug Eq. (4), with the summation index $n$ ' replaced with $n$ ", into both parts of Eq. (2):

$$
\begin{equation*}
\sum_{n^{\prime \prime}}\left\langle n^{\prime \prime}(0) \mid n\right\rangle \hat{H}^{(0)}\left|n^{\prime \prime}(0)\right\rangle+\sum_{n^{\prime \prime}}\left\langle n^{\prime \prime}(0) \mid n\right\rangle \hat{H}^{(1)}\left|n^{\prime \prime}(0)\right\rangle=\sum_{n^{\prime \prime}}\left\langle n^{\prime \prime}(0) \mid n\right\rangle E_{n}\left|n^{\prime \prime(0)}\right\rangle, \tag{6.5}
\end{equation*}
$$

and then inner-multiply all terms by an arbitrary unperturbed bra-vector $\left\langle n^{,(0)}\right|$. Assuming that the system of unperturbed eigenstates is orthonormal, $\left\langle n^{,(0)} \mid n^{\prime(0)}\right\rangle=\delta_{n^{\prime} n^{\prime \prime}, \text {, and using Eq. (3) in the first term of the }}$ left-hand part, we get the following system of linear equations

$$
\begin{equation*}
\sum_{n^{\prime \prime}}\left\langle n^{\prime \prime(0)} \mid n\right\rangle H_{n^{\prime} n^{\prime \prime}}^{(1)}=\left\langle n^{\prime(0)} \mid n\right\rangle\left(E_{n}-E_{n^{\prime}}^{(0)}\right), \tag{6.6}
\end{equation*}
$$

where the matrix elements of the perturbation are calculated in unperturbed bra-kets:

$$
\begin{equation*}
H_{n^{\prime} n^{\prime \prime}}^{(1)} \equiv\left\langle n^{\prime(0)}\right| \hat{H}^{(1)}\left|n^{\prime \prime(0)}\right\rangle \tag{6.7}
\end{equation*}
$$

The linear equation system (6) is still exact, ${ }^{1}$ and is frequently used for numerical calculations. (Since the matrix coefficients (7) typically decrease when $n$ ' and/or $n$ " become very large, the sum in the left-hand part of Eq. (6) may be typically truncated, still giving acceptable accuracy of the solution.) For getting analytical results we need to make more explicit approximations. In the simple perturbation theory we are discussing now, this is achieved by the expansion of both eigenenergies and coefficients into the Taylor series in a certain small parameter $\mu$ of the problem:

$$
\begin{gather*}
E_{n}=E_{n}^{(0)}+E_{n}^{(1)}+E_{n}^{(2)} \ldots  \tag{6.8}\\
\left\langle n^{\prime(0)} \mid n\right\rangle=\left\langle n^{\prime(0)} \mid n\right\rangle^{(0)}+\left\langle n^{(0)} \mid n\right\rangle^{(1)}+\left\langle n^{\prime(0)} \mid n\right\rangle^{(2)} \ldots \tag{6.9}
\end{gather*}
$$

where ${ }^{2}$

$$
\begin{equation*}
E_{n}^{(k)} \propto\left\langle n^{\prime(0)} \mid n\right\rangle^{(k)} \propto \mu^{k} . \tag{6.10}
\end{equation*}
$$

[^636]In order to explore the $1^{\text {st }}$-order approximation, which ignores all terms $O\left(\mu^{2}\right)$ and higher, let us plug only the two first terms of expansions (8) and (9) into the basic system of equations (6):

$$
\begin{equation*}
\sum_{n^{\prime \prime}} H_{n^{\prime} n^{\prime \prime}}^{(1)}\left(\delta_{n^{\prime \prime} n}+\left\langle n^{\prime \prime}(0) \mid n\right\rangle^{(1)}\right)=\left(\delta_{n^{\prime} n}+\left\langle n^{(0)} \mid n\right\rangle^{(1)}\right)\left(E_{n}^{(0)}+E_{n}^{(1)}-E_{n^{\prime}}^{(0)}\right) . \tag{6.11}
\end{equation*}
$$

Now let us open the parentheses, and disregard all the remaining terms $O\left(\mu^{2}\right)$. The result is

$$
\begin{equation*}
H_{n^{\prime} n}^{(1)}=\delta_{n^{\prime} n} E_{n}^{(1)}+\left\langle n^{\prime(0)} \mid n\right\rangle^{(1)}\left(E_{n}^{(0)}-E_{n^{\prime}}^{(0)}\right), \tag{6.12}
\end{equation*}
$$

This equation is valid for any set of indices $n$ and $n$ '; let us start from the case $n=n$ ' and immediately get a very simple (and the most important!) result:
$1^{\text {st }}$ - order correction energies

$$
\begin{equation*}
E_{n}^{(1)}=H_{n n}^{(1)} \equiv\left\langle n^{(0)}\right| \hat{H}^{(1)}\left|n^{(0)}\right\rangle . \tag{6.13}
\end{equation*}
$$

For example, let us see what does this result give for two first perturbation terms in the weakly anharmonic oscillator (1b)

$$
\begin{equation*}
E_{n}^{(1)}=\alpha\left\langle n^{(0)}\right| \hat{X}^{3}\left|n^{(0)}\right\rangle+\beta\left\langle n^{(0)}\right| \hat{X}^{4}\left|n^{(0)}\right\rangle . \tag{6.14}
\end{equation*}
$$

As the reader should know from the solution of Problem 5.6, the first term is zero, while the second one yields ${ }^{3}$

$$
\begin{equation*}
E_{n}^{(1)}=\frac{3}{4} \beta x_{0}^{4}\left(2 n^{2}+2 n+1\right) . \tag{6.15}
\end{equation*}
$$

Naturally, there should be some contribution from the (typically, larger) term proportional to $\alpha$, so we need to explore the $2^{\text {nd }}$ approximation of the perturbation theory. However, before doing that, let us complete our discussion of its $1^{\text {st }}$ order. For $n^{\prime} \neq n$, Eq. (12) may be used to calculate the eigenstates rather than the eigenvalues:

$$
\begin{equation*}
\left\langle n^{\prime(0)} \mid n\right\rangle^{(1)}=\frac{H_{n^{\prime} n}^{(1)}}{E_{n}^{(0)}-E_{n^{\prime}}^{(0)}}, \quad \text { for } n^{\prime} \neq n . \tag{6.16}
\end{equation*}
$$

This means that the eigenket's expansion (4), in the $1^{\text {st }}$ order, may be represented as
vectors

$$
\begin{equation*}
\left|n^{(1)}\right\rangle=\sum_{n^{\prime} \neq n} \frac{H_{n^{\prime} n}^{(1)}}{E_{n}^{(0)}-E_{n^{\prime}}^{(0)}}\left|n^{\prime(0)}\right\rangle+C\left|n^{(0)}\right\rangle . \tag{6.17}
\end{equation*}
$$

Coefficient $C$ cannot be found from Eq. (12), however, requiring the final state $n$ to be normalized, we see that other terms may provide only corrections $O\left(\mu^{2}\right)$, so in the $1^{\text {st }}$ order we should take $C=1$. The
${ }^{3}$ The result for $n=0$ may be readily calculated in the wave-mechanics style as well, using Eq. (2.269) for unperturbed ground state wavefunction, and the table integral MA Eq. (6.9d):

$$
\left\langle n^{(0)}\right| \hat{x}^{4}\left|n^{(0)}\right\rangle_{n=0}=\int\left(\psi_{0}^{(0)}\right)^{*} x^{4} \psi_{0}^{(0)} d x=\left(\frac{1}{\pi x_{0}}\right)^{1 / 2} \int_{-\infty}^{+\infty} x^{4} \exp \left\{-\frac{x^{2}}{x_{0}^{2}}\right\} d x=\frac{3}{4} x_{0}^{4},
$$

but for higher values of $n$, such calculations are much harder, because of more involved Eq. (2.279) for $\psi_{n}^{(0)}$. Note also that at $n \gg 1$, Eq. (15) gives predictions which coincide with those of the classical theory of weakly nonlinear oscillations - see, e.g., CM Sec. 4.2, in particular, Eq. (4.49).
most important feature of Eq. (17) is its denominator: the closer the (unperturbed) eigenenergies of two states, the larger is their mutual contribution (hybridization), created by the perturbation.

This feature also affects the $1^{\text {st }}$ approximation's validity condition that may be quantified using Eq. (16): the magnitudes of all the bra-kets it describes have to be much less then the unperturbed product $\langle n \mid n\rangle^{(0)}=1$, so that all elements of the perturbation matrix have to be much less that the difference between the corresponding unperturbed energies. For the anharmonic oscillator's energy correction (15), this requirement is reduced to $E_{n}{ }^{(1)} \ll \hbar \omega_{0}$.

Now we are ready for going after the $2^{\text {nd }}$ second order approximation to Eq. (6). Let us focus on the case $n^{\prime}=n$, because as we already know, only this term will give us a correction to eigenenergies. Moreover, we see that since the left-hand side of Eq. (6) already has the small factor $H^{(1)}{ }_{n^{\prime} n^{n}} \propto \mu$, the bra-ket coefficients in that part may be taken from the $1^{\text {st }}$ order result (16). As a result, we get

$$
\begin{equation*}
E_{n}^{(2)}=\sum_{n^{\prime \prime}}\left\langle n^{\prime \prime}(0) \mid n\right\rangle^{(1)} H_{n n^{\prime \prime}}^{(1)}=\sum_{n^{\prime \prime} \neq n} \frac{H_{n^{\prime \prime} n}^{(1)} H_{n n^{\prime \prime}}^{(1)}-E_{n^{\prime \prime}}^{(0)}}{E_{n}^{(0)} .} \tag{6.18}
\end{equation*}
$$

Since $\hat{H}^{(1)}$ represents an observable (energy), and hence has to be Hermitian, we may rewrite this expression as

$$
E_{n}^{(2)}=\sum_{n^{\prime} \neq n} \frac{\left|H_{n^{\prime} n}^{(1)}\right|^{2}}{E_{n}^{(0)}-E_{n^{\prime}}^{(0)}}=\sum_{n^{\prime} \neq n} \frac{\left.\left|\left\langle n^{\prime(0)}\right| \hat{H}^{(1)}\right| n^{(0)}\right\rangle\left.\right|^{2}}{E_{n}^{(0)}-E_{n^{\prime}}^{(0)}} .
$$

This is the much celebrated $2^{\text {nd }}$ order perturbation result that frequently (in sufficiently symmetric problems) is the first nonvanishing correction to the state energy - for example, from the cubic term (proportional to $\alpha$ ) in our weakly anharmonic oscillator problem (1). In order to calculate the corresponding correction, we may use another result of Problem 5.6:

$$
\begin{align*}
& \left\langle n^{\prime}\right| \hat{X}^{3}|n\rangle=\left(\frac{x_{0}}{\sqrt{2}}\right)^{3}  \tag{6.20}\\
& \times\left\{[n(n-1)(n-2)]^{1 / 2} \delta_{n^{\prime}, n-3}+3 n^{3 / 2} \delta_{n^{\prime}, n-1}+3(n+1)^{3 / 2} \delta_{n^{\prime}, n+1}+[(n+1)(n+2)(n+3)]^{1 / 2} \delta_{n^{\prime}, n+3}\right\} .
\end{align*}
$$

So, according to Eq. (19), we need to calculate

$$
\begin{align*}
& E_{n}^{(2)}=\alpha^{2}\left(\frac{x_{0}}{\sqrt{2}}\right)^{6} \\
& \times \sum_{n^{\prime} \neq n} \frac{\left[[n(n-1)(n-2)]^{1 / 2} \delta_{n^{\prime}, n-3}+3 n^{3 / 2} \delta_{n^{\prime}, n-1}+3(n+1)^{3 / 2} \delta_{n^{\prime}, n+1}+[(n+1)(n+2)(n+3)]^{1 / 2} \delta_{n^{\prime}, n+3}\right\}^{2}}{\hbar \omega_{0}\left(n-n^{\prime}\right)} \tag{6.21}
\end{align*}
$$

The summation is actually not as cumbersome as may look, because all mixed products are proportional to different Kronecker deltas and hence vanish, so that we need to sum up only the squares of each term:

$$
\begin{align*}
E_{n}^{(2)} & =\frac{\alpha^{2}}{\hbar \omega_{0}}\left(\frac{x_{0}}{\sqrt{2}}\right)^{6}\left[\frac{n(n-1)(n-2)}{3}+\frac{9 n^{3}}{1}+\frac{9(n+1)^{3}}{-1}+\frac{(n+1)(n+2)(n+3)}{-3}\right]  \tag{6.22}\\
& =-\frac{15}{4} \frac{\alpha^{2} x_{0}^{6}}{\hbar \omega_{0}}\left(n^{2}+n+\frac{11}{30}\right) .
\end{align*}
$$

Please notice that all energy level corrections are negative, regardless of the sign of $\alpha$. On the contrary, the $1^{\text {st }}$ order correction $E_{n}{ }^{(1)}(15)$ depends on the sign of parameter $\beta$, so that the net correction, $E_{n}{ }^{(1)}+E_{n}{ }^{(2)}$, may be of any sign.

Results (17) and (19) are clearly inapplicable to the degenerate case where, in the absence of perturbation, several states correspond to the same energy level, because of the divergence of their denominators. ${ }^{4}$ This divergence hints that the largest effect of the perturbation in that case is the degeneracy lifting, e.g., splitting of the initially degenerate energy level $E^{(0)}$ (Fig. 2), and that for the analysis of this case we can, to the first approximation, ignore the effect of all other energy levels. (A careful analysis shows that this is indeed the case until the level splitting becomes comparable with the distance to other energy levels.)

$$
\hat{H}=\hat{H}^{(0)} \quad \hat{H}=\hat{H}^{(0)}+\hat{H}^{(1)}
$$

Fig. 5.2. Lifting the energy level degeneracy by a perturbation (schematically).

Limiting the summation in Eq. (6) to the group of $N$ degenerate states with equal $E_{n}{ }^{(0)} \equiv E^{(0)}$, we reduce it to

$$
\begin{equation*}
\sum_{n^{\prime \prime}=1}^{N}\left\langle n^{\prime \prime(0)} \mid n\right\rangle H_{n^{\prime} n^{\prime \prime}}^{(1)}=\left\langle n^{\prime(0)} \mid n\right\rangle\left(E_{n}-E^{(0)}\right) . \tag{6.23}
\end{equation*}
$$

where $n$ ' and $n "$ number $N$ states of the degenerate group. ${ }^{5}$ For $n=n$ ', Eq. (23) may be rewritten as

$$
\begin{equation*}
\sum_{n^{\prime \prime}=1}^{N}\left\langle n^{\prime \prime}(0) \mid n^{\prime}\right\rangle\left(H_{n^{\prime} n^{\prime \prime}}^{(1)}-E_{n^{\prime \prime}}^{(1)} \delta_{n^{\prime} n^{\prime \prime}}\right)=0, \quad \text { where } E_{n}^{(1)} \equiv E_{n}-E^{(0)} \tag{6.24}
\end{equation*}
$$

For each $n=1,2, \ldots N$, this is a system of $N$ linear, homogenous equations (with $N$ terms each) for unknown coefficients $\left\langle n^{\prime(0)} \mid n^{\prime}\right\rangle$. In this problem, we readily recognize the problem of diagonalization of the perturbation matrix $\mathrm{H}^{(1)}$ - cf. Sec. 4.4 and in particular Eq. (4.101). As in the general case, in the condition of self-consistency of the system, we can change the notation of the lower index of $E^{(1)}$, for example to $n$ :

[^637]According to the definition (24) of $E_{n}{ }^{(1)}$, the resulting $N$ energy levels $E_{n}$ may be found as $E^{(0)}+E_{n}{ }^{(1)}$, where $E_{n}{ }^{(1)}$ are the $N$ roots of Eq. (25).

If the perturbation matrix is diagonal, the result is extremely simple,

$$
\begin{equation*}
E_{n}-E^{(0)} \equiv E_{n}^{(1)}=H_{n n}^{(1)}, \tag{6.26}
\end{equation*}
$$

and formally coincides with Eq. (13) for the non-degenerate case, but now may give a different result for each of $N$ previously degenerate states $n$.

Let us see what does this theory give for several important examples. First of all, let us consider a two-level system (or a system with two degenerate states with energy far from all others levels), with an arbitrary perturbation matrix ${ }^{6}$

$$
\mathrm{H}^{(1)}=\left(\begin{array}{ll}
H_{11} & H_{12}  \tag{6.27a}\\
H_{21} & H_{22}
\end{array}\right) .
$$

Since that both the unperturbed Hamiltonian and the operator of its perturbation are Hermitian, the diagonal elements of matrix $\mathrm{H}^{(1)}$ are real, and its off-diagonal elements are complex conjugates of each other. As a result, we can present the matrix in the same form as in Eq. (4.106):

$$
\mathrm{H}^{(1)}=\left(\begin{array}{cc}
a_{0}+a_{z} & a_{x}-i a_{y}  \tag{6.27b}\\
a_{x}+i a_{y} & a_{0}-a_{z}
\end{array}\right)=a_{0} \mathrm{I}+a_{x} \sigma_{x}+a_{y} \sigma_{y}+a_{z} \sigma_{z}=a_{0} \mathrm{I}+\mathbf{a} \cdot \boldsymbol{\sigma} .
$$

where scalar $a_{0}$ and the Cartesian components of vector a are real c-number coefficients. The corresponding characteristic equation,

$$
\left|\begin{array}{cc}
a_{0}+a_{z}-E_{n}^{(1)} & a_{x}-i a_{y}  \tag{6.28}\\
a_{x}+i a_{y} & a_{0}-a_{z}-E_{n}^{(1)}
\end{array}\right|=0
$$

has the solution that is familiar to the reader from Chapters 2 and 4:

$$
\begin{equation*}
E_{ \pm}^{(1)} \equiv E_{ \pm}-E^{(0)}=a_{0} \pm a=a_{0} \pm\left(a_{x}^{2}+a_{y}^{2}+a_{z}^{2}\right)^{1 / 2}=\frac{H_{11}+H_{22}}{2} \pm\left[\left(\frac{H_{11}-H_{22}}{2}\right)^{2}+H_{12} H_{21}\right]^{1 / 2} \tag{6.29}
\end{equation*}
$$

Let us discuss physics of this simple result. Parameter $a_{0}=\left(H_{11}+H_{22}\right) / 2$ is evidently the correction to the average energy of both states, that does not give any contribution to the level splitting. The splitting, $\Delta E=E_{+}-E_{-}$, is a hyperbolic function of coefficient $a_{z}=\left(\mathrm{H}_{11}-\mathrm{H}_{22}\right) / 2$ that describes the direct contributions (13) to the eigenstates due to the perturbation. A plot of this function is the famous level-anticrossing diagram (Fig. 3) that has already been discussed in Sec. 2.5 in a particular context of the weak potential limit of the 1D band theory - see Fig. 2.29.

Now we see that this is a general result for any two-level system. The examples of this behavior that we already know include the coupled quantum wells (see Fig. 2.29 and its discussion), band theory in the weak coupling limit (Sec. 2.5), and spin $-1 / 2$ systems discussed through Chapter 4 and in Sec. 5.1. By the way, from Sec. 4.4 we already know the perturbed states in the middle of the anticrossing

[^638]diagram (at $a_{z}=0$ ). For example, if $a_{y}=0$, then our perturbation Hamiltonian matrix (27), besides the trivial term proportional to $a_{0}$, is proportional to $\sigma_{x}$, and hence we can use the result (4.114) to write: ${ }^{7}$
where $1^{(0)}$ and $2^{(0)}$ are system's states in the absence of the perturbation.


Fig. 6.3. Level-anticrossing diagram for an arbitrary two-level system.

This analysis shows that other results of our discussions of particular two-level systems in Sec. 2.6 and 4.6 are also general. For example, if we put such any two-level system into an initial state different from one of the eigenstates $\pm$, the probability of its finding it in any of states $1^{(0)}$ or $2^{(0)}$ will oscillate with frequency

$$
\begin{equation*}
\Omega=\frac{\Delta E}{\hbar} \equiv \frac{E_{+}-E_{-}}{\hbar} . \tag{6.31}
\end{equation*}
$$

Hence, for a spin- $1 / 2$ particle in a $z$-oriented magnetic field, the periodic oscillations of the $x$ - and $y$ components of spin vector, described by Eqs. (4.196) and (4.202), may be interpreted not only as the torque-induced precession of spin within the $[x, y]$ plane, but alternatively as the quantum oscillations of the of the z-component of spin between states $\uparrow$ and $\downarrow$ with energies $E \uparrow$ and $E \downarrow$ given by Eq. (4.167).

Some other examples of such oscillations may be rather unexpected. For example, the ammonium molecule $\mathrm{NH}_{3}$ (Fig. 4) has two symmetric states which differ by the inversion of the nitrogen atom relative to the plane of the three hydrogen atoms, and are coupled due to quantummechanical tunneling of the nitrogen atom through the plane of hydrogen atoms. ${ }^{8}$ Since for this molecule, the level splitting $\Delta E$ corresponds to an experimentally convenient frequency $\Omega / 2 \pi \approx 24 \mathrm{GHz}$, it played an important historic role for the initial development of first atomic frequency standards and microwave quantum generators (masers) in the 1950s, ${ }^{9}$ which paved the way toward the development of the laser technology.

[^639]

Fig. 6.4. Ammonia molecule and its inversion.

### 6.2. The Stark effect

Another example of the level degeneracy lifted by a perturbation is the linear Stark effect atomic level splitting by an external electric field. Let us study this effect, in the linear approximation, for a hydrogen-like atom. Taking the direction of external electric field $\varepsilon$ (which is practically uniform on the atomic scale) for the $z$-axis, the perturbation may be represented by the following Hamiltonian: ${ }^{10}$

$$
\begin{equation*}
\hat{H}^{(1)}=-q \varepsilon \hat{\mathbf{z}}=-q \varepsilon r \cos \theta \tag{6.32}
\end{equation*}
$$

(Since we will work in the coordinate representation, we may skip the operator sign from this point on.)
As you (should :-) remember, energy levels of a hydrogen-like atom depend only on the main quantum number $n$ - see Eq. (3.191); hence all states but the ground state $n=1$ (" $1 s$ " in the spectroscopic nomenclature) in which $l=m=0$, have some degeneracy that grows rapidly with $n$. This is why I will carry out the calculations only for the lowest degenerate level with $n=2$. Since generally 0 $\leq l \leq n-1$, here $l$ may be equal either 0 (one $2 s$ state, with $m=0$ ) or 1 (three $2 p$ states, with $m=0, \pm 1$ ). Due to this 4 -fold degeneracy, $\mathrm{H}^{(1)}$ is a $4 \times 4$ matrix with 16 elements:

$$
\begin{align*}
& \overbrace{m=0}^{l=0} \overbrace{m=0 m=+1 m=-1}^{l=1} \\
& \mathrm{H}^{(1)}=  \tag{6.33}\\
&\left(\begin{array}{llll}
H_{11} & H_{12} & H_{13} & H_{14} \\
H_{21} & H_{22} & H_{23} & H_{24} \\
H_{31} & H_{32} & H_{33} & H_{34} \\
H_{41} & H_{42} & H_{43} & H_{44}
\end{array}\right) \begin{array}{l}
m=0, \\
m=0, \\
m=+1, \\
m=-1,
\end{array} \quad l=0,
\end{align*}
$$

However, please do not be scared. First, due to the Hermitian character of the operator, only 10 of the matrix elements ( 4 diagonal ones and 6 off-diagonal elements) may be substantially different. Moreover, due to a high symmetry of the problem, there are a lot of zeros even among these elements. Indeed, let us have a look at the angular components $Y_{l}^{m}$ of the corresponding wavefunctions, described by Eqs. (3.174)-(3.175). For states with $m= \pm 1$, the azimuthal parts of wavefunctions are proportional to $\exp \{ \pm i \varphi\}$; hence the off-diagonal elements $H_{34}$ and $H_{43}$ of matrix (33), relating these functions, are proportional to

[^640]\[

$$
\begin{equation*}
\oint d \Omega Y_{1}^{ \pm^{*}} \hat{H}^{(1)} Y_{1}^{\mp} \propto \int_{0}^{2 \pi} d \varphi\left(e^{ \pm i \varphi}\right)^{*}\left(e^{\mp i \varphi}\right)=0 . \tag{6.34}
\end{equation*}
$$

\]

The azimuthal-angle symmetry also kills the off-diagonal elements $H_{13}, H_{14}, H_{23}, H_{24}$ (and hence their complex conjugates $H_{31}, H_{41}, H_{32}$, and $H_{42}$ ), because they relate states with $m=0$ and $m \neq 0$, and are proportional to

$$
\begin{equation*}
\oint d \Omega Y_{1}^{0^{*}} \hat{H}^{(1)} Y_{1}^{ \pm 1} \propto \int_{0}^{2 \pi} d \varphi e^{ \pm i \varphi}=0 . \tag{6.35}
\end{equation*}
$$

For the diagonal elements $H_{33}$ and $H_{44}$, corresponding to $m= \pm 1$, the azimuthal-angle integral does not vanish, but since the spherical functions depend on the polar angle as $\sin \theta$, the matrix elements are proportional to

$$
\begin{equation*}
\oint d \Omega Y_{1}^{ \pm^{*}} \hat{H}^{(1)} Y_{1}^{ \pm} \propto \int_{0}^{\pi} \sin \theta d \theta \sin \theta \cos \theta \sin \theta=\int_{-1}^{+1} \cos \theta\left(1-\cos ^{2} \theta\right) d(\cos \theta) \tag{6.36}
\end{equation*}
$$

i.e. are equal to zero as any limit-symmetric integral of an odd function. Finally, for states $2 s$ and $2 p$ with $m=0$, the diagonal elements $H_{11}$ and $H_{22}$ are also killed by the polar-angle integration:

$$
\begin{align*}
& \oint d \Omega Y_{0}^{0^{*}} \hat{H}^{(1)} Y_{0}^{0} \propto \int_{0}^{\pi} \sin \theta d \theta \cos \theta=\int_{-1}^{1} \cos \theta d(\cos \theta)=0  \tag{6.37a}\\
& \oint d \Omega Y_{0}^{1^{*}} \hat{H}^{(1)} Y_{0}^{1} \propto \int_{0}^{\pi} \sin \theta d \theta \cos ^{3} \theta=\int_{-1}^{+1} \cos ^{3} \theta d(\cos \theta)=0 \tag{6.37b}
\end{align*}
$$

Hence, the only nonvanishing matrix elements are two off-diagonal elements $H_{12}$ and $H_{21}$ relating different states with $m=0$, because they are proportional to

$$
\begin{equation*}
\oint d \Omega Y_{0}^{0^{*}} \cos \theta Y_{1}^{0}=\frac{\sqrt{3}}{4 \pi} \int_{0}^{2 \pi} d \varphi \int_{0}^{\pi} \sin \theta d \theta \cos ^{2} \theta=\frac{1}{\sqrt{3}} \neq 0 . \tag{6.38}
\end{equation*}
$$

What remains is to use Eqs. (3.199) for the radial parts of these functions to finish the calculation of those two matrix elements:

$$
\begin{equation*}
H_{12}=H_{21}=-\frac{q \varepsilon}{\sqrt{3}} \int_{0}^{\infty} r^{2} d r R_{2,0}(r) r R_{2,1}(r) \tag{6.39}
\end{equation*}
$$

where the radial functions are given by Eqs. (3.199). Due to the structure of function $R_{2,0}(r)$, the integral falls into a sum of two parts, both of the type we have already met. ${ }^{11}$ The final result is

$$
\begin{equation*}
H_{12}=H_{21}=3 q \varepsilon r_{0}, \tag{6.40}
\end{equation*}
$$

where $r_{0}$ is the radius scale given by Eq. (3.183); for the hydrogen atom it is just the Bohr radius $r_{\mathrm{B}}$ (1.13).

Thus, for our case the perturbation matrix (33) is reduced to

[^641]\[

\mathrm{H}^{(1)}=\left($$
\begin{array}{cccc}
0 & 3 q \varepsilon r_{0} & 0 & 0  \tag{6.41}\\
3 q \varepsilon r_{0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array}
$$\right)
\]

so that the condition (25) of self-consistency is

$$
\left|\begin{array}{cccc}
-E_{n}^{(1)} & 3 q \varepsilon r_{0} & 0 & 0  \tag{6.42}\\
3 q \varepsilon r_{0} & -E_{n}^{(1)} & 0 & 0 \\
0 & 0 & -E_{n}^{(1)} & 0 \\
0 & 0 & 0 & -E_{n}^{(1)}
\end{array}\right|=0
$$

giving a very simple characteristic equation

$$
\begin{equation*}
\left(E_{n}^{(1)}\right)^{2}\left[\left(E_{n}^{(1)}\right)^{2}-\left(3 q \varepsilon r_{0}\right)^{2}\right]=0 . \tag{6.43}
\end{equation*}
$$

with the roots

$$
\begin{equation*}
E_{1,2}^{(1)}=0, \quad E_{3,4}^{(1)}= \pm 3 q \varepsilon r_{0} \tag{6.44}
\end{equation*}
$$

Linear
Stark
effect
for $n=2$
so that the degeneracy is only partly lifted - see Fig. 5.


Fig. 6.5. Linear Stark effect for level $n$ $=2$ of a hydrogen-like atom.

Generally, in order to understand the nature of states corresponding to these levels, we should go back to Eq. (24) with each calculated value of $E_{n}{ }^{(1)}$, and calculate the corresponding expansion coefficients $\left\langle n "{ }^{(0)} \mid n\right\rangle$, which describe the perturbed states. However, in our simple case the outcome of the procedure is clear in advance. Indeed, since the states with $m= \pm 1$ are not affected by the perturbation (in the linear approximation in electric field), their degeneracy is not lifted, and energy unaffected - see the middle level in Fig. 5. On the other hand, the perturbation matrix connecting states $2 s$ and $2 p$, i.e. the top left $2 \times 2$ part of the full matrix (41), is proportional to the Pauli matrix $\sigma_{x}$, and we already know the result of its diagonalization - see Eqs. (4.114). This means that the upper and lower split levels correspond to very simple linear combinations of the previously degenerate states,
both with $m=0$.

Finally, let us estimate the magnitude of the linear Stark effect for a hydrogen atom. For a very high electric field of $\mathcal{E}=3 \times 10^{6} \mathrm{~V} / \mathrm{m},{ }^{12} q=e \approx 1.6 \times 10^{-19} \mathrm{C}$, and $r_{0}=r_{\mathrm{B}} \approx 0.5 \times 10^{-10} \mathrm{~m}$, we get a level splitting of $3 q \delta_{0} \approx 0.8 \times 10^{-22} \mathrm{~J} \approx 0.5 \mathrm{meV}$. This number is much lower than the unperturbed energy of the level, $E_{2}=-E_{H} / 2 \times 2^{2} \approx-3.4 \mathrm{eV}$, so that the perturbation result is quite valid. On the other hand, the splitting is much larger than the resolution limit imposed by the natural linewidth $\left(\sim 10^{-7} E_{2}\right.$, see Chapter 9 ), so that the effect is quite observable even in substantially lower electric fields.

### 6.3. Fine structure of atomic levels

Now let us analyze, for the simplest case of a hydrogen-like atom, the so-called fine structure of atomic levels - their degeneracy lifting even in the absence of external fields. In the limit when the effective speed $v$ of electron motion is much smaller than the speed of light $c$ (as it is in the hydrogen atom), the fine structure may be analyzed as a sum of two small relativistic effects. To analyze the first of these effects, let us expand the well-known classical relativistic expression ${ }^{13}$ for the kinetic energy $T$ $=E-m c^{2}$ of a free particle with the rest mass $m$,

$$
\begin{equation*}
T=\left(m^{2} c^{4}+p^{2} c^{2}\right)^{1 / 2}-m c^{2}=m c^{2}\left[\left(1+\frac{p^{2}}{m^{2} c^{2}}\right)^{1 / 2}-1\right], \tag{6.46}
\end{equation*}
$$

into the Taylor series with respect to the small ratio $(p / m c)^{2} \approx(v / c)^{2}$ :

$$
\begin{equation*}
T=m c^{2}\left[1+\frac{1}{2}\left(\frac{p}{m c}\right)^{2}-\frac{1}{8}\left(\frac{p}{m c}\right)^{4}+\ldots-1\right]=\frac{p^{2}}{2 m}-\frac{p^{4}}{8 m^{3} c^{2}}+\ldots \tag{6.47}
\end{equation*}
$$

and neglect all the terms besides the first (non-relativistic) one and the next term representing the first nonvanishing relativistic correction of $T$.

In accordance with the correspondence principle, the quantum-mechanical problem in this approximation may be described by the perturbative Hamiltonian (1a), where the unperturbed (nonrelativistic) Hamiltonian of the problem, whose eigenstates and eigenenergies were discussed in Sec. 3.5 , is

$$
\begin{equation*}
\hat{H}^{(0)}=\frac{\hat{p}^{2}}{2 m}+\hat{U}(r), \quad \hat{U}(r)=-\frac{C}{r}, \tag{6.48}
\end{equation*}
$$

while the small kinetic-relativistic perturbation is

Kineticrelativistic perturbation

$$
\begin{equation*}
\hat{H}^{(1)}=-\frac{\hat{p}^{4}}{8 m^{3} c^{2}}=-\frac{1}{2 m c^{2}}\left(\frac{\hat{p}^{2}}{2 m}\right)^{2} \tag{6.49a}
\end{equation*}
$$

Using Eq. (48), we may rewrite the last formula as

[^642]\[

$$
\begin{equation*}
\hat{H}^{(1)}=-\frac{1}{2 m c^{2}}\left(\hat{H}^{(0)}-\hat{U}(r)\right)^{2}, \tag{6.49b}
\end{equation*}
$$

\]

so that its matrix elements, participating in the characteristic equation (25) for a given degenerate energy level (3.191), i.e. a given principal quantum number $n$, are

$$
\begin{equation*}
\langle n \operatorname{lm}| \hat{H}^{(1)}\left|n l^{\prime} m^{\prime}\right\rangle=-\frac{1}{2 m c^{2}}\langle n \operatorname{lm}|\left(\hat{H}^{(0)}-\hat{U}(r)\right)\left(\hat{H}^{(0)}-\hat{U}(r)\right)\left|n l^{\prime} m^{\prime}\right\rangle, \tag{6.50}
\end{equation*}
$$

where the bra- and ket vectors describe the unperturbed eigenstates whose eigenfunctions (in the coordinate representation) are given by Eq. (3.190): $\psi_{n, l, m}=R_{n, l}(r) Y_{l}^{m}(\theta, \varphi)$.

It is straightforward (and hence left for the reader :-) to prove that all off-diagonal elements of the set (50) are equal to 0 . Thus we may use Eq. (26) for each set of quantum numbers $\{n, l, m\}$ :

$$
\begin{align*}
E_{n, l, m}^{(1)} & \equiv E_{n, l, m}-E_{n}^{(0)}=\langle n \operatorname{lm}| \hat{H}^{(1)}|n l m\rangle=-\frac{1}{2 m c^{2}}\left\langle\left(\hat{H}^{(0)}-\hat{U}(r)\right)^{2}\right\rangle_{n, l, m} \\
& =-\frac{1}{2 m c^{2}}\left(E_{n}^{2}-2 E_{n}\langle\hat{U}\rangle_{n, l}+\left\langle\hat{U}^{2}\right\rangle_{n, l}\right)=-\frac{1}{2 m c^{2}}\left[\frac{E_{0}^{2}}{4 n^{4}}-\frac{E_{0}}{n^{2}} C\left\langle\frac{1}{r}\right\rangle_{n, l}+C^{2}\left\langle\frac{1}{r^{2}}\right\rangle_{n, l}\right], \tag{6.51}
\end{align*}
$$

where index $m$ has been dropped, because the radial wavefunctions $R_{n, l}(r)$, which affect the averages, do not depend on that quantum number. Now using Eqs. (3.183), (3.191) and the first two of Eqs. (3.201), we finally get

$$
\begin{equation*}
E_{n, l}^{(1)}=-\frac{m C^{2}}{2 \hbar^{2} c^{2} n^{4}}\left(\frac{n}{l+1 / 2}-\frac{3}{4}\right)=-\frac{2 E_{n}^{2}}{m c^{2}}\left(\frac{n}{l+1 / 2}-\frac{3}{4}\right) . \tag{6.52}
\end{equation*}
$$

Let us discuss this result. First of all, its last form confirms that that correction (52) is indeed much smaller than the unperturbed energy $E_{n}$ (and hence the perturbation theory is solid) if the latter is much smaller than the relativistic rest energy $m c^{2}$ of the particle. Next, since in the Bohr problem $n \geq l+$ 1, the first fraction in the parentheses of Eq. (52) is always larger than 1, so that the relativistic correction to kinetic energy is negative for all $n$ and $l$. (This is already evident from Eqs. (6.49), which show that the correction Hamiltonian is a negatively defined form.) Finally, at a fixed principal number $n$, the negative correction's magnitude decreases with the growth of $l$. This fact may be classically interpreted using Eq. (3.200): the larger is $l$ (at fixed $n$ ), the smaller is particle's average distance from the center, and hence the smaller is its effective velocity, the smaller is the magnitude of the quantummechanical average of the negative relativistic correction (49a) to the kinetic energy.

Result (52) is conceptually valid for any physics of interaction $U(r)=-C / r$. However, if the interaction is Coulombic, say between an electron with charge $(-e)$ and a nucleus of charge $(+Z e)$, there is also another relativistic correction to energy, due to the so-called spin-orbit interaction. Its physics may be understood from the following semi-qualitative, classical reasoning: from the "the point of view" of an electron rotating about the nucleus at constant distance $r$ with velocity $v$, it is the nucleus, of charge $Z e$, that rotates about the electron with velocity $(-v)$ and hence time period $T=2 \pi r / v$. From the point of view of magnetostatics, such circular motion of electric charge $Q=Z e$ is equivalent to the
constant circular electric current $I=Q v=(Z e)(v / 2 \pi r)$ which creates, at electron's location, i.e. in the center of the current loop, a magnetic field with magnitude ${ }^{14}$

$$
\begin{equation*}
\mathcal{B}_{a}=\frac{\mu_{0}}{2 r} I=\frac{\mu_{0}}{2 r} \frac{Z e v}{2 \pi r}=\frac{\mu_{0} Z e v}{4 \pi r^{2}} . \tag{6.53}
\end{equation*}
$$

The field's direction $\mathbf{n}$ is perpendicular to the apparent plane of the nucleus' rotation (i.e. that of the real rotation of the electron), and hence its vector may be readily expressed via the similarly directed vector $\mathbf{L}$ of electron's angular (orbital) momentum:

$$
\begin{equation*}
\mathcal{B}_{a}=\frac{\mu_{0} Z e v}{4 \pi r^{2}} \mathbf{n}=\frac{\mu_{0} Z e}{4 \pi r^{3} m_{e}} m_{e} v r \mathbf{n}=\frac{\mu_{0} Z e}{4 \pi r^{3} m_{e}} \mathbf{L}=\frac{Z e}{4 \pi \varepsilon_{0} r^{3} m_{e} c^{2}} \mathbf{L} \tag{6.54}
\end{equation*}
$$

where the last transition is due to the basic relation between the SI unit constants: $\mu_{0} \equiv 1 / \varepsilon_{0} c^{2}$.
A more careful (but still classical) analysis of the problem ${ }^{15}$ brings both good and bad news. The bad news is that result (54) is wrong by a factor of 2 even for the circular motion, because the electron moves with acceleration, and the reference frame bound to its cannot be considered inertial (as was implied in the above reasoning), so that the actual magnetic field felt by the electron is

$$
\begin{equation*}
\boldsymbol{B}=\frac{Z e}{8 \pi \varepsilon_{0} r^{3} m_{e} c^{2}} \mathbf{L} . \tag{6.55}
\end{equation*}
$$

The good news is that, so corrected, the result is valid (on the average) for not only circular but arbitrary (elliptic ${ }^{16}$ ) orbital motion in the Coulomb field $U(r)$. Hence from the discussion in Sec. 4.1 and Sec. 4.4 we may expect that the quantum-mechanical description of the interaction between this apparent magnetic field and electron's spin moment (4.116) is given by the following perturbation Hamiltonian

$$
\begin{equation*}
\hat{H}^{(1)}=-\hat{\boldsymbol{\mu}} \cdot \hat{\boldsymbol{B}}=-\left(-\frac{e}{m_{e}} \hat{\mathbf{S}}\right) \cdot\left(\frac{Z e}{8 \pi \varepsilon_{0} r^{3} m_{e} c^{2}} \hat{\mathbf{L}}\right)=\frac{1}{2 m_{e}^{2} c^{2}} \frac{Z e^{2}}{4 \pi \varepsilon_{0}} \frac{1}{r^{3}} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}}, \tag{6.56a}
\end{equation*}
$$

Spinorbit perturbation
where the small correction to value $g_{e}=2$ of electron's $g$-factor has been ignored, because Eq. (56) is already a small correction. This expression is confirmed by the fully-relativistic Dirac theory, to be discussed in Sec. 9.7 below: it yields, for an arbitrary central potential $U(r)$, the following Hamiltonian of the spin-orbit coupling:

$$
\begin{equation*}
\hat{H}^{(1)}=\frac{1}{2 m_{e}^{2} c^{2}} \frac{1}{r} \frac{d U(r)}{d r} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}} . \tag{6.56b}
\end{equation*}
$$

For the Coulomb potential $U(r)=-Z e^{2} / 4 \pi \varepsilon_{0} r$, this formula is reduced to Eq. (56a).
As we already know from the discussion in Sec. 5.7, such Hamiltonian commutes with all operators diagonal in the coupled representation (inside the blue line in Fig. 5.10): $\hat{L}^{2}, \hat{S}^{2}, \hat{J}^{2}$, and $\hat{J}_{z}$. Hence, using Eq. (5.208) to rewrite the spin-orbit Hamiltonian as

[^643]\[

$$
\begin{equation*}
\hat{H}^{(1)}=\frac{1}{2 m_{e}^{2} c^{2}} \frac{Z e^{2}}{4 \pi \varepsilon_{0}} \frac{1}{r^{3}} \frac{1}{2}\left(\hat{J}^{2}-\hat{L}^{2}-\hat{S}^{2}\right), \tag{6.57}
\end{equation*}
$$

\]

we may conclude that this operator is diagonal in the coupled representation with fixed quantum numbers $l, s, j$, and $m_{j}$. As a result, in this representation, we may again use Eq. (26) for each set $\{l, j$, $\left.m_{j}\right\}:$

$$
\begin{equation*}
E_{n, j, l}^{(1)}=\frac{1}{2 m_{e}^{2} c^{2}} \frac{Z e^{2}}{4 \pi \varepsilon_{0}}\left\langle\frac{1}{r^{3}}\right\rangle_{n, l} \frac{1}{2}\left\langle\hat{J}^{2}-\hat{L}^{2}-\hat{S}^{2}\right\rangle_{j, s}, \tag{6.58}
\end{equation*}
$$

where the indices irrelevant for each particular term have been dropped. (As a reminder, the spin quantum number $s$ is fixed by particle's nature; for our case of an electron, $s=1 / 2$.) Now using the last of Eqs. (3.201), and similar expressions (5.192), (5.197), and (5.203), we get an explicit expression for the spin-orbit corrections ${ }^{17}$

$$
\begin{equation*}
E_{n, j, l}^{(1)}=\frac{1}{2 m_{e}^{2} c^{2}} \frac{Z e^{2}}{4 \pi \varepsilon_{0}} \frac{\hbar^{2}}{2 r_{0}^{3}} \frac{j(j+1)-l(l+1)-3 / 4}{n^{3} l(l+1 / 2)(l+1)}=\frac{E_{n}^{2}}{m_{e} c^{2}} n \frac{j(j+1)-l(l+1)-3 / 4}{l(l+1 / 2)(l+1)} . \tag{6.59}
\end{equation*}
$$

The last form of its right-hand part shows very clearly that this correction has the same scale as the kinetic correction (52), ${ }^{18}$ so that they should be considered together. In the first order of the perturbation they may be just added, giving a very simple formula for the net fine structure of level $n$ :

$$
\begin{equation*}
E_{\text {fine }}^{(1)}=\frac{E_{n}^{2}}{2 m_{e} c^{2}}\left(3-\frac{4 n}{j+1 / 2}\right) \tag{6.60}
\end{equation*}
$$



Fine structure of H-like atom's levels

This simplicity, as well as the independence of the result of the orbital quantum number $l$, will become less surprising when (in Sec. 9.7) we see that this formula follows in one shot from the Dirac theory, in which the Bohr atom's energy spectrum in numbered only with $n$ and $j$, but not $l$.

Let us recall (see Sec. 5.7) that for an electron ( $s=1 / 2$ ), the quantum number $j$ may take $n$ positive half-integer values, from $1 / 2$ to $n-1 / 2$. With the account of this fact, Eq. (60) shows that the fine structure of $n^{\text {th }}$ Bohr's energy level has $n$ sub-levels - see Fig. 6.


Fig. 6.6. Fine structure of a hydrogen-like atom's level.

[^644]Please note that according to Eq. (5.203), each of these sub-levels is still $(2 j+1)$-times degenerate in quantum number $m_{j}$. This degeneracy is very natural, because in the absence of external field the system is still isotropic. Moreover, on each fine-structure level, besides the lowest $(j=1 / 2)$ and the highest $(j=n-1 / 2)$ ones, each of the $m_{j}$-states is doubly-degenerate in the orbital quantum number $l=$ $j \mp 1 / 2$ - see the labels of $l$ in Fig. 6. (According to Eq. (5.215), each of these states, with fixed $j$ and $m_{j}$, may be represented as a linear combination of two states with adjacent values of $l$, and hence different electron spin orientations, $m_{s}= \pm 1 / 2$, weighed with the Clebsch-Gordan coefficients.)

These details aside, one may crudely say that the relativistic corrections make the total eigenenergy to grow with $l$, contributing to the effect already mentioned at our analysis of the periodic table of elements in Sec. 3.7. The relative scale of this increase may be evaluated from the largest deviation from the unperturbed energy $E_{n}$, reached for the state with $j=1 / 2($ and hence $l=0)$ :

$$
\begin{equation*}
\frac{\left|E_{\max }^{(1)}\right|}{E_{n}}=\frac{E_{n}}{m_{e} c^{2}}\left(2 n-\frac{3}{2}\right)=\left(\frac{Z e^{2}}{4 \pi \varepsilon_{0} \hbar c}\right)^{2}\left(\frac{1}{n}-\frac{3}{4 n^{2}}\right)=Z^{2} \alpha^{2}\left(\frac{1}{n}-\frac{3}{4 n^{2}}\right) . \tag{6.61}
\end{equation*}
$$

where $\alpha$ is the fine structure ("Sommerfeld") constant,

$$
\begin{equation*}
\alpha \equiv \frac{e^{2}}{4 \pi \varepsilon_{0} \hbar c} \approx \frac{1}{137}, \tag{6.62}
\end{equation*}
$$

that was already mentioned in Sec. 4.4. ${ }^{19}$ These expressions show that the fine structure is indeed a very small effect $\left(\sim \alpha^{2} \sim 10^{-6}\right.$ ) for the hydrogen atom, but it rapidly grows (as $Z^{2}$ ) with the nuclear charge (i.e. the atomic number) $Z$, and becomes rather substantial for the heaviest atoms with $Z \sim 100$.

### 6.4. The Zeeman effect

Now, we are ready to review the Zeeman effect - the lifting of atomic level degeneracy by an external magnetic field. ${ }^{20}$ Using Eq. (3.26) (with $q=-e$ ) for the description of electron's orbital motion in the field, and Eq. (4.116) for the operator of electron's magnetic moment due to its spin- $1 / 2$, we see that even for a hydrogen-like (i.e. single-electron) atom, neglecting the relativistic effects, the full Hamiltonian is rather bulky:

$$
\begin{equation*}
\hat{H}=\frac{1}{2 m_{e}}(\hat{\mathbf{p}}+e \hat{\mathbf{A}})^{2}-\frac{Z e^{2}}{4 \pi \varepsilon_{0} r}+\frac{e}{m_{e}} \boldsymbol{B} \cdot \hat{\mathbf{S}} . \tag{6.63}
\end{equation*}
$$

There are several simplifications we may make. First, let us assume that the external field is spatial-uniform on the atomic scale (which is a very good approximation for most cases), so that we can take the vector-potential in an axially-symmetric gauge - cf. Eq. (3.132):

[^645]\[

$$
\begin{equation*}
\mathbf{A}=\frac{1}{2} \boldsymbol{B} \times \mathbf{r} . \tag{6.64}
\end{equation*}
$$

\]

Second, let us neglect the terms proportional to $B^{2}$, which are small in practical magnetic fields of the order of a few Tesla. ${ }^{21}$ The remaining term in the effective kinetic energy, describing the interaction with the magnetic field, is linear in the momentum operator, so that we may repeat the standard classical calculation ${ }^{22}$ to reduce it to the product of $\mathcal{B}$ by the orbital magnetic moment's component $m_{z}=-$ $e L_{z} / 2 m_{e}$ - besides that both $m_{z}$ and $L_{z}$ should be understood as operators now. As a result, the Hamiltonian reduces to Eq. (1a), $\hat{H}^{(0)}+\hat{H}^{(1)}$, where $\hat{H}^{(0)}$ is that of the atom at $\mathcal{B}=0$, and

$$
\begin{equation*}
\hat{H}^{(1)}=\frac{e B}{2 m_{e}}\left(\hat{L}_{z}+2 \hat{S}_{z}\right) . \tag{6.65}
\end{equation*}
$$

The form of the perturbation immediately reveals the major complication with the Zeeman effect description. Namely, in comparison with its contribution (5.198) to the total angular momentum of the electron, its spin- $1 / 2$ produces a twice larger contribution into the magnetic moment, so that the righthand part of Eq. (65) is not proportional to the total angular moment. As a result, the effect description is simple only in two limits.

If the magnetic field is so high that its effects are much stronger than the relativistic (finestructure) effects discussed in the last section, we may treat two terms in Eq. (48) as independent perturbations of different (orbital and spin) degrees of freedom. Since in the $z$-basis each of the perturbation matrices is diagonal, we can again use Eq. (26):

$$
\begin{align*}
E-E^{(0)} & =\frac{e B}{2 m_{e}}\left(\left\langle n, l, m_{l}\right| \hat{L}_{z}\left|n, l, m_{l}\right\rangle+2\left\langle m_{s}\right| \hat{S}_{z}\left|m_{s}\right\rangle\right)=\frac{e B}{2 m_{e}}\left(\hbar m_{l}+2 \hbar m_{s}\right)  \tag{6.66}\\
& =\mu_{B} B\left(m_{l} \pm 1\right) .
\end{align*}
$$

This result describes splitting of each $2 \times(2 l+1)$-degenerate energy level, with certain $n$ and $l$, into ( $2 l$ +3 ) levels (Fig. 7), with the adjacent level splitting of $\mu_{\mathrm{B}} \mathcal{B}$, equal to $\sim 10^{-23} \mathrm{~J} \sim 10^{-4} \mathrm{eV} / \mathrm{T}$. Note that all levels, besides the top and bottom one, remain doubly degenerate. This limit of the Zeeman effect is sometimes called the Paschen-Back effect - which simplicity was recognized only in the 1920s, due to the need in very high magnetic fields for its observation.


Fig. 6.7. The Paschen-Back effect.

[^646]In the opposite limit of low magnetic field, the Zeeman effect takes place on the background of the fine structure splitting. As was discussed in Sec. 3, at $\mathcal{B}=0$ each split sub-level has a $2(2 l+1)$-fold degeneracy corresponding to $(2 l+1)$ different values of the half-integer quantum number $m_{j}$, ranging from $-j$ to $+j$, and 2 values of integer $l=j \mp 1 / 2$ - see Fig. 6. The magnetic field lifts this degeneracy. ${ }^{23}$ Indeed, in the coupled representation discussed in Sec. 5.7, perturbation (48) is described by the matrix with elements

$$
\begin{align*}
H^{(1)} & =\frac{e B}{2 m_{e}}\left\langle j, m_{j}\right| \hat{L}_{z}+2 \hat{S}_{z}\left|j^{\prime}, m_{j^{\prime}}\right\rangle=\frac{e B}{2 m_{e}}\left\langle j, m_{j}\right| \hat{J}_{z}+\hat{S}_{z}\left|j^{\prime}, m_{j^{\prime}}\right\rangle \\
& =\frac{e B}{2 m_{e}}\left(\hbar m_{j} \delta_{m_{j} m_{j^{\prime}}}+\left\langle j, m_{j}\right| \hat{S}_{z}\left|j^{\prime}, m_{j^{\prime}}\right\rangle\right) . \tag{6.67}
\end{align*}
$$

Now plugging into the last term the Clebsh-Gordan expansions (5.216a) for the bra- and ket-vectors, and taking into account that operator $\hat{S}_{z}$ gives non-zero bra-kets only for $m_{s}=m^{\prime}$, matrix (67) becomes diagonal, and may again use Eq. (26) to get

Anomalous
Zeeman
effect for $s=1 / 2$

$$
\begin{align*}
E-E^{(0)} & =\frac{e B}{2 m_{e}}\left[\hbar m_{j}+\frac{\hbar}{2} \frac{\left(l \pm m_{j}+1 / 2\right)}{2 l+1}-\frac{\hbar}{2} \frac{\left(l \mp m_{j}+1 / 2\right)}{2 l+1}\right]  \tag{6.68}\\
& =\frac{e B}{2 m_{e}} \hbar m_{j}\left(1 \pm \frac{1}{2 l+1}\right)=\mu_{\mathrm{B}} B m_{j}\left(1 \pm \frac{1}{2 l+1}\right), \quad \text { for }-j \leq m_{j} \leq+j
\end{align*}
$$

where two signs correspond to the two possible values of $l=j \mp 1 / 2-$ see Fig. 8 .


Fig. 6.8. Anomalous Zeeman effect in a hydrogen-like atom - schematically.

We see that the magnetic field splits each sub-level of the fine structure, with a given $l$, into $2 j+$ 1 levels, with the distance between the levels depending on l. In the end of the 1890 s, when the Zeeman effect was first observed, there was no notion of spin at all, so that this puzzling result was called the anomalous Zeeman effect. (In this terminology, the normal Zeeman effect is the one with no spin splitting, i.e. without the second terms in the parentheses of Eqs. (66)-(68); it may be observed experimentally in atoms with the net $\operatorname{spin} s=0$.)

[^647]The strict quantum-mechanical analysis of the anomalous Zeeman effect for arbitrary $s$ (which is important for applications to multi-electron atoms) is not that complex, but requires explicit expressions for the corresponding Clebsch-Gordan coefficients, which are rather bulky. Let me just cite the unexpectedly simple result of this analysis:

$$
\begin{equation*}
\Delta E=\mu_{\mathrm{B}} B m_{j} g, \tag{6.69}
\end{equation*}
$$

where $g$ is the so-called Lande factor: ${ }^{24}$

$$
\begin{equation*}
g=1+\frac{j(j+1)+s(s+1)-l(l+1)}{2 j(j+1)} \tag{6.70}
\end{equation*}
$$

For $s=1 / 2$ (and hence $j=l \pm 1 / 2$ ), this factor is reduced to the parentheses in the last form of Eq. (68).
It is remarkable that Eqs. (69)-(70) may be readily derived using very plausible classical arguments, similar to those used in Sec. 5.7-see Fig. 5.11 and its discussion. As we have seen above, in the absence of spin, the quantization of observable $L_{z}$ is an extension of the classical torque-induced precession of the corresponding vector (say, $\mathbf{L}$ ) about the magnetic field direction, so that the interaction energy, proportional to $B L_{z}=\boldsymbol{B} \cdot \mathbf{L}$, remains constant (Fig. 9a). At the spin-orbit interaction without external magnetic field, the Hamiltonian includes the operator of product $\mathbf{S} \cdot \mathbf{L}$, so that it has to be quantized, i.e. constant, together with $J^{2}, L^{2}$, and $S^{2}$. Hence, this system's classical image is a rapid precession of vectors $\mathbf{S}$ and $\mathbf{L}$ about the direction of vector $\mathbf{J}=\mathbf{L}+\mathbf{S}$, so that the spin-orbit interaction energy, proportional to product $\mathbf{L} \cdot \mathbf{S}$, remains constant (Fig. 9b). On this backdrop, the anomalous Zeeman effect in a relatively weak magnetic field $\boldsymbol{B}=\mathcal{B}_{\mathbf{z}}$ corresponds to a slow precession of vector $\mathbf{J}$ ("dragging" the rapidly rotating vectors $\mathbf{L}$ and $\mathbf{S}$ with it) about axis $z$.


Fig. 6.9. Classical images of (a) the orbital angular momentum's quantization in external magnetic field and (b) the fine-structure level splitting.

This picture allows us to conjecture that what is important for the slow precession rate are only the vectors $\mathbf{L}$ and $\mathbf{S}$ averaged over the period of the much faster precession about vector $\mathbf{J}$ - in other words, only their components $\mathbf{L}_{J}$ and $\mathbf{S}_{J}$ directed along vector $\mathbf{J}$. Classically, these components may be calculated as

$$
\begin{equation*}
\mathbf{L}_{J}=\frac{\mathbf{L} \cdot \mathbf{J}}{J^{2}} \mathbf{J}, \quad \mathbf{S}_{J}=\frac{\mathbf{S} \cdot \mathbf{J}}{J^{2}} \mathbf{J} \tag{6.71}
\end{equation*}
$$

The scalar products participating in these expressions may be readily expressed via the squared length of the vectors, using the following evident formulas:

[^648]\[

$$
\begin{equation*}
S^{2}=(\mathbf{J}-\mathbf{L})^{2}=J^{2}+L^{2}-2 \mathbf{L} \cdot \mathbf{J}, \quad L^{2}=(\mathbf{J}-\mathbf{S})^{2}=J^{2}+S^{2}-2 \mathbf{J} \cdot \mathbf{S} . \tag{6.72}
\end{equation*}
$$

\]

As a result, we get the following time average:

$$
\begin{align*}
\overline{L_{z}+2 S_{z}} & =\left(\mathbf{L}_{J}+2 \mathbf{S}_{J}\right)_{z}=\left(\frac{\mathbf{L} \cdot \mathbf{J}}{J^{2}} \mathbf{J}+2 \frac{\mathbf{S} \cdot \mathbf{J}}{J^{2}} \mathbf{J}\right)_{z}=\frac{J_{z}}{J^{2}}(\mathbf{L} \cdot \mathbf{J}+2 \mathbf{S} \cdot \mathbf{J}) \\
& =J_{z} \frac{\left(J^{2}+L^{2}-S^{2}\right)+2\left(J^{2}+S^{2}-L^{2}\right)}{2 J^{2}}=J_{z}\left(1+\frac{J^{2}+S^{2}-L^{2}}{2 J^{2}}\right) . \tag{6.73}
\end{align*}
$$

The last move is to smuggle in some quantum mechanics by using, instead of vector lengths squared, and the $z$-component of $J_{z}$, their eigenvalues given by Eqs. (5.197), (5.203), and (5.204). As a result, we immediately arrive at the exact result given by Eqs. (69)-(70). This coincidence encourages thinking about quantum mechanics of angular momenta in classical terms of torque-induced precession, and turns out to be very fruitful in more complex problems of atomic and molecular physics.

The high-field limit and low-field limits of the Zeeman effect, described respectively by Eqs. (66) and (68), are separated by a medium field strength range in which the Zeeman splitting is of the order of the fine-structure splitting analyzed in Sec. 3. There is no time in this course for a quantitative analysis of this crossover. ${ }^{25}$

### 6.5. Time-dependent perturbations

Now let us proceed to the case when perturbation $\hat{H}^{(1)}$ in Eq. (1a) is a function of time, while $\hat{H}^{(0)}$ is time-independent. The adequate perturbative approach to this problem, and its results, depend critically on the relation between the characteristic frequency (or the characteristic reciprocal time) $\omega$ of the perturbation and the distance between the initial system's energy levels:

$$
\begin{equation*}
\hbar \omega \leftrightarrow\left|E_{n}-E_{n^{\prime}}\right| . \tag{6.74}
\end{equation*}
$$

In the easiest case when all essential frequencies of a perturbation are very small in the sense of Eq. (74), we are dealing with the so-called adiabatic change of parameters, that may be treated essentially as a time-independent perturbation (see the previous sections of this chapter). The most interesting observation here is that the adiabatic perturbation does not allow any significant transfer of system's probability from one eigenstate to another. For example, in the WKB limit of the orbital motion, the Bohr-Sommerfeld quantization rule (2.110), and its multi-dimensional generalization, guarantee that integral

$$
\begin{equation*}
\oint_{C} \mathbf{p} \cdot d \mathbf{r}, \tag{6.75}
\end{equation*}
$$

taken along the particle's classical trajectory, is an adiabatic invariant, i.e. does not change at a slow change of system's parameters. (It is curious that classical mechanics also guarantees the invariance of integral (75), but its proof there ${ }^{26}$ is much harder than the quantum-mechanical derivation of this fact,

[^649]carried out in Sec. 2.4.) This is why even if the perturbation becomes large with time (while changing sufficiently slowly), we can expect the eigenstate and eigenvalue classification to persist.

Now let us proceed to the more important (and more complex) case when both sides of Eq. (74) are comparable, and use for its discussion the Schrödinger picture of quantum mechanics given by Eqs. (4.157) and (4.158). Combining these equations, we get the Schrödinger equation in the form

$$
\begin{equation*}
\left.i \hbar \frac{\partial}{\partial t}|\alpha(t)\rangle=\left(\hat{H}^{(0)}+H^{(1)}(t)\right) \alpha(t)\right\rangle . \tag{6.76}
\end{equation*}
$$

Very much in the spirit of our treatment of the time-independent case in Sec. 1, let us represent the timedependent ket-vector of the system with its expansion,

$$
\begin{equation*}
|\alpha(t)\rangle=\sum_{n}|n\rangle\langle n \mid \alpha(t)\rangle, \tag{6.77}
\end{equation*}
$$

over the full and orthonormal set of the unperturbed, stationary ket-vectors defined by equation

$$
\begin{equation*}
\hat{H}^{(0)}|n\rangle=E_{n}|n\rangle, \tag{6.78}
\end{equation*}
$$

where bra-kets $\langle n \mid \alpha(t)\rangle$ are time-dependent coefficients. Plugging expansion (77), with $n$ replaced with $n$ ', into both sides of Eq. (76), and then inner-multiplying both its parts by bra-vector $\langle n|$ of another unperturbed (and hence time-independent) state of the system, we get a set of linear, ordinary differential equations for the expansion coefficients:

$$
\begin{equation*}
i \hbar \frac{d}{d t}\langle n \mid \alpha(t)\rangle=E_{n}\langle n \mid \alpha(t)\rangle+\sum_{n^{\prime}} H_{n n^{\prime}}^{(1)}(t)\left\langle n^{\prime} \mid \alpha(t)\right\rangle, \tag{6.79}
\end{equation*}
$$

where the matrix elements of the perturbation in the unperturbed state basis, defined similarly to Eq. (7), are now functions of time:

$$
\begin{equation*}
H_{n n^{\prime}}^{(1)}(t) \equiv\langle n| \hat{H}^{(1)}(t)\left|n^{\prime}\right\rangle . \tag{6.80}
\end{equation*}
$$

The set of differential equations (79), which are still exact, may be useful for numerical calculations, because for virtually all practical problems the set of eigenstates $n$ ' may be restricted with an acceptable error in the final result. ${ }^{27}$ However, Eq. (79) has a certain technical inconvenience, which becomes clear if we consider its (evident) solution in the absence of perturbation: ${ }^{28}$

$$
\begin{equation*}
\langle n \mid \alpha(t)\rangle=\langle n \mid \alpha(0)\rangle \exp \left\{-i \frac{E_{n}}{\hbar} t\right\} . \tag{6.81}
\end{equation*}
$$

We see that the solution oscillates very fast, and its numerical modeling may present a challenge for even fastest computers. These spurious oscillations (whose frequency, in particular, depends of the energy reference level) may be partly tamed by looking for the general solution of Eqs. (79) in a form inspired by Eq. (81):

[^650]\[

$$
\begin{equation*}
\langle n \mid \alpha(t)\rangle \equiv a_{n}(t) \exp \left\{-i \frac{E_{n}}{\hbar} t\right\} . \tag{6.82}
\end{equation*}
$$

\]

Here $a_{n}(t)$ are new functions of time (essentially, the stationary states' probability amplitudes), which may be used, in particular, to calculate the time-dependent level occupancies, i.e. the probabilities $W_{n}$ to find the perturbed system on the corresponding energy levels of the unperturbed system:

$$
\begin{equation*}
W_{n}(t)=|\langle n \mid \alpha(t)\rangle|^{2}=\left|a_{n}(t)\right|^{2} \tag{6.83}
\end{equation*}
$$

Plugging Eq. (65) into Eq. (79), for these functions we readily get a slightly modified system of equations:

General equations probability amplitude evolution

$$
\begin{equation*}
i \hbar \dot{a}_{n}=\sum_{n^{\prime}} a_{n^{\prime}} H_{n n^{\prime}}^{(1)}(t) \exp \left\{i \frac{E_{n}-E_{n^{\prime}}}{\hbar} t\right\} \equiv \sum_{n^{\prime}} a_{n^{\prime}} H_{n n^{\prime}}^{(1)}(t) e^{i \omega_{n n^{\prime}} t} \tag{6.84}
\end{equation*}
$$

where factors $\omega_{n n^{\prime}}$, defined by relation

$$
\begin{equation*}
\hbar \omega_{n n^{\prime}} \equiv E_{n}-E_{n^{\prime}} \tag{6.85}
\end{equation*}
$$

have the physical sense of frequencies of potential quantum transitions between the $n$-th and $n$ '-th energy levels of the unperturbed system. (The conditions when such transitions indeed take place will be discussed later in this chapter.) An advantage of Eq. (84) over Eq. (79) for numerical calculations is the absence of any dependence on the energy reference selection, and lower frequencies of oscillations of the right hand part terms, especially when the energy levels of interest are close to each other.

In order to continue our analytical treatment, let us restrict ourselves to a particular but very important case of a sinusoidal perturbation turned on at some moment - for example, at $t=0$ :

Turning on sinusoidal perturbation

$$
\hat{H}^{(1)}(t)= \begin{cases}0, & \text { for } t<0  \tag{6.86}\\ \hat{A} e^{-i \omega t}+\hat{A}^{\dagger} e^{+i \omega t} & \text { for } t \geq 0\end{cases}
$$

where the perturbation amplitude operators $\hat{A}$ and $\hat{A}^{\dagger}$, and hence their matrix elements,

$$
\begin{equation*}
\langle n| \hat{A}\left|n^{\prime}\right\rangle \equiv A_{n n^{\prime}}, \quad\langle n| \hat{A}^{\dagger}\left|n^{\prime}\right\rangle=A_{n^{\prime} n}^{*}, \tag{6.87}
\end{equation*}
$$

are time-independent. ${ }^{29}$ In this case, for $t>0$, Eq. (84) yields

$$
\begin{equation*}
i \hbar \dot{a}_{n}=\sum_{n^{\prime}} a_{n^{\prime}}\left[A_{n n^{\prime}} e^{i\left(\omega_{n n^{\prime}}-\omega\right) t}+A_{n^{\prime} n}^{*} e^{i\left(\omega_{n n^{\prime}}+\omega\right) t}\right] . \tag{6.88}
\end{equation*}
$$

This is, generally, still a complex system of coupled differential equations; however, it allows simple and explicit solutions in two very important cases. First, let us assume that our system is initially in one eigenstate $n$ ' (say, on the ground energy level), and that the occupancies $W_{n}$ of all other levels stays very low all the time. (We will find the corresponding condition a posteriori - from the solution.) With the corresponding assumption

[^651]\[

$$
\begin{equation*}
a_{n^{\prime}}=1 ; \quad\left|a_{n}\right| \ll 1, \quad \text { for } n \neq n^{\prime}, \tag{6.89}
\end{equation*}
$$

\]

Eq. (88) may be readily integrated, giving

$$
\begin{equation*}
a_{n}=-\frac{A_{n n^{\prime}}}{\hbar\left(\omega_{n n^{\prime}}-\omega\right)}\left[e^{i\left(\omega_{n n^{\prime}}-\omega\right) t}-1\right]-\frac{A_{n^{\prime} n}^{*}}{\hbar\left(\omega_{n n^{\prime}}+\omega\right)}\left[e^{i\left(\omega_{n n^{\prime}}+\omega\right) t}-1\right], \quad \text { for } n \neq n^{\prime} \tag{6.90}
\end{equation*}
$$

We see that the probability $W_{n}$ (83) of finding the system on each energy level of the system oscillates in time, and that our assumption (89) is satisfied as soon as the excitation amplitude is not too large, ${ }^{30}$

$$
\begin{equation*}
\left|A_{n n^{\prime}}\right| \ll \hbar\left|\omega \pm \omega_{n n^{\prime}}\right| . \tag{6.91}
\end{equation*}
$$

Expression (90) also shows that this phenomenon has a clearly resonant character: the maximum occupancy $W_{n}$ of a level grows infinitely when the corresponding detuning, ${ }^{31}$

$$
\begin{equation*}
\Delta_{n n^{\prime}} \equiv \omega-\omega_{n n^{\prime}}, \tag{6.92}
\end{equation*}
$$

tends to zero. In this limit, our initial assumption (89) may become a liability; in order to overcome it we may perform the following trick - very similar to the one we used for transfer to the degenerate case in Sec. 1. Let us assume that for a certain level $n$,

$$
\begin{equation*}
\left|\Delta_{n n^{\prime}}\right| \ll \omega,\left|\omega \pm \omega_{n^{\prime \prime} n}\right|, \mid \omega \pm \omega_{n^{\prime \prime} n^{\prime}}, \quad \text { for all } n^{\prime \prime} \neq n, n^{\prime} \tag{6.93}
\end{equation*}
$$

- the condition illustrated in Fig. 10. Then, according to Eq. (90), we may ignore the occupancy of all but two levels, $n$ and $n^{\prime}$, and also the second, non-resonant terms with frequency $\omega_{n n^{\prime}}+\omega \approx 2 \omega \gg\left|\Delta_{n n^{\prime}}\right|$ in Eqs. (88) written for $a_{n}$ and $a_{n},{ }^{32}$


Fig. 6.10. Resonant excitation of one of the higher energy levels.

As a result, in this two-level approximation (that is of course not an approximation at all for twolevel systems, such as spin- $1 / 2$ - see Sec. 5.1 ), we get a simple system of two linear equations:

$$
\begin{align*}
& i \hbar \dot{a}_{n}=a_{n^{\prime}} A e^{-i \Delta t} \\
& i \hbar \dot{a}_{n^{\prime}}=a_{n} A^{*} e^{+i \Delta t} \tag{6.94}
\end{align*}
$$

[^652]where I have used shorthand notation $A \equiv A_{n n}$, and $\Delta \equiv \Delta_{n n}$, - and will use it for a while - until other energy levels become involved (in the beginning of the next section). This system of linear differential equations may be solved exactly by the introduction of a new variable (for one of the levels only!)
\[

$$
\begin{equation*}
b_{n} \equiv a_{n} e^{+i \Delta t} \tag{6.95}
\end{equation*}
$$

\]

According to this formula,

$$
\begin{equation*}
a_{n}=b_{n} e^{-i \Delta t}, \quad \dot{a}_{n}=\left(\dot{b}_{n}-i \Delta b_{n}\right) e^{-i \Delta t} \tag{6.96}
\end{equation*}
$$

Plugging these relations into Eq. (94), we see that both equations of the system loose their explicit time dependence:

$$
\begin{equation*}
i \hbar\left(\dot{b}_{n}-i \Delta b_{n}\right)=a_{n^{\prime}} A, \quad i \hbar \dot{a}_{n^{\prime}}=b_{n} A^{*} \tag{6.97}
\end{equation*}
$$

and now may be readily solved by regular methods. For example, we may differentiate the first equation, and then use the second one to eliminate variable $a_{n}$ :

$$
\begin{equation*}
i \hbar\left(\ddot{b}_{n}-i \Delta \dot{b}_{n}\right)=\dot{a}_{n^{\prime}} A=\frac{b_{n} A^{*}}{i \hbar} A=b_{n} \frac{|A|^{2}}{i \hbar} . \tag{6.98}
\end{equation*}
$$

From mathematics we know that the resulting linear, second-order differential equation, with time-independent coefficients, has the following general solution,

$$
\begin{equation*}
b_{n}(t)=b_{+} e^{\lambda_{+} t}+b_{-} e^{\lambda_{-} t} \tag{6.99}
\end{equation*}
$$

whose characteristic exponents $\lambda$ may be readily found by plugging any of the exponential functions into Eq. (98). In our case, both roots of the resulting characteristic equation,

$$
\begin{equation*}
\lambda^{2}-i \Delta \lambda+\frac{|A|^{2}}{\hbar^{2}}=0 \tag{6.100}
\end{equation*}
$$

are purely imaginary: $\lambda_{ \pm}=i(\Delta / 2 \pm \Omega)$, where

$$
\begin{equation*}
\Omega \equiv\left(\frac{\Delta^{2}}{4}+\frac{|A|^{2}}{\hbar^{2}}\right)^{1 / 2} \tag{6.101}
\end{equation*}
$$

The coefficients $b_{ \pm}$are determined by initial conditions. If, as before, the system was completely on level $n^{\prime}$ initially, i.e. $a_{n^{\prime}}(0)=1, a_{n}(0)=b_{n}(0)=0$; then Eq. (99) immediately yields $b_{-}=-b_{+}$, so that

$$
\begin{equation*}
b_{n}(t)=2 i b_{+} e^{i \Delta t / 2} \sin \Omega t, \quad a_{n}(t)=2 i b_{+} e^{-i \Delta t / 2} \sin \Omega t, \quad \dot{a}_{n}(0)=2 i b_{+} \Omega \tag{6.102}
\end{equation*}
$$

Now the coefficient $b_{+}$may be readily found from the comparison of the last equality in Eq. (102) with the first of Eqs. (94), taken for $t=0$, when $a_{n},=1$. This comparison yields $2 i b_{+} \Omega=A / i \hbar$, and hence

$$
\begin{equation*}
a_{n}(t)=-\frac{A}{\hbar \Omega} e^{-i \Delta t / 2} \sin \Omega t, \tag{6.103}
\end{equation*}
$$

so that the $n^{\text {th }}$ level occupancy is

$$
\begin{equation*}
W_{n}=\left|a_{n}\right|^{2}=\frac{|A|^{2}}{\hbar^{2} \Omega^{2}} \sin ^{2} \Omega t=\frac{|A|^{2}}{|A|^{2}+(\hbar \Delta / 2)^{2}} \sin ^{2} \Omega t \tag{6.104}
\end{equation*}
$$

This is the famous Rabi formula. ${ }^{33}$ It shows that an increase of the perturbation amplitude $|A|$ leads not only to an increase of the amplitude of the probability oscillations, but also of their frequency $2 \Omega$ described by Eq. (101) - see Fig. 11.


Fig. 6.11. Rabi oscillations.

Ultimately, at $|A| \gg \hbar|\Delta|$ (for example, at the exact resonance, $\Delta=0$ ) Eqs. (101)-(102) give $\Omega=$ $|A| / \hbar$ and $\left(W_{n}\right)_{\max }=1$, i.e. describe a periodic, full "repumping" of the system from one level to another and back, with a frequency proportional to the perturbation amplitude. This effect gives a very convenient tool for manipulating two-level-systems (qubits, in the quantum information context). For example, limiting the external excitation time to $\Delta t=\pi / 2 \Omega$ (or an odd number of such intervals) we may completely transfer the system from one eigenstate (say, $\downarrow$ ) to the opposite one ( $\uparrow$ ). ${ }^{34}$ On the Bloch sphere (Fig. 5.1), this transfer corresponds to the representing point's drive from the South Pole to the North Pole.

Note, however, that according to Eq. (90), if the system has energy levels other than $n$ and $n$ ', they also become occupied to some extent. Since the sum of occupancies should be 1 , this means that $\left(W_{n}\right)_{\text {max }}$ may approach 1 only if the excitation amplitude is very small, and hence the state switching time $\Delta t=\pi / 2 \Omega=\pi \hbar / 2|A|$ is very long. The ultimate limit in this sense is provided by the harmonic oscillator where all energy levels are equidistant, and probability repumping between all of them occurs with the same rate. Hence, in that particular system, the implementation of the full Rabi oscillations is impossible even at the exact resonance. ${ }^{35}$ In the opposite limit, when the detuning is large in comparison with $|A| / \hbar$, though still small in the sense of Eq. (93), the frequency of Rabi oscillations is completely determined by the detuning, and their amplitude is small:

[^653]\[

$$
\begin{equation*}
W_{n}(t)=4 \frac{|A|^{2}}{\hbar^{2} \Delta^{2}} \sin ^{2} \frac{\Delta t}{2} \ll 1, \text { for }|A|^{2} \ll(\hbar \Delta)^{2} \tag{6.105}
\end{equation*}
$$

\]

However, I would not like these quantitative details to obscure from the reader the most important qualitative (OK, maybe semi-quantitative :-) conclusion of this section's analysis: the resonant increase of interlevel transition intensity at $\omega \rightarrow \omega_{n n}$. Using the fundamental Kramer-Kronig dispersion relations, ${ }^{36}$ based essentially only on very general causality arguments, it is easy to show (and hence left for reader's exercise) that in a medium incorporating many similar quantum systems (e.g., atoms or molecules), this increase of quantum transitions is accompanied by a sharp increase of external field's absorption. This effect has numerous practical applications including systems based on the electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR) spectroscopies, which are broadly used in material science, chemistry, and medicine. Unfortunately, I will not have time to discuss the related technical issues (in particular, interesting pulsing spectroscopy techniques) in detail, and have to refer the reader to special literature. ${ }^{37}$

### 6.6. Quantum-mechanical Golden Rule

The last result of the past section, Eq. (105), may be used to derive one of the most important results of quantum mechanics - its so-called Golden Rule. For that, let us consider the case when the perturbation causes quantum transitions from a discrete energy level $E_{n}$, into a group of eigenstates $E_{n}$ with a dense (virtually continuous) spectrum - see Fig. 12a. If, for all states $n$ of the group, the following conditions are satisfied

$$
\begin{equation*}
\left|A_{n n^{\prime}}\right|^{2} \ll\left(\hbar \Delta_{n n^{\prime}}\right)^{2} \ll\left(\hbar \omega_{n n^{\prime}}\right)^{2}, \tag{6.106}
\end{equation*}
$$

then Eq. (105) coincides with the result that would follow from Eq. (90). This means that we may apply Eq. (105), with indices $n$ and $n$ ' duly restored, to any level $n$ of our tight group. As a result, the total probability of having our system transferred from level $n$ ' to that group is

$$
\begin{equation*}
W_{\Sigma}(t)=\sum_{n} W_{n}(t)=\frac{4}{\hbar^{2}} \sum_{n} \frac{\left|A_{n n^{\prime}}\right|^{2}}{\Delta_{n n^{\prime}}^{2}} \sin ^{2} \frac{\Delta_{n n^{\prime}} t}{2} . \tag{6.107}
\end{equation*}
$$


(b)

Fig. 6.12. Deriving the Golden Rule: (a) the energy level scheme, and (b) the function under integral (108).

[^654]Now comes the main, absolutely beautiful trick: let us assume that the summation over $n$ will be limited to a tight group of very similar states for which the matrix elements $A_{n n}$, are virtually similar (we will check the validity of this assumption later on), so that we can take it out of the sum (107) and then replace the sum with the corresponding integral:

$$
\begin{equation*}
W_{\Sigma}(t)=\frac{4\left|A_{n n^{\prime}}\right|^{2}}{\hbar^{2}} \int \frac{1}{\Delta_{n n^{\prime}}^{2}} \sin ^{2} \frac{\Delta_{n n^{\prime}} t}{2} d n=\frac{4\left|A_{n n^{\prime}}\right|^{2} \rho_{n} t}{\hbar} \int \frac{1}{\left(\Delta_{n n^{\prime}} t\right)^{2}} \sin ^{2}\left(\frac{\Delta_{n n^{\prime}} t}{2}\right) d\left(-\Delta_{n n^{\prime}} t\right), \tag{6.108}
\end{equation*}
$$

where $\rho_{n}$ is the density of eigenstates $n$ on the energy axis:

$$
\begin{equation*}
\rho_{n} \equiv \frac{d n}{d E_{n}} \tag{6.109}
\end{equation*}
$$

This density, as well as the matrix element $A_{n n^{\prime}}$, have to be evaluated at $\Delta_{n n^{\prime}}=0$, i.e. at energy $E_{n}=E_{n},+$ $\hbar \omega$, and are assumed to be constant within the final state group. At fixed $E_{n^{\prime}}$, the function under integral (108) is even and decreases fast at $\left|\Delta_{n n}, t\right| \gg 1$ - see Fig. 12b. Hence we may introduce a dimensionless integration variable $\xi \equiv \Delta_{n n}$ t, and extend integration over this variable formally from $-\infty$ to $+\infty$. Then Eq. (108) is reduced to a table integral, ${ }^{38}$ and yields

$$
\begin{equation*}
W_{\Sigma}(t)=\frac{4\left|A_{n n^{\prime}}\right|^{2} \rho_{n}}{\hbar} \int_{-\infty}^{+\infty} \frac{1}{\xi^{2}} \sin ^{2} \frac{\xi}{2} d \xi=\frac{4\left|A_{n n^{\prime}}\right|^{2} \rho_{n} t}{\hbar} \frac{\pi}{2} \equiv \Gamma t \tag{6.110}
\end{equation*}
$$

where constant

$$
\begin{equation*}
\Gamma=\frac{2 \pi}{\hbar}\left|A_{n n^{\prime}}\right|^{2} \rho_{n} \tag{6.111}
\end{equation*}
$$

Density
of states
is the called the transition rate. ${ }^{39}$
This is one of the most famous and useful results of quantum mechanics, its Golden Rule (sometimes, rather unfairly, called the "Fermi Golden Rule" ${ }^{40}$ ), which deserves much discussion. First of all, let us reproduce the reasoning already used in Sec. 2.5 to show that the meaning of rate $\Gamma$ is much deeper than Eq. (110) seems to imply. Indeed, due to the conservation of the total probability, $W_{n},+W_{\Sigma}$ $=1$, we can rewrite that equation as

$$
\begin{equation*}
\left.\dot{W}_{n^{\prime}}\right|_{t=0}=-\Gamma . \tag{6.112}
\end{equation*}
$$

Evidently, this result cannot be true for $t \rightarrow \infty$, otherwise probability $W_{n}$, would become negative. The reason for that apparent contradiction is that result (110) was obtained in the assumption that initially the system was completely on level $n^{\prime}: W_{n^{\prime}}(0)=1$. Now, if in the initial moment the value of $W_{n^{\prime}}$, is
${ }^{38}$ See, e.g., MA Eq. (6.12).
${ }^{39}$ In some texts, the density of states in Eq. (111) is replaced with expression $\sum_{n} \delta\left(E_{n}-E_{n^{\prime}}-\hbar \omega\right)$. Indeed, the integration of this expression over any final energy interval $\Delta E_{n}$ gives the same result $\Delta n=\left(d n / d E_{n}\right) \Delta E_{n}=\rho_{n} \Delta E_{n}$ as Eq. (111). Such replacement may be useful in some cases, but should be used with utmost care, and for most applications the more explicit form (111) is preferable.
${ }^{40}$ Actually, this result was developed mostly by the same P. A. M. Dirac in 1927; E. Fermi's role was not much more than advertising it, under the name of "Golden Rule No. 2", in his lecture notes on nuclear physics, which were published much later, in 1950. (To be fair to Fermi, he has never tried to pose as the Golden Rule's author.)
different, result (110) has to be multiplied by that number, due to the linear relation (88) between $d a_{n} / d t$ and $a_{n}$. Hence, instead of Eq. (112) we get a differential equation similar to Eq. (2.159),

$$
\begin{equation*}
\dot{W}_{n^{\prime}}=-\Gamma W_{n^{\prime}}, \tag{6.113}
\end{equation*}
$$

Initial state's occupancy decay
which, for time-independent $\Gamma$, has the evident solution,

$$
\begin{equation*}
W_{n^{\prime}}(t)=W_{n^{\prime}}(0) e^{-\Gamma t} \tag{6.114}
\end{equation*}
$$

describing an exponential decay of the initial state's occupancy, with time constant $\tau=1 / \Gamma$.
I would ask the reader to think again about this fascinating mathematical result: by summation of periodic oscillations (105) over many levels $n$, we have got an exponential evolution (114) of the probability. The main trick here is of course that the effective range $\Delta E$ of states $E_{n}$, giving the dominating contribution into integral (108), shrinks with time: $\Delta E_{n} \sim \hbar / t .{ }^{41}$ By the way, since most of the decay takes place at times $t \sim \tau \equiv 1 / \Gamma$, the range of participating final energies may be estimated as

$$
\begin{equation*}
\Delta E_{n} \sim \frac{\hbar}{\tau}=\hbar \Gamma . \tag{6.115}
\end{equation*}
$$

This estimate is very instrumental for the formulation of conditions of validity of the Golden Rule (111). First, we have assumed that the matrix elements of the perturbation and the density of states do not depend on energy within interval (115). This gives the following requirement

$$
\begin{equation*}
\Delta E_{n} \sim \hbar \Gamma \ll E_{n}-E_{n^{\prime}} \sim \hbar \omega, \tag{6.116}
\end{equation*}
$$

Second, for the transfer from sum (107) to integral (108), we need the number of states within that energy interval, $\Delta N_{n}=\rho_{n} \Delta E_{n}$, to be much larger than 1. Merging Eq. (116) with Eq. (93) for all energy levels $n " \neq n, n$ ' not participating in the resonant transfer, we may summarize all conditions of the Golden Rule validity as

Golden
Rule's validity

$$
\begin{equation*}
\rho_{n}^{-1} \ll \hbar \Gamma \ll \hbar\left|\omega \pm \omega_{n^{\prime} n^{\prime \prime}}\right| \tag{6.117}
\end{equation*}
$$

(The reader may ask whether I have forgotten the condition expressed by the first of Eqs. (106). However, for $\Delta_{n n}, \sim \Delta E_{n} / \hbar \sim \Gamma$, this condition is just $\left|A_{n n}\right|^{2} \ll(\hbar \Gamma)^{2}$, so that plugging it into Eq. (111),

$$
\begin{equation*}
\Gamma \ll \frac{2 \pi}{\hbar}(\hbar \Gamma)^{2} \rho_{n}, \tag{6.118}
\end{equation*}
$$

and canceling one $\Gamma$ and one $\hbar$, we see that this requirement coincides with the left relation in Eq. (117) above.)

Let us have a look at whether these conditions may be satisfied in practice, at least in some cases. For example, let us consider the optical ionization of an atom, with the released electron confined in a volume of the order of $1 \mathrm{~cm}^{3}=10^{-6} \mathrm{~m}^{3}$. According to Eq. (1.82), with $E$ of the order of the atomic ionization energy $E_{n}-E_{m}=\hbar \omega \sim 1 \mathrm{eV}$, the density of electron states in that volume is of the order of $10^{17} 1 / \mathrm{eV}$. Thus conditions (117) provide an approximately 15 -orders-of magnitude range for acceptable

[^655]values of $\hbar \Gamma$. This illustration should give the reader a taste of why the Golden Rules is applicable to so many situations.

Finally, the physical picture of initial state's decay (which will also be the key for our discussion of quantum mechanics of "open" systems in the next chapter) is also very important. According to Eq. (114), the external excitation transfers the system onto the continuous spectrum of levels $n$, and it never comes back on the initial level $n$ '. However, it was derived from quantum mechanics of Hamiltonian systems, whose equations are invariant with respect to time reversal. This paradox is a result of the generalization (113) of the exact result (112), that breaks the time reversal symmetry, but is absolutely adequate for the physics under study. Some gut feeling of the physical sense of this irreversibility may be obtained from the following observation. From our wave-mechanics experience, we know that the distance between adjacent orbital energy levels tends to zero only if the system size goes to infinity. This means that the assumption of continuous energy spectrum of final states $n$ essentially requires these states to be infinitely extended in space - essentially being free de Broglie waves. The Golden Rule approach corresponds to the (physically justified) assumption that in an infinitely large system the traveling waves excited by a local source and propagating outward from it, would never come back, and even if they do, the unpredictable phase shifts introduced by the uncontrollable perturbations on their way would never allow them to sum up in the way necessary to bring the system back into the initial state $n^{\prime}$. ${ }^{42}$

Maybe the best illustration of this interpretation is given by the following problem - which is a toy model of the photoelectric effect that was briefly discussed in Sec. 1.1(iii). A 1D particle is initially trapped in the ground state of a narrow quantum well,

$$
\begin{equation*}
U(x)=-w \delta(x) \tag{6.119}
\end{equation*}
$$

Let us use the Golden Rule to find rate $\Gamma$ of particle's "ionization" (i.e. its excitation into an extended, delocalized state) by a weak classical sinusoidal force of amplitude $F_{0}$ and frequency $\omega$. As a reminder, finding the initial, localized state ( $n$ ') of such particle was the task of Problem 2.14, and its solution was

$$
\begin{equation*}
\psi_{n^{\prime}}(x)=\kappa^{1 / 2} \exp \{-\kappa|x|\}, \quad \kappa \equiv \frac{m w}{\hbar^{2}}, \quad E_{n^{\prime}}=-\frac{\hbar^{2} \kappa^{2}}{2 m}=-\frac{m w^{2}}{2 \hbar^{2}} . \tag{6.120}
\end{equation*}
$$

Extended states $n$ with continuous spectrum, for this problem exist only at energies $E_{n}>0$, so that the excitation rate is different from zero only for frequencies

$$
\begin{equation*}
\omega>\omega_{t} \equiv \frac{\left|E_{n^{\prime}}\right|}{\hbar}=\frac{m w^{2}}{2 \hbar^{3}} . \tag{6.121}
\end{equation*}
$$

The weak sinusoidal force may be described by the following perturbation Hamiltonian,

$$
\begin{equation*}
\hat{H}^{(1)}=-F(t) \hat{x}=-F_{0} \hat{x} \cos \omega t=-\frac{F_{0}}{2} \hat{x}\left(e^{i \omega t}+e^{-i \omega t}\right), \quad \text { for } t>0, \tag{6.122}
\end{equation*}
$$

so that according to Eq. (86), that serves as the amplitude operator definition, in this case

[^656]\[

$$
\begin{equation*}
\hat{A}=\hat{A}^{\dagger}=-\frac{F_{0}}{2} \hat{x} . \tag{6.123}
\end{equation*}
$$

\]

Now the matrix elements $A_{n n}$, that participate in Eq. (111) may be calculated in the coordinate representation:

$$
\begin{equation*}
A_{n n^{\prime}}=\int_{-\infty}^{+\infty} \psi_{n}^{*}(x) \hat{A}(x) \psi_{n^{\prime}}(x) d x=-\frac{F_{0}}{2} \int_{-\infty}^{+\infty} \psi_{n}^{*}(x) x \psi_{n^{\prime}}(x) d x \tag{6.124}
\end{equation*}
$$

Since, according to Eq. (120), the initial $\psi_{n}$, is a symmetric function of $x$, a nonvanishing contribution to this integral is given only by asymmetric functions $\psi_{n}(x)$, proportional to $\sin k_{n} x$, with wavenumber $k_{n}$ related to the final energy by the well-familiar equality (1.77):

$$
\begin{equation*}
\frac{\hbar^{2} k_{n}^{2}}{2 m}=E_{n} . \tag{6.125}
\end{equation*}
$$

As we know from Sec. 2.5 (see in particular Eq. (2.124) and its discussion), such asymmetric functions, with $\psi_{n}(0)=0$, are not affected by the zero-centered delta-functional potential (119), and their density $\rho_{n}$ is the same as in a completely free space, and we can use Eq. (1.94). (Actually, since that relation was derived for traveling waves, it is more prudent to repeat the calculation that has led to that result, confining the waves on an artificial segment $[-l / 2,+l / 2]$ - so long,

$$
\begin{equation*}
k_{n} l, k l \gg 1, \tag{6.126}
\end{equation*}
$$

that it does not affect the initial localized state and the excitation process. Then the confinement requirement $\psi_{n}( \pm l / 2)=0$ immediately yields the condition $k_{n} l / 2=n \pi$, so that Eq. (1.94) is indeed valid, but only for positive values of $k_{n}$, because $\sin k_{n} X$ with $k_{n} \rightarrow-k_{n}$ does not give an independent standingwave eigenstate.) Hence the final state density is

$$
\begin{equation*}
\rho_{n} \equiv \frac{d n}{d E_{n}}=\frac{d n}{d k_{n}} / \frac{d E_{n}}{d k_{n}}=\frac{l}{2 \pi} / \frac{\hbar^{2} k_{n}}{m}=\frac{l m}{2 \pi \hbar^{2} k_{n}} . \tag{6.127}
\end{equation*}
$$

It may look troubling that the density of states depends on artificial segment's length $l$, but the same $l$ also participates in the final wavefunction normalization factor, ${ }^{43}$

$$
\begin{equation*}
\psi_{n}=\left(\frac{2}{l}\right)^{1 / 2} \sin k_{n} x \tag{6.128}
\end{equation*}
$$

and hence the matrix element (124):

$$
\begin{equation*}
A_{n n^{\prime}}=-\frac{F_{0}}{2}\left(\frac{2 \kappa}{l}\right)^{1 / 2} \int_{-l}^{+l} \sin k_{n} x e^{-\kappa|x|} x d x .=-\frac{F_{0}}{2 i}\left(\frac{2 \kappa}{l}\right)^{1 / 2}\left(\int_{0}^{l} e^{\left(i k_{n}-\kappa\right) x} x d x-\int_{0}^{l} e^{-\left(i k_{n}+\kappa\right) x} x d x\right) \tag{6.129}
\end{equation*}
$$

These two integrals may be readily worked out by parts. Taking into account that, according to condition (126), their upper limits may be extended to $\infty$, the result is

[^657]\[

$$
\begin{equation*}
A_{n n^{\prime}}=-\left(\frac{2 \kappa}{l}\right)^{1 / 2} F_{0} \frac{2 k_{n} \kappa}{\left(k_{n}^{2}+\kappa^{2}\right)^{2}} \tag{6.130}
\end{equation*}
$$

\]

so that finally we get an expression for the rate, which is independent of the artificially introduced $l$ :

$$
\begin{equation*}
\Gamma=\frac{2 \pi}{\hbar}\left|A_{n n^{\prime}}\right|^{2} \rho_{n}=\frac{2 \pi}{\hbar}\left[\left(\frac{2 \kappa}{l}\right)^{1 / 2} F_{0} \frac{2 k_{n} \kappa}{\left(k_{n}^{2}+\kappa^{2}\right)^{2}}\right]^{2} \frac{l m}{2 \pi \hbar^{2} k_{n}}=\frac{8 F_{0}^{2} m k_{n} \kappa^{3}}{\hbar^{3}\left(k_{n}^{2}+\kappa^{2}\right)^{4}} \tag{6.131}
\end{equation*}
$$

Note that due to the above definitions of $k_{n}$ and $\kappa$, the expression in parentheses in the denominator of the last formula does not depend on the quantum well parameter $W$, and is a function of only the excitation frequency $\omega$ (and particle's mass):

$$
\begin{equation*}
\frac{\hbar^{2}\left(k_{n}^{2}+\kappa^{2}\right)}{2 m}=E_{n}-E_{n^{\prime}}=\hbar \omega . \tag{6.132}
\end{equation*}
$$

As a result, Eq. (131) may be recast simply as

$$
\begin{equation*}
\hbar \Gamma=\frac{F_{0}^{2} w^{3} k_{n}}{2(\hbar \omega)^{4}} . \tag{6.133}
\end{equation*}
$$

What is still hidden here is that $k_{n}$, defined by to Eq. (125) with $E_{n}=E_{n},+\hbar \omega$, is a function of frequency, changing as $\omega^{1 / 2}$ at $\omega \gg \omega_{t}$ (so that $\Gamma$ drops as $\omega^{-7 / 2}$ at $\omega \rightarrow \infty$ ), and as $\left(\omega-\omega_{t}\right)^{1 / 2}$ when $\omega$ approaches the "red boundary" $\omega_{t} \equiv\left|E_{n}\right| / \hbar=m \omega^{2} / 2 \hbar^{3}$ of the ionization effect, so that $\Gamma \propto\left(\omega-\omega_{t}\right)^{1 / 2} \rightarrow$ 0 in that limit as well. We see that our toy model does describe this main feature of the photoelectric effect, whose explanation by Einstein was essentially the starting point of quantum mechanics - see Sec. 1.1. The (very similar) analysis of this effect in a more realistic model, the hydrogen atom's ionization, is left for reader's exercise.

### 6.7. Golden Rule for step-like perturbations

Now let us reuse some of our results for a perturbation being turned on at $t=0$, but after that time-independent:

$$
\hat{H}^{(1)}(t)= \begin{cases}0, & t<0  \tag{6.134}\\ \hat{H}^{(1)}=\text { const }, & t \geq 0\end{cases}
$$

A superficial comparison of this equation and our former Eq. (69) seems to indicate that we may use all our previous results, taking $\omega=0$. However, that conclusion does not take into account the fact that analyzing both the two-level approximation and the Golden Rule for continuous spectrum, we have neglected the second (non-resonant) term in Eq. (90). This why it is more prudent to use the general Eq. (86),

$$
\begin{equation*}
i \hbar \dot{a}_{n}=\sum_{n^{\prime}} a_{n^{\prime}} \cdot H_{n n^{\prime}}^{(1)} e^{i \omega_{n n^{\prime}} t} \tag{6.135}
\end{equation*}
$$

in which the matrix element of the perturbation is now time-independent. We see that it is formally equivalent to Eq. (88) with only the first (resonant) term kept, if we make the following replacements:

Step-like perturbation

$$
\begin{equation*}
\hat{A} \rightarrow \hat{H}^{(1)}, \quad \Delta_{n n^{\prime}} \equiv \omega-\omega_{n n^{\prime}} \rightarrow-\omega_{n n^{\prime}} . \tag{6.136}
\end{equation*}
$$

As a sanity check, let us revisit a two-level system such as two quantum wells coupled by tunneling - see Fig. 13a. It is convenient to include the energy difference $E_{n}-E_{n}$, between the two levels into the unperturbed Hamiltonian, so that perturbation (134) describes only the localized state coupling due to tunneling through the energy barrier separating the wells. (The turning on of the coupling, described by Eq. (134), may be achieved, for example, by a rapid lowering of the barrier at $t=0$.) Then, after replacements (136), we are getting an analog of Eq. (104):

$$
\begin{equation*}
W_{n}=\left|a_{n}\right|^{2}=\frac{\left|H_{n n^{\prime}}^{(1)}\right|^{2}}{\hbar^{2} \Omega^{2}} \sin ^{2} \Omega t, \tag{6.137}
\end{equation*}
$$

where frequency $\Omega$ of the periodic "probability repumping" between levels $n$ ' and $n$ is now described, instead of Eq. (104), by relation

$$
\begin{equation*}
2 \Omega=\left(\omega_{n n^{\prime}}^{2}+4 \frac{\left|H_{n n^{\prime}}^{(1)}\right|^{2}}{\hbar^{2}}\right)^{1 / 2}=\frac{1}{\hbar}\left[\left(E_{n}-E_{n^{\prime}}\right)^{2}+4 H_{n n^{\prime}}^{(1)} H_{n^{\prime} n}^{(1)}\right]^{1 / 2} . \tag{6.138}
\end{equation*}
$$

But these are exactly the quantum oscillations that have already been discussed in Sec. 2.6 - now derived for an arbitrary quantum wells and tunnel barrier shape.
(a)
(b)


Fig. 6.13. Quantum-well implementation of coupling of a discrete-energy state $n$ ' to (a) another discrete-energy state, and (b) a state continuum, due to tunneling through a potential barrier.

The similarity of Eqs. (104) and (137) shows that the Rabi oscillations and the "usual" quantum oscillations have essentially the same physical nature, besides that in the former case the external rf signal quantum $\hbar \omega$ bridges over the state energy difference. We may also compare result (138) with our analysis of a two-level system, with a similar time-independent perturbation, in Sec. 1. According to Eq. (29), its eigenenergies differ by

$$
\begin{equation*}
E_{+}-E_{-}=\left[\left(H_{11}-H_{22}\right)^{2}+4 H_{12} H_{21}\right]^{1 / 2} . \tag{6.139}
\end{equation*}
$$

But this is exactly the result given by Eq. (138), provided that we consider $\left(H_{11}-H_{22}\right)$ as the difference ( $E_{n}-E_{n}$ ) of unperturbed state energies rather than as a perturbation, as we certainly have a right to do.

Now let us consider the effect of perturbation (134) in the case when it creates coupling between the initial (discrete) energy level and a dense group of states with a quasi-continuum spectrum, in the same energy range. Figure 13 b shows an example of such a system: a quantum well separated by a
penetrable tunnel barrier from an extended region with a quasi-continuous energy spectrum. Making replacements (136) in Eq. (111), we may present the Golden Rule for this case as

$$
\begin{equation*}
\Gamma=\frac{2 \pi}{\hbar}\left|H_{n n^{\prime}}^{(1)}\right|^{2} \rho_{n}, \tag{6.140}
\end{equation*}
$$

where states $n$ and $n$ ' now have the same energy. ${ }^{44}$
It is very informative to compare this result with Eq. (138) for a symmetric ( $E_{n}=E_{n^{\prime}}$ ) double quantum well using the same tunnel barrier - see Fig. 13. For the latter case, Eq. (138) yields

$$
\begin{equation*}
\Omega=\frac{1}{\hbar}\left|H_{n n^{\prime}}^{(1)}\right|_{\text {con }} . \tag{6.141}
\end{equation*}
$$

Here I have used index "con" (from "confinement") to emphasize that this matrix element is rather different from the one participating in Eq. (140). Indeed, in the latter case, the matrix element,

$$
\begin{equation*}
H_{n n^{\prime}}^{(1)}=\langle n| \hat{H}^{(1)}\left|n^{\prime}\right\rangle=\int \psi_{n^{\prime}}^{*} \hat{H}^{(1)} \psi_{n} d x, \tag{6.142}
\end{equation*}
$$

has to be calculated for two similar wavefunctions $\psi_{n}$ and $\psi_{n}$, confined to spatial intervals of the same scale $l_{\text {con }}$, while in Eq. (140), wavefunctions $\psi_{n}$ are extended to a much larger distance $l \gg l_{\text {con }}-$ see Fig. 13. As Eq. (129) tells us, in the 1D model we are considering now, this means an additional factor small factor of the order of $\left(l_{\text {con }} / l\right)^{1 / 2}$. Now using Eq. (128) as a crude but suitable model for the finalstate wavefunctions, we arrive at the following estimate:

$$
\begin{equation*}
\hbar \Gamma \sim 2 \pi\left|H_{n n^{\prime}}^{(1)}\right|_{\text {con }}^{2} \frac{l_{\text {con }}}{l} \rho_{n} \sim 2 \pi\left|H_{n n^{\prime}}^{(1)}\right|_{\text {con }}^{2} \frac{l_{\text {con }}}{l} \frac{l m}{2 \pi \hbar^{2} k_{n}} \sim \frac{\left|H_{n n^{\prime}}^{(1)}\right|_{\text {con }}^{2}}{\Delta E_{n^{\prime}}}=\frac{(\hbar \Omega)^{2}}{\Delta E_{n^{\prime}}} \tag{6.143}
\end{equation*}
$$

where $\Delta E_{n}, \sim \hbar^{2} / m l^{2}$ con is the scale of the differences between eigenenergies of the particle in an unperturbed quantum well. Since the condition of validity of the perturbative formula (140) is $\hbar \Omega \ll$ $\Delta E_{n}$, we see that ${ }^{45}$

$$
\begin{equation*}
\hbar \Gamma \sim \frac{\hbar \Omega}{\Delta E_{m}} \hbar \Omega \ll \hbar \Omega . \tag{6.144}
\end{equation*}
$$

Hence the rate of (irreversible) quantum tunneling into continuum is always much lower that the frequency of (reversible) quantum oscillations between states separated with the same potential barrier at least for the case when both are much lower than $\Delta E_{n^{\prime}} / \hbar$, so that the perturbation theory is valid. A handwaving interpretation of this result is that the confined particle wonders beyond the barrier and back many times before finally "deciding" to perform an irreversible transition into unconfined continuum. ${ }^{46}$

[^658]Let me conclude this section (and this chapter) with the application of Eq. (140) to an important case, which will provide us with a smooth transition to the next chapter's topics. Consider a composite system consisting of two parts, $a$ and $b$, with the energy spectra sketched in Fig. 14.


Fig. 6.14. Energy relaxation in system $a$ due to its coupling with system $b$ (which serves as the environment of $a$ ).

Let the systems be completely independent initially. The independence means that in the absence of perturbation, the total Hamiltonian of the system at $t<0$ may be presented as a sum

$$
\begin{equation*}
\hat{H}^{(0)}=\hat{H}_{a}(a)+\hat{H}_{b}(b), \tag{6.145}
\end{equation*}
$$

where arguments $a$ and $b$ symbolize the non-overlapping sets of variables of the two systems. Then eigenkets of the system may be naturally factored as ${ }^{47}$

$$
\begin{equation*}
|n\rangle=\left|n_{a}\right\rangle \otimes\left|n_{b}\right\rangle \tag{6.146}
\end{equation*}
$$

while its eigenenergies separate into a sum, just as the Hamiltonian (145) does:

$$
\begin{align*}
\hat{H}^{(0)}|n\rangle & \left.=\left(\hat{H}_{a}+\hat{H}_{b}\right) n_{a}\right\rangle \otimes\left|n_{b}\right\rangle=\left(\hat{H}_{a}\left|n_{a}\right\rangle\right) \otimes\left|n_{b}\right\rangle+\left(\hat{H}_{b}\left|n_{b}\right\rangle\right) \otimes\left|n_{a}\right\rangle  \tag{6.147}\\
& =\left(E_{n a}\left|n_{a}\right\rangle\right) \otimes\left|n_{b}\right\rangle+\left(E_{n b}\left|n_{b}\right\rangle\right) \otimes\left|n_{a}\right\rangle=\left(E_{n a}+E_{n b}\right)|n\rangle .
\end{align*}
$$

Analysis of such a composite system is much easier when the interaction of its components may be presented as a product of two Hermitian operators, each depending only on the degrees of freedom of only one component system:

$$
\begin{equation*}
\hat{H}^{(1)}=\hat{A}(a) \hat{B}(b) . \tag{6.148}
\end{equation*}
$$

A typical example of such a bilinear interaction Hamiltonian is the electric-dipole interaction between an atomic-scale electron system (with a size of the order of the Bohr radius $r_{\mathrm{B}} \sim 10^{-10} \mathrm{~m}$ ) and the electromagnetic field at optical frequencies $\omega \sim 10^{16} \mathrm{~s}^{-1}$, with wavelength $\lambda=2 \pi c / \omega \sim 10^{-6} \mathrm{~m} \gg r_{\mathrm{B}}$ : ${ }^{48}$

$$
\begin{equation*}
\hat{H}^{(1)}=-\hat{\mathbf{d}} \cdot \hat{\boldsymbol{\varepsilon}}, \quad \text { with } \hat{\mathbf{d}} \equiv \sum_{k} q_{k} \hat{\mathbf{r}}_{k}, \tag{6.149}
\end{equation*}
$$

where the dipole electric moment $\mathbf{d}$ depends only on positions $\mathbf{r}_{k}$ of charged particles (numbered with index $k$ ), while that of electric field $\varepsilon$ is a function of only the electromagnetic field's degrees of freedom - see Chapter 9 below.

[^659]Returning to the general situation shown in Fig. 14, if the component system $a$ was initially in an excited state $n^{\prime}{ }_{a}$, interaction (148) may bring it to another discrete state $n_{a}$ of a lower energy - for example, the ground state. In the process of this transition, the released energy, in the form of energy quantum

$$
\begin{equation*}
\hbar \omega \equiv E_{n^{\prime} a}-E_{n a}, \tag{6.150}
\end{equation*}
$$

is picked up by system $b$ :

$$
\begin{equation*}
E_{n b}-E_{n^{\prime} b}=\hbar \omega . \tag{6.151}
\end{equation*}
$$

(In typical applications, though not always, the initial state $n_{b}$ of that system is its ground state.) If the final state $n_{b}$ of the system is inside a state group with quasi-continuous energy spectrum (Fig. 14), the process has the exponential character (114) ${ }^{49}$ and may be interpreted as the effect of energy relaxation of system $a$, with the released energy quantum $\hbar \omega$ absorbed by system $b$. Note that since the quasicontinuous spectrum essentially requires a system of large spatial size, such model is very convenient for description of the environment of system $a$. (In physics, the "environment" typically means all the Universe less the system under consideration.)

The relaxation rate $\Gamma$ may be described by the Golden Rule. Since perturbation (148) does not depend on time explicitly, and the total energy of the composite system does not change, we may use Eq. (140) that, with the account of Eqs. (146) and (148), takes the form

$$
\begin{equation*}
\Gamma=\frac{2 \pi}{\hbar}\left|A_{n n^{\prime}}\right|^{2}\left|B_{n n^{\prime}}\right|^{2} \rho_{n}, \quad \text { where } A_{n n^{\prime}} \equiv\left\langle n_{a}\right| \hat{A}\left|n_{a}^{\prime}\right\rangle, B_{n n^{\prime}}=\left\langle n_{b}\right| \hat{B}\left|n_{b}^{\prime}\right\rangle, \tag{6.152}
\end{equation*}
$$

with $\rho_{n}$ being the density of the final states of system $b$, at the relevant energy $E_{n b}=E_{n^{\prime} b}+\hbar \omega=E_{n^{\prime} b}+$ $\left(E_{n}{ }^{\prime} a-E_{n a}\right)$. In particular, Eq. (152), with the dipole Hamiltonian (149), enables a very simple calculation of the natural linewidth of atomic electric dipole transitions. However, such calculation has to be postponed until Chapter 9 in which we will discuss the electromagnetic field quantization - i.e., the exact nature of states $n_{b}$ and $n^{\prime} b$ for this problem. Instead, I will proceed to a discussion of the effects of interaction of quantum systems with their environment, toward which the situation shown in Fig. 14 provides a clear path.

### 6.8. Exercise problems

6.1. Use Eq. (13) to prove the Hellmann-Feynman theorem: ${ }^{50}$

$$
\frac{\partial E_{n}}{\partial \lambda}=\langle n| \frac{\partial \hat{H}}{\partial \lambda}|n\rangle,
$$

where $\lambda$ is an arbitrary $c$-number parameter.
6.2. Analyze the relation between Eq. (15) and the results of classical analysis ${ }^{51}$ of a similar anharmonic ("nonlinear") oscillator.

[^660]6.3. A weak additional force $F$ is applied to a 1D particle that was placed into a hard-wall quantum well with
\[

U(x)= $$
\begin{cases}0, & \text { for } 0<x<a \\ +\infty, & \text { otherwise }\end{cases}
$$
\]

Calculate, sketch, and discuss the first-order perturbation of its ground-state wavefunction.
6.4. A 2 D quantum particle is confined in a square-shaped quantum well with infinitely high walls and slightly skewed floor:

$$
U=\left\{\begin{array}{lr}
\mu x y, & \text { for } 0<x<L \text { and } 0<y<L \\
+\infty, & \text { otherwise } .
\end{array}\right.
$$

In the first order in the small parameter $\mu$, find energies of the ground state and the lowest excited state of the system. Formulate the conditions of validity of your result.

Hint: To save reader's time on a straightforward but longish integration by parts, I can offer the following integral:

$$
\int_{0}^{1} \sin (\pi \xi) \sin (2 \pi \xi) \xi d \xi=-\frac{8}{9 \pi^{2}}
$$

6.5. Calculate the lowest-order relativistic correction to the ground-state energy of a 1D harmonic oscillator.
6.6. A 1 D particle of mass $m$ is localized at a narrow potential well which may be approximated with a delta-function:

$$
U(x)=-w \delta(x), \quad \text { with } w>0
$$

Calculate the change of its ground state energy by an additional weak, time-independent force $F$, in the first nonvanishing approximation of the perturbation theory. Discuss the limits of validity of this result, taking into account that at $F \neq 0$, the localized state of the particle is metastable.
6.7. Use the perturbation theory results to calculate the eigenvalues of the observable $L^{2}$, in the limit $l \approx|m| \gg 1$, by purely wave-mechanical means.

Hint: Try the following substitution: $\Theta(\theta)=f(\theta) / \sin ^{1 / 2} \theta$.
6.8. In the first nonvanishing order of the perturbation theory, calculate the shift of the groundstate energy of an electrically charged spherical rotator (i.e. a particle of mass $m$, free to move over a spherical surface of radius $R$ ) due to a weak, uniform, time-independent electric field $\boldsymbol{\varepsilon}$.
6.9. Use the perturbation theory to evaluate the effect of a constant electric field $\mathbf{E}$ on the ground state energy $E_{g}$ of a hydrogen atom. In particular:

[^661](i) calculate the $1^{\text {stt }}$-order shift of $E_{g}$,
(ii) bring the expression for the $2^{\text {nd }}$-order shift (neglecting the extended unperturbed states with $E$ $>0$ ) to the simplest possible analytical form,
(iii) find the lower and upper bounds on the result, and
(iv) discuss the simplest manifestations of the shift (called the quadratic Stark effect).
6.10.* A particle of mass $m$, with electric charge $q$, is in its ground $s$-state with known energy $E_{g}$ $<0$, being localized by a very short-range, spherically-symmetric potential well. Calculate its electric polarizability $\alpha$.
6.11. In the first nonvanishing order of the perturbation theory, calculate the correction to energies of the ground state and all lowest excited states of a hydrogen-like atom/ion, due to electron's penetration into its nucleus, modeling it as a spinless, uniformly charged sphere of radius $R \ll r_{\mathrm{B}} / Z$.
6.12. A spin $-1 / 2$ particle is placed into a magnetic field
$$
\boldsymbol{B}=\mathcal{B}_{z} \mathbf{n}_{z}+\mathcal{B}_{x} \mathbf{n}_{x}, \quad \text { with }\left|\mathcal{B}_{x}\right| \ll\left|\mathcal{B}_{z}\right| .
$$

Calculate its energy levels:
(i) exactly, and
(ii) in the first nonvanishing order of the perturbation theory in small $B_{x}$.

Compare the results of the two approaches.
6.13. Use the perturbation theory to analyze the orbital diamagnetism. Namely, calculate the magnetic susceptibility $\chi_{m}$ of a dilute gas due to the orbital motion of a single electron confined inside each gas particle.

Hint: You may like to use the well-known formula for the magnetic energy $u$ per unit volume of a linear medium:

$$
u=\mathcal{B}^{2} / 2 \mu
$$

where $\mathcal{B}$ is the applied magnetic field, and $\mu$ is the magnetic permeability, related to the susceptibility as $\mu \equiv \mu_{0}\left(1+\chi_{m}\right) .{ }^{52}$
6.14. ${ }^{*}$ Analyze the statistics of the spacing $S \equiv E_{+}-E$. between energy levels of a two-level system, assuming that all elements $H_{j j}$, of its Hamiltonian matrix (6.27) are independent random numbers, with equal and constant probability densities within the energy interval of interest. Compare the result with that for a purely diagonal matrix, with the similar probability distribution of the diagonal elements.
6.15. Discuss how to calculate the energy level degeneracy lifting in the second order of the perturbation theory, assuming that it is not lifted in the first order. Carry out such a calculation for a plane rotator of mass $m$ and radius $R$, carrying electric charge $q$, and placed into a weak, uniform, constant electric field $\varepsilon$.

[^662]6.16. Use the single-particle approximation to find the complex dielectric constant $\varepsilon(\omega)$ of a dilute gas of similar atoms, due to their induced electric polarization by a weak external ac field, for a field frequency $\omega$ very close to one of quantum transition frequencies $\omega_{n n}$, defined by Eq. (85).

Hint: In the single-particle approximation, atom's response to an external field is described as that of $Z$ similar, non-interacting electrons moving in an effective static attracting potential - generally induced not only by the nuclei but also by other electrons.
6.17. Use the solution of the previous problem to generalize the expression for the London dispersion force between two electroneutral molecules (whose calculation in the harmonic oscillator model was the subject of Problems 3.18 and 5.11) to the single-particle model with an arbitrary energy spectrum.
6.18. Use the solution of the previous problem to express the potential energy of interaction of two hydrogen atoms, both in their ground state and separated by distance $r \gg r_{\mathrm{B}}$, in the simplest analytical form, and use the result to estimate the energy.
6.19. In a certain quantum system, distances between three lowest energy levels are slightly different - see Fig. on the right $\left(|\xi| \ll \omega_{1,2}\right)$. Find the time necessary to populate the first excited level almost completely (with a given precision $\varepsilon \ll 1$ ), using the Rabi oscillation effect, if at $t=0$ the system is completely in its ground state.

Hint: Assume that all matrix elements of the perturbation Hamiltonian
 are known, and are all proportional to the external rf field amplitude.
6.20. A weak external force pulse $F(t)$, of a finite time duration, is applied to a 1 D harmonic oscillator that initially was in its ground state.
(i) Calculate, in the lowest nonvanishing order of the perturbation theory, the probability that the pulse drives the oscillator into an excited state.
(ii) Formulate the condition of validity of the result, and compare it with the exact solution of the problem.
(iii) Spell out the perturbative result for a Gaussian-shaped waveform,

$$
F(t)=F_{0} \exp \left\{-t^{2} / \tau^{2}\right\}
$$

and analyze its dependence on the effective duration $\tau$ of the pulse.
6.21. A charged plane rotator, initially in its ground state, is placed into a spatially-uniform, but time-dependent external field $\boldsymbol{\mathcal { E }}(t)$, applied at $t=0$.
(i) Calculate, in the lowest nonvanishing order in field's strength, the probability that the pulse drives the rotator oscillator into its $n^{\text {th }}$ excited state.
(ii) Spell out and analyze your results for a rotating field.
(iii) Same for an ac field with fixed polarization.
6.22 .
(i) Develop the general theory of excitations of the higher levels of a discrete-spectrum system, initially in the ground state, by a weak time-dependent perturbation, up to the $2^{\text {nd }}$ order.
(ii) Apply the theory to the system analyzed in the previous problem (a plane rotator driven by a time-dependent electric field) to find out what excitations, forbidden in the $1^{\text {st }}$ order of the perturbation theory, are allowed in its $2^{\text {nd }}$ order.
6.23. A heavy, relativistic particle, with the electric charge $q=Z e$, passes by a hydrogen atom, initially in its ground state, with the impact parameter (shortest distance) $b$ within the limits $r_{\mathrm{B}} \ll b \ll$ $r_{\mathrm{B}} / \alpha$, where $\alpha \approx 1 / 137$ is the fine structure constant. Calculate the probability of atom's transition to its lowest excited states.
6.24. ${ }^{*}$ A particle of mass $m$ is initially in the localized ground state, with the known energy $E_{g}<$ 0 , of a very small, spherically-symmetric potential well. Calculate the rate of its delocalization ("ionization") by an applied force $\mathbf{F}(t)=\mathbf{n}_{F} F_{0} \cos \omega t$, with a time-independent orientation $\mathbf{n}_{F}$, and discuss its dependence on frequency $\omega$.
6.25.* Calculate the rate of ionization of a hydrogen atom, initially in its ground state, by a classical, linearly polarized electromagnetic wave with electric field's amplitude $\varepsilon_{0}$, and frequency $\omega$ within the range

$$
\frac{\hbar}{m_{e} r_{\mathrm{B}}^{2}} \ll \omega \ll \frac{c}{r_{\mathrm{B}}},
$$

where $r_{\mathrm{B}}$ is the Bohr radius. Recast your result in terms of the cross-section of this electromagnetic wave absorption process. Discuss semi-quantitatively what changes would be necessary in the theory if either of the above conditions had been violated.
6.26. For the system of two weakly coupled quantum wells (see Fig. 13a), write the system of differential equations for the probability amplitudes $a_{n}$ defined by Eq. (2.199), and in particular prove Eqs. (2.201) - which were just guessed in Sec. 2.7.
6.27.* Use the quantum-mechanical Golden Rule to derive the general expression for the electric current $I$ through a weak tunnel junction between two conductors, biased with dc voltage $V$, treating the conduction electrons as a Fermi gas, in which the electron-electron interaction is limited to the Pauli exclusion principle. Simplify the result in the low-voltage limit.

Hint: The electric current flowing through a weak tunnel junction is so low that its perturbation of the electron states inside each conductor is negligible.
6.28. ${ }^{*}$ Generalize the result of the previous problem to the case when a weak tunnel junction is biased with voltage $V(t)=\bar{V}+A \cos \omega t$, with $\hbar \omega$ generally comparable with $e|\bar{V}|$ and $e A$.
6.29.* Use the quantum-mechanical Golden Rule to derive the Landau-Zener formula (2.266).
6.30. Calculate, in the $2^{\text {nd }}$ order of the perturbation theory, the rate $\Gamma$ of transitions between different states of a continuous group (of virtually the same energy $E_{n}$ ), induced by a monochromatic perturbation of frequency $\omega$, with $\hbar \omega$ comparable to the distances between other, discrete levels of the system.


## Chapter 7. Open Quantum Systems

This chapter discusses the effects of interaction of a quantum system with its environment, and in particular, with the instruments used for measurements. Some part of this material is on the fine line between quantum mechanics and (quantum) statistical physics. Here I will only cover those aspects of this field which are of key importance for the basic goals of this course, in particular for the discussion of quantum measurements in the end of the chapter. ${ }^{1}$

### 7.1. Open systems and the density matrix

All the way until the very end of the previous chapter, we have discussed quantum systems isolated from their environment. Indeed, from the very beginning we have assumed that we are dealing with the statistical ensembles of systems as similar to each other as only allowed by laws of quantum mechanics. Each member of such an ensemble, called pure or coherent, may be described by the same quantum state $\alpha$ - in the wave mechanics case, by the same wavefunction $\Psi_{\alpha}$. Even our discussion of the Golden Rule in the end of the last chapter, in particular its form in which one component system (in Fig. 6.13, system $b$ ) may be used as a model of the environment of another component ( $a$ ), was still based on the assumption of a pure initial state (6.146) of the system. Since the interaction of two component systems was described by a certain Hamiltonian (the one given by Eq. (6.145) for example), for the state $\alpha$ of the system as a whole at arbitrary instant we might write

$$
\begin{equation*}
|\alpha\rangle=\sum_{n} \alpha_{n}|n\rangle=\sum_{n} \alpha_{n}\left|n_{a}\right\rangle \otimes\left|n_{b}\right\rangle, \tag{7.1}
\end{equation*}
$$

with a unique correspondence between eigenstates states $n_{a}$ and $n_{b}$.
However, in many important cases our knowledge of quantum system's state is incomplete. This is especially unavoidable ${ }^{2}$ when a relatively simple quantum system $s$ of our interest (say, an electron or an atom) is in a contact with environment $e$ - here understood in a most general sense, say, as all the whole Universe less system $s-$ see Fig. 1. Then there is virtually no chance of making two or more experiments with exactly the same composite system, because it would imply a repeated preparation of the whole environment (including the experimenter :-) in a certain quantum state - a rather challenging task, to put it mildly. In this case, it makes much more sense to consider a statistical ensemble of another kind, with random quantum states of the environment, though possibly with known macroscopic parameters (e.g., temperature, pressure, etc.).

In classical physics, such mixed ensembles are the subject of statistical (classical) mechanics. ${ }^{3}$ Let us see how they may be described in quantum mechanics. For the beginning, we need to assume

[^663]again that the coupling between the system of interest and its environment is weak in the sense accepted in the perturbation theory. ${ }^{4}$ In this case we can still use the bra- and ket-vectors of unperturbed states, that depend on different sets of variables (again, "belonging to different Hilbert spaces"). Then the most general quantum state of the whole Universe, still assumed to be pure, ${ }^{5}$ may be described as the following linear superposition:
\[

$$
\begin{equation*}
|\alpha\rangle=\sum_{j, k} \alpha_{j k}\left|s_{j}\right\rangle \otimes\left|e_{k}\right\rangle . \tag{7.2}
\end{equation*}
$$

\]

Assumed quantum state of Universe

The "only" difference between the description of such an entangled state and the superposition of separable states, described by Eq. (1), is that coefficients $\alpha_{j k}$ in the right-hand part of Eq. (2) are numbered with two indices: index $j$ listing the quantum states of system $s$, and $k$ numbering the (enormously large) set of quantum states of the environment. So, in a mixed ensemble a certain state $s_{j}$ of the system of interest may coexist with different states of its environment. ${ }^{6}$ Of course, the enormity of the Hilbert space of the environment, i.e. the number of $k$-components in sum (2), strips us of any opportunity to make direct calculations using that sum. For example, according to the basic Eq. (4.125), in order to find the expectation value of an arbitrary observable $A$ in state (2), we would need to calculate

$$
\begin{equation*}
\langle A\rangle=\langle\alpha| \hat{A}|\alpha\rangle=\sum_{\substack{i, j^{\prime} \\ k, k^{\prime}}} \alpha_{j k}^{*} \alpha_{j^{\prime} k^{\prime}}\left\langle e_{k}\right| \otimes\left\langle s_{j}\right| \hat{A}\left|s_{j^{\prime}}\right\rangle \otimes\left|e_{k^{\prime}}\right\rangle \tag{7.3}
\end{equation*}
$$

Even if we assume that $\{s\}$ and $\{e\}$ are sets of the basis states of, respectively, the system and the environment, and that each is full and orthonormal, Eq. (3) still includes a double sum over the enormous basis state set of the environment!


However, let us consider a limited but the most important subset of operators - those of intrinsic observables, which depend only on the degrees of freedom of the system of interest $(s)$. These operators commute do not act on environment's degrees of freedom, and hence in Eq. (3) we may move the environment bra-vector $\left\langle e_{k}\right|$ over all the way to ket-vector $\left|e_{k^{\prime}}\right\rangle$. Assuming, again, that the set of environmental eigenstates is full and orthonormal, Eq. (3) is now reduced to

[^664]\[

$$
\begin{equation*}
\langle A\rangle=\sum_{\substack{j, j^{\prime} \\ k, k^{\prime}}} \alpha_{j k}^{*} \alpha_{j k^{\prime}}\left\langle s_{j}\right| \hat{A}\left|s_{j^{\prime}}\right\rangle\left\langle e_{k} \mid e_{k^{\prime}}\right\rangle=\sum_{i j^{\prime}} A_{j j^{\prime}} \sum_{k} \alpha_{j k}^{*} \alpha_{j^{\prime} k} . \tag{7.4}
\end{equation*}
$$

\]

This is already some relief, because we have "only" a single sum over $k$, but the main trick 7 is still ahead. After the summation over $k$, the second sum in the last form of Eq. (4) is some function $w$ of indices $j$ and $j$ ', so that, according to Eq. (4.96), this relation may be presented as

Expectation value of intrinsic observable

$$
\begin{equation*}
\langle A\rangle=\sum_{i j j^{\prime}} A_{i j j^{\prime}} w_{j^{\prime} j}=\operatorname{Tr}(\mathrm{Aw}) \tag{7.5}
\end{equation*}
$$

where matrix w , with elements

Density matrix: definition

$$
\begin{equation*}
w_{j^{\prime} j} \equiv \sum_{k} \alpha_{j k}^{*} \alpha_{j^{\prime} k}, \quad \text { i.e. } w_{j j^{\prime}} \equiv \sum_{k} \alpha_{j k} \alpha_{j^{\prime} k}^{*} \tag{7.6}
\end{equation*}
$$

is called the density matrix of the system. Most importantly, Eq. (5) shows that the knowledge of this matrix allows the calculation of the expectation value of any intrinsic observable $A$ (and, according to Eqs. (1.33)-(1.34), its r.m.s. fluctuation as well if necessary), even for the very general statistical ensemble of states (2). This is why let us have a very good look at the density matrix.

First of all, as we know very well by now that the expansion coefficients in superpositions of the type (2) may be always expressed as bra-kets; in our current case, we may write

$$
\begin{equation*}
\alpha_{j k}=\left\langle e_{k}\right| \otimes\left\langle s_{j} \| \alpha\right\rangle \tag{7.7}
\end{equation*}
$$

Plugging this expression into Eq. (6), we get

$$
\begin{equation*}
w_{j j^{\prime}}=\sum_{k} \alpha_{j k} \alpha_{j^{\prime k}}^{*}=\left\langle s_{j}\right| \otimes\left(\sum_{k}\left\langle e_{k} \mid \alpha\right\rangle\left\langle\alpha \mid e_{k}\right\rangle\right) \otimes\left|s_{j^{\prime}}\right\rangle=\left\langle s_{j}\right| \hat{w}\left|s_{j^{\prime}}\right\rangle . \tag{7.8}
\end{equation*}
$$

We see that from the point of our system (i.e. in its Hilbert space whose basis states may be numbered by indices $j$ only), the density matrix is indeed just the matrix of some construct, ${ }^{8}$

Statistical operator: definition

$$
\begin{equation*}
\hat{w} \equiv \sum_{k}\left\langle e_{k} \mid \alpha\right\rangle\left\langle\alpha \mid e_{k}\right\rangle, \tag{7.9}
\end{equation*}
$$

that is called the statistical (or "density") operator. As evident from its definition (9), in contrast to the density matrix this operator does not depend on the choice of a particular basis $s_{j}$ - just as all previous operators considered in this course, but in contrast to them, the statistical operator does depend on composite system's state $\alpha$, including the state of system $s$ as well. However, in the $j$-space it is mathematically still an operator whose matrix elements obey all formulas of the bra-ket formalism.

In particular, due to its definition (6), the density operator is Hermitian:

$$
\begin{equation*}
w_{i j^{\prime}}^{*}=\sum_{k} \alpha_{j k}^{*} \alpha_{j^{\prime} k}=\sum_{k} \alpha_{j^{\prime} k} \alpha_{j k}^{*}=w_{j j^{\prime}} \tag{7.10}
\end{equation*}
$$

[^665]so that according to the general analysis of Sec. 4.3, there should be a certain basis $\{w\}$ in which the matrix of this operator is diagonal:
\[

$$
\begin{equation*}
\left.w_{i j^{\prime}}\right|_{\text {in } w}=w_{j} \delta_{j j^{\prime}} . \tag{7.11}
\end{equation*}
$$

\]

Since any operator, in any basis may be presented in form (4.59), in basis $\{w\}$ we may write

$$
\begin{equation*}
\hat{w}=\sum_{j}\left|w_{j}\right\rangle w_{j}\left\langle w_{j}\right| . \tag{7.12}
\end{equation*}
$$

Statistical operator in diagonalizing
basis

This expression reminds, but is not equivalent to Eq. (4.44) for the identity operator, that has been used so many times in this course, and in the basis $w_{j}$ has the form

$$
\begin{equation*}
\hat{I}=\sum_{j}\left|w_{j}\right\rangle\left\langle w_{j}\right| . \tag{7.13}
\end{equation*}
$$

In order to comprehend the meaning of coefficients $w_{j}$ participating in Eq. (12), let us use Eq. (5) to calculate the expectation value of any observable $A$ whose eigenstates coincide with those of the special basis set $\{w\}$ :

$$
\begin{equation*}
\langle A\rangle=\operatorname{Tr}(\mathrm{Aw})=\sum_{i j j^{\prime}} A_{i j^{\prime}} w_{j} \delta_{i j^{\prime}}=\sum_{j} A_{j} w_{j} \tag{7.14}
\end{equation*}
$$

Expectation value of $w_{j}$-compatible variable
where $A_{j}$ is just the expectation value of observable $A$ in state $w_{j}$. Hence, in order to comply with the general Eq. (1.37), real $c$-numbers $w_{j}$ must have the physical sense of probabilities $W_{j}$ of finding the system in state $j$. As the result, we can rewrite Eq. (12) in the form

$$
\begin{equation*}
\hat{w}=\sum_{j}\left|w_{j}\right\rangle W_{j}\left\langle w_{j}\right| . \tag{7.15}
\end{equation*}
$$

In one ultimate case when only one of probabilities (say, $W_{j^{\prime \prime}}$ ) is different from zero,

$$
\begin{equation*}
W_{j}=\delta_{j j^{\prime \prime}}, \tag{7.16}
\end{equation*}
$$

the system is evidently in a coherent (pure) state $w_{j^{\prime \prime}}$. Indeed, it is fully described by one ket-vector $\left|w_{j^{\prime \prime}}\right\rangle$, and we can use the general rule (4.86) to present it in another (arbitrary) basis $\{s\}$ as a coherent superposition

$$
\begin{equation*}
\left|w_{j^{\prime \prime}}\right\rangle=\sum_{j^{\prime}}\left(U^{\dagger}\right)_{j j^{\prime}}\left|s_{j^{\prime}}\right\rangle=\sum_{j^{\prime}} U_{i j^{\prime}}^{*}\left|s_{j^{\prime}}\right\rangle, \tag{7.17}
\end{equation*}
$$

where U is the unitary matrix of transform from basis $\{w\}$ to basis $\{s\}$. According to Eqs. (11) and (16), in such a pure state the density matrix is diagonal in the $\{w\}$ basis,

$$
\begin{equation*}
\left.w_{i j^{\prime}}\right|_{\text {in } w}=\delta_{j, j^{\prime \prime}} \delta_{j^{\prime}, j^{\prime \prime}}, \tag{7.18a}
\end{equation*}
$$

but not in an arbitrary basis. Indeed, using the general rule (4.92), we get

$$
\begin{equation*}
\left.w_{i j^{\prime}}\right|_{\text {in } s}=\left.\sum_{l, l^{\prime}} U_{j l}^{\dagger} w_{l l^{\prime}}\right|_{\text {in } w} U_{l j^{\prime}}=U_{i j^{\prime}}^{\dagger} U_{j^{\prime \prime} j^{\prime}}=U_{j^{\prime \prime} j}^{*} U_{j^{\prime \prime} j^{\prime}} . \tag{7.18b}
\end{equation*}
$$

To make this result more transparent, let us denote matrix elements $U_{j^{\prime \prime} j}=\left\langle w_{j^{\prime}} \mid S_{j}\right\rangle$ (that, for fixed $j$ ', depend on just one index $j$ ) by $\alpha_{j}$; then

Density matrix in a pure state

$$
\begin{equation*}
\left.w_{i j^{\prime}}\right|_{\text {in } s}=\alpha_{j}^{*} \alpha_{j^{\prime}}, \tag{7.19}
\end{equation*}
$$

so that $N^{2}$ elements of the whole $N \times N$ matrix is determined by just one string of $N c$-numbers $\alpha_{j}$. For example, for a two-level system ( $N=2$ ),

$$
\left.\mathrm{w}\right|_{\mathrm{in} s}=\left(\begin{array}{ll}
\alpha_{1} \alpha_{1}^{*} & \alpha_{2} \alpha_{1}^{*}  \tag{7.20}\\
\alpha_{1} \alpha_{2}^{*} & \alpha_{2} \alpha_{2}^{*}
\end{array}\right) .
$$

We see that the off-diagonal terms are, colloquially, "as large as the diagonal ones", in the following sense:

$$
\begin{equation*}
w_{12} w_{21}=w_{11} w_{22} \tag{7.21}
\end{equation*}
$$

Since the diagonal terms have the sense of probabilities $W_{1,2}$ to find the system in the corresponding state, we may present Eq. (20) in the form

$$
\mathrm{w}=\left(\begin{array}{cc}
W_{1} & \left(W_{1} W_{2}\right)^{1 / 2} e^{i \varphi}  \tag{7.22}\\
\left(W_{1} W_{2}\right)^{1 / 2} e^{-i \varphi} & W_{2}
\end{array}\right) .
$$

The physical sense of the (real) constant $\varphi$ is the phase shift between the coefficients in the linear superposition (17) that presents the pure state $w_{j " \prime}$ in basis $s_{1,2}$.

Now let us consider a different statistical ensemble of two-level systems, that includes member states identical in all aspects (including similar probabilities $W_{1,2}$ in the same basis $s_{1,2}$ ), besides that the phase shifts $\varphi$ are random, with the phase probability uniformly distributed over the trigonometric circle. Then the ensemble averaging is equivalent to averaging over $\varphi$ from 0 to $2 \pi$, so that it kills the offdiagonal terms of the density matrix (22), and the matrix becomes diagonal. For a system with a timeindependent Hamiltonian, such averaging is especially plausible in the basis of stationary states $n$ of the system, in which phase $\varphi$ is just the difference of integration constants in Eq. (4.158), and randomness is naturally produced by minor fluctuations of the energy difference $E_{1}-E_{2}$. (In Sec. 3 we will study the dynamics of such dephasing process.) The mixed statistical ensemble of systems with the density matrix diagonal in the stationary state basis is called the classical mixture, and presents the limit opposite to the pure (coherent) state.

After that example, the reader should not be much shocked by the main claim ${ }^{9}$ of statistical mechanics that any large ensemble of similar systems in thermodynamic (or "thermal") equilibrium is exactly such a classical mixture. Moreover, for systems in the thermal equilibrium with a much larger environment with fixed temperature $T$ (such environment is usually called a heat bath or a thermostat) statistical physics gives ${ }^{10}$ a very simple expression, called the Gibbs distribution, for probabilities $W_{n}$ :

Gibbs distribution

$$
\begin{equation*}
W_{n}=\frac{1}{Z} \exp \left\{-\frac{E_{n}}{k_{\mathrm{B}} T}\right\} \tag{7.23a}
\end{equation*}
$$

[^666]where $E_{n}$ is the eigenenergy of the corresponding stationary state, and $Z$ is the normalization coefficient called the statistical sum
\[

$$
\begin{equation*}
Z \equiv \sum_{n} \exp \left\{-\frac{E_{n}}{k_{\mathrm{B}} T}\right\} . \tag{7.23b}
\end{equation*}
$$

\]

A detailed analysis of classical and quantum ensembles in thermodynamic equilibrium is the focus of statistical physics courses (such as my SM) rather than this course of quantum mechanics. However, I would still like to attract reader's attention to the key fact that, in contrast with the similarlylooking Boltzmann distribution for single particles, ${ }^{11}$ the Gibbs distribution is absolutely general and is not limited to classical statistics. In particular, for quantum gases of indistinguishable particles, it is absolutely compatible with quantum statistics (such as the Bose-Einstein or Fermi-Dirac distributions) of the component particles. For example, if we use Eq. (23) to calculate the average energy of a 1D harmonic oscillator of frequency $\omega_{0}$ in thermal equilibrium, we easily get ${ }^{12}$

$$
\begin{gather*}
W_{n}=\exp \left\{-n \frac{\hbar \omega_{0}}{k_{\mathrm{B}} T}\right\}\left(1-\exp \left\{-\frac{\hbar \omega_{0}}{k_{\mathrm{B}} T}\right\}\right),  \tag{7.24}\\
Z=\exp \left\{-\frac{\hbar \omega_{0}}{2 k_{\mathrm{B}} T}\right\} /\left(1-\exp \left\{-\frac{\hbar \omega_{0}}{k_{\mathrm{B}} T}\right\}\right),  \tag{7.25}\\
\langle E\rangle=\sum_{n=0}^{\infty} W_{n} E_{n}=\frac{\hbar \omega_{0}}{2} \operatorname{coth} \frac{\hbar \omega_{0}}{2 k_{\mathrm{B}} T}=\frac{\hbar \omega_{0}}{2}+\frac{\hbar \omega_{0}}{\exp \left\{\hbar \omega_{0} / k_{\mathrm{B}} T\right\}-1} . \tag{7.26a}
\end{gather*}
$$

An alternative way to present the last result is to write

$$
\begin{equation*}
\langle E\rangle=\frac{\hbar \omega_{0}}{2}+\hbar \omega_{0}\langle n\rangle, \quad \text { with }\langle n\rangle=\frac{1}{\exp \left\{\hbar \omega_{0} / k_{\mathrm{B}} T\right\}-1} \tag{7.26b}
\end{equation*}
$$

and to interpret it as the fact that in addition to the so-called zero-point energy $\hbar \omega_{0} / 2$ of the ground state, the oscillator (on the average) has $\langle n\rangle$ thermally-induced excitations, with energy $\hbar \omega_{0}$ each. In the harmonic oscillator, whose energy levels are equidistant, such a language is completely appropriate, because the transfer from any level to one just above it adds the same amount of energy, $\hbar \omega_{0}$, to the system. The above expression for $\langle n\rangle$ is actually the Bose-Einstein distribution (for the particular case of zero chemical potential); ${ }^{13}$ we see that it does not only contradict the Gibbs distribution (for the total energy of the system), but immediately follows from it. ${ }^{14}$

[^667]
### 7.2. Coordinate representation and the Wigner function

For many applications of the density matrix to wave mechanics, its coordinate representation is convenient. (I will only discuss it for 1D case; the generalization to multi-dimension case is straightforward.) Following Eq. (4.47), it is natural to define the following function of two arguments (frequently also called the density matrix):

$$
\begin{equation*}
w\left(x, x^{\prime}\right) \equiv\langle x| \hat{w}\left|x^{\prime}\right\rangle . \tag{7.27}
\end{equation*}
$$

Inserting, into the right-hand part of this definition, two closure conditions (4.44) for an arbitrary (full and orthonormal) basis $\{\mathrm{s}\}$, and then using Eq. (5.19), we get ${ }^{15}$

$$
\begin{equation*}
w\left(x, x^{\prime}\right)=\sum_{j, j^{\prime}}\left\langle x \mid s_{j}\right\rangle\left\langle s_{j}\right| \hat{w}\left|s_{j^{\prime}}\right\rangle\left\langle s_{j^{\prime}} \mid x^{\prime}\right\rangle=\sum_{j, j^{\prime}} \psi_{j}(x) w_{j j^{\prime}} \mid \text { ins } \psi_{j^{\prime}}^{*}\left(x^{\prime}\right) . \tag{7.28}
\end{equation*}
$$

In the special basis $\{w\}$, in which the density matrix is diagonal, this expression is reduced to

$$
\begin{equation*}
w\left(x, x^{\prime}\right)=\sum_{j} \psi_{j}(x) W_{j} \psi_{j}^{*}\left(x^{\prime}\right) \tag{7.29}
\end{equation*}
$$

Let us discuss the properties of this function. At coinciding arguments, $x=x$, this is just the probability density: ${ }^{16}$

$$
\begin{equation*}
w(x, x)=\sum_{j} \psi_{j}(x) W_{j} \psi_{j}^{*}(x)=\sum_{j} w_{j}(x) W_{j}=w(x) . \tag{7.30}
\end{equation*}
$$

However, the density matrix gives more information about the system than just the probability density. As the simplest example, let us consider a pure quantum state, with $W_{j}=\delta_{j, j}$, so that $\psi(x)=\psi_{j}(x)$, and

$$
\begin{equation*}
w\left(x, x^{\prime}\right)=\psi_{j^{\prime}}(x) \psi_{j^{\prime}}^{*}\left(x^{\prime}\right)=\psi(x) \psi^{*}\left(x^{\prime}\right) . \tag{7.31}
\end{equation*}
$$

We see that the density matrix carries the information not only about the modulus but also the phase of the wavefunction. (Of course one may argue rather convincingly that in this ultimate limit the densitymatrix description is redundant, because all this information is contained in the wavefunction itself.)

How may be the density matrix interpreted? In the simple case (31), we can write

$$
\begin{equation*}
\left|w\left(x, x^{\prime}\right)\right|^{2}=w\left(x, x^{\prime}\right) w^{*}\left(x, x^{\prime}\right)=\psi(x) \psi^{*}(x) \psi\left(x^{\prime}\right) \psi^{*}\left(x^{\prime}\right)=w(x) w\left(x^{\prime}\right), \tag{7.32}
\end{equation*}
$$

so that the modulus squared of the density matrix may is just as the joint probability density to find the system at point $x$ and point $x^{\prime}$. For example, for a simple wave packet with the spatial extent $\delta x, w\left(x, x^{\prime}\right)$ is appreciable only if the both points are not farther than $\delta x$ from the packet center, and hence from each other. The interpretation becomes more complex if we deal with an incoherent mixture of several wavefunctions, for example the classical mixture describing the thermodynamic equilibrium. In this case, we can use Eq. (23) to rewrite Eq. (29) as follows:

[^668]\[

$$
\begin{equation*}
w\left(x, x^{\prime}\right)=\sum_{n} \psi_{n}(x) W_{n} \psi_{n}^{*}\left(x^{\prime}\right)=\frac{1}{Z} \sum_{n} \psi_{n}(x) \exp \left\{-\frac{E_{n}}{k_{B} T}\right\} \psi_{n}^{*}\left(x^{\prime}\right) . \tag{7.33}
\end{equation*}
$$

\]

As the simplest example, let us see what is the density matrix of a free (1D) particle in the thermal equilibrium. As we know very well, in this case, the set of energies $E_{p}=p^{2} / 2 m$ of stationary states (monochromatic waves) forms a continuum, so that we need to replace sum (33) by an integral, taking "delta-normalized" traveling wavefunctions (5.59) as eigenstates:

$$
\begin{equation*}
w\left(x, x^{\prime}\right)=\frac{1}{2 \pi \hbar Z} \int_{-\infty}^{+\infty} \exp \left\{-\frac{i p x}{\hbar}\right\} \exp \left\{-\frac{p^{2}}{2 m k_{B} T}\right\} \exp \left\{\frac{i p x^{\prime}}{\hbar}\right\} d p \tag{7.34}
\end{equation*}
$$

This is a usual Gaussian integral, and may be worked out, as we have done repeatedly in Chapter 2 and beyond, by complementing the exponent to the full square of momentum plus a constant. The statistical sum $Z$ may be also readily calculated, ${ }^{17}$

$$
\begin{equation*}
Z=\left(2 \pi m k_{B} T\right)^{1 / 2} \tag{7.35}
\end{equation*}
$$

However, for what follows it is more useful to write the result for product $w Z$ (the so-called unnormalized density matrix):

$$
\begin{equation*}
w\left(x, x^{\prime}\right) Z=\left(\frac{m k_{\mathrm{B}} T}{2 \pi \hbar^{2}}\right)^{1 / 2} \exp \left\{-\frac{m k_{\mathrm{B}} T\left(x-x^{\prime}\right)^{2}}{2 \hbar^{2}}\right\} \tag{7.36}
\end{equation*}
$$

This is a very interesting result: the density matrix depends only on the difference of its arguments, dropping to zero fast as the distance between points $x$ and $x$ ' exceeds the following characteristic scale (called the correlation length)

$$
\begin{equation*}
x_{c} \equiv\left\langle\left(x-x^{\prime}\right)^{2}\right\rangle^{1 / 2}=\frac{\hbar}{\left(m k_{\mathrm{B}} T\right)^{1 / 2}} \tag{7.37}
\end{equation*}
$$

This length may be interpreted in the following way. It is straightforward to use Eq. (23) to verify that the average energy $E_{p}=p^{2} / 2 m$ of a particle in the thermal equilibrium, i.e. in the classical mixture (33), equals $k_{\mathrm{B}} T / 2$ - this is just one more manifestation of the equipartition theorem. Hence the average momentum magnitude may be estimated as

$$
\begin{equation*}
p_{c} \equiv\left\langle p^{2}\right\rangle^{1 / 2}=(2 m\langle E\rangle)^{1 / 2}=\left(m k_{B} T\right)^{1 / 2} \tag{7.38}
\end{equation*}
$$

so that $x_{c}$ is of the order of the minimal length allowed by the Heisenberg-like "uncertainty relation":

$$
\begin{equation*}
x_{c}=\frac{\hbar}{p_{c}} . \tag{7.39}
\end{equation*}
$$

[^669]Notice that with the growth of temperature, the correlation length (37) goes to zero, and the density matrix (36) tends to the $\delta$-function:

$$
\begin{equation*}
\left.w\left(x, x^{\prime}\right) Z\right|_{T \rightarrow \infty} \rightarrow \delta\left(x-x^{\prime}\right) \tag{7.40}
\end{equation*}
$$

Since in this limit the average kinetic energy of the particle is larger than its potential energy in any fixed potential profile, Eq. (40) is the general property of the density matrix (33).

Let us discuss the following curious feature of Eq. (36): if we replace $k_{\mathrm{B}} T$ with $\hbar / i\left(t-t_{0}\right)$, and $x$, with $x_{0}$, the un-normalized density matrix $w Z$ for a free particle turns into the particle's propagator - see Eq. (2.49). This is not just an occasional coincidence. Indeed, in Chapter 2 we saw that the propagator of a system with an arbitrary stationary Hamiltonian may be expressed via the stationary eigenfunction as

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\sum_{n} \psi_{n}(x) \exp \left\{-i \frac{E_{n}}{\hbar}\left(t-t_{0}\right)\right\} \psi_{n}^{*}\left(x_{0}\right) . \tag{7.41}
\end{equation*}
$$

Comparing this expression with Eq. (33), we see that the replacements

$$
\begin{equation*}
\frac{i\left(t-t_{0}\right)}{\hbar} \rightarrow \frac{1}{k_{\mathrm{B}} T}, \quad x_{0} \rightarrow x^{\prime} \tag{7.42}
\end{equation*}
$$

turn the pure-state propagator $G$ into the un-normalized density matrix $w Z$ of the same system in thermodynamic equilibrium. This important fact, rooted in the formal similarity of the Gibbs distribution (23) with the Schrödinger equation's solution (1.67), enables a theoretical technique of the so-called thermodynamic Green's functions, which is especially productive in condensed matter physics. ${ }^{18}$

For our purposes, we can use Eq. (42) to recycle some of wave mechanics results, in particular the following formula for the harmonic oscillator's propagator

$$
\begin{equation*}
G\left(x, t ; x_{0}, t_{0}\right)=\left(\frac{m \omega_{0}}{2 \pi i \hbar \sin \left[\omega_{0}\left(t-t_{0}\right)\right]}\right)^{1 / 2} \exp \left\{-\frac{m \omega_{0}\left[\left(x^{2}+x_{0}^{2}\right) \cos \left[\omega_{0}\left(t-t_{0}\right)\right]-2 x x_{0}\right]}{2 i \hbar \sin \left[\omega_{0}\left(t-t_{0}\right)\right]}\right\} . \tag{7.43}
\end{equation*}
$$

that may be readily proved to satisfy the Schrödinger equation for Hamiltonian (5.95), with the appropriate initial condition, $G\left(x, t_{0} ; x_{0}, t_{0}\right)=\delta\left(x-x_{0}\right)$. Making substitution (42), we immediately get

Harmonic oscillator in thermal equilibrium

$$
\begin{equation*}
w\left(x, x^{\prime}\right) Z=\left(\frac{m \omega_{0}}{2 \pi \hbar \sinh \left[\hbar \omega_{0} / k_{B} T\right]}\right)^{1 / 2} \exp \left\{-\frac{m \omega_{0}\left[\left(x^{2}+x^{\prime 2}\right) \cosh \left[\hbar \omega_{0} / k_{B} T\right]-2 x x^{\prime}\right]}{2 \hbar \sinh \left[\hbar \omega_{0} / k_{B} T\right]}\right\} . \tag{7.44}
\end{equation*}
$$

As a sanity check, at very low temperatures, $k_{\mathrm{B}} T \ll \hbar \omega_{0}$, both hyperbolic functions, participating in this expression, are very large and nearly equal, and Eq. (44) yields

$$
\begin{equation*}
\left.w\left(x, x^{\prime}\right) Z\right|_{T \rightarrow 0} \rightarrow\left[\left(\frac{m \omega_{0}}{\pi \hbar}\right)^{1 / 4} \exp \left\{-\frac{m \omega_{0} x^{2}}{\hbar}\right\}\right] \times \exp \left\{-\frac{\hbar \omega_{0}}{2 k_{B} T}\right\} \times\left[\left(\frac{m \omega_{0}}{\pi \hbar}\right)^{1 / 4} \exp \left\{-\frac{m \omega_{0} x^{\prime 2}}{\hbar}\right\}\right] . \tag{7.45}
\end{equation*}
$$

[^670]In each of the square brackets we can readily recognize the ground state's wavefunction (2.269), while the middle exponent is just the statistical sum (24) in the low-temperature limit when it is dominated by the ground-level contribution:

$$
\begin{equation*}
\left.Z\right|_{T \rightarrow 0} \rightarrow \exp \left\{-\frac{\hbar \omega_{0}}{2 k_{B} T}\right\} \tag{7.46}
\end{equation*}
$$

As a result, $Z$ in both parts of Eq. (45) may be cancelled, and the density matrix in this limit is described by Eq. (31), with the ground state as the only state of the system. This is natural when temperature is too low for the excitation of any other state.

Returning to arbitrary temperatures, Eq. (44) in coinciding arguments gives the following expression for the probability density: ${ }^{19}$

$$
\begin{equation*}
w(x, x) Z=w(x) Z=\left(\frac{m \omega_{0}}{2 \pi \hbar \sinh \left[\hbar \omega_{0} / k_{B} T\right]}\right)^{1 / 2} \exp \left\{-\frac{m \omega_{0} x^{2}}{\hbar} \tanh \frac{\hbar \omega_{0}}{2 k_{B} T}\right\} \tag{7.47}
\end{equation*}
$$

This is just a Gaussian function of $x$, with the following variance:

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=\frac{\hbar}{2 m \omega_{0}} \operatorname{coth} \frac{\hbar \omega_{0}}{2 k_{B} T} . \tag{7.48}
\end{equation*}
$$

In order to compare this result with our earlier ones, it is useful to recast it as

$$
\begin{equation*}
\langle U\rangle=\frac{m \omega_{0}^{2}}{2}\left\langle x^{2}\right\rangle=\frac{\hbar \omega_{0}}{4} \operatorname{coth} \frac{\hbar \omega_{0}}{2 k_{B} T} . \tag{7.49}
\end{equation*}
$$

Comparing this expression with Eq. (26), we see that the average value of potential energy is exactly one half of the total energy - the other half being the average kinetic energy. This is what we could expect, because according to Eqs. (5.129)-(5.130), such relation holds for each Fock state and hence should also hold for their classical mixture.

Unfortunately, besides the trivial case (30) of coinciding arguments, it is hard to give a straightforward interpretation of the density function in terms of system measurements. This is a fundamental difficulty that has been well explored in terms of the Wigner function (sometimes called the "Wigner-Ville distribution") ${ }^{20}$ defined as

$$
\begin{equation*}
W(X, P) \equiv \frac{1}{2 \pi \hbar} \int w\left(X+\frac{\tilde{X}}{2}, X-\frac{\widetilde{X}}{2}\right) \exp \left\{-\frac{i P \tilde{X}}{\hbar}\right\} d \widetilde{X} \tag{7.50}
\end{equation*}
$$

[^671]From the mathematical standpoint, this is just the Fourier expansion of the density matrix in one of two new coordinates (Fig. 2) defined by relations

$$
\begin{equation*}
x=X+\frac{\tilde{X}}{2}, \quad x^{\prime}=X-\frac{\tilde{X}}{2} . \tag{7.51}
\end{equation*}
$$

Physically, the new argument $X=\left(x+x^{\prime}\right) / 2$ may be understood as the average position of the particle during the time interval $\left(t-t^{\prime}\right)$, while $\tilde{X}=x-x^{\prime}$ as the distance passed by the particle during that time interval, so that $P$ may be interpreted as the characteristic momentum of a particle during that motion. As a result, the Wigner function is a construct intended to characterize the system spread simultaneously in the coordinate and momentum space - for 1D systems, on the phase plane $[X, P]$ that we considered before - see Fig. 5.6. Let us see how fruitful these intentions are.


Fig. 7.2. Coordinates $X$ and $\tilde{X}$ employed in the WeylWigner transform (50). They differ from the coordinates obtained by the rotation of the reference frame by angle $\pi / 2$ only by coefficients $\sqrt{ } 2$, describing scale stretching.

First of all, we may write the Fourier transform reciprocal to Eq. (50):

$$
\begin{equation*}
w\left(X+\frac{\tilde{X}}{2}, X-\frac{\tilde{X}}{2}\right)=\int W(X, P) \exp \left\{+\frac{i P \tilde{X}}{\hbar}\right\} d P \tag{7.52}
\end{equation*}
$$

For the particular case $\tilde{X}=0$, this relation yields

$$
\begin{equation*}
w(X) \equiv w(X, X)=\int W(X, P) d P \tag{7.53}
\end{equation*}
$$

Hence the integral of the Wigner function over momentum $P$ gives the probability density to find the system at point $X$.

Actually, the function has the same property for integration over $X$. To prove that, we should first introduce the momentum representation of the density matrix, in the full analogy with its coordinate representation (27):

$$
\begin{equation*}
w\left(p, p^{\prime}\right) \equiv\langle p| \hat{w}\left|p^{\prime}\right\rangle . \tag{7.54}
\end{equation*}
$$

Inserting, as usual, two identity operators, in the form given by Eq. (5.21), into the right hand part of this equality, we can get the following relation between the momentum and coordinate representations:

$$
\begin{equation*}
w\left(p, p^{\prime}\right) \equiv\langle p| \hat{w}\left|p^{\prime}\right\rangle=\iint d x d x^{\prime}\langle p \mid x\rangle\langle x| \hat{w}\left|x^{\prime}\right\rangle\left\langle x^{\prime} \mid p^{\prime}\right\rangle=\frac{1}{2 \pi \hbar} \iint d x d x^{\prime} \exp \left\{-\frac{i p x}{\hbar}\right\} w\left(x, x^{\prime}\right) \exp \left\{\frac{i p^{\prime} x^{\prime}}{\hbar}\right\} \cdot( \tag{7.55}
\end{equation*}
$$

This is of course nothing else than the unitary transform of an operator from the $x$-basis to $p$-basis, and is similar to the first form of Eq. (5.67). ${ }^{21}$ For coinciding arguments, $p=p$, Eq. (55) is reduced to

$$
\begin{equation*}
w(p) \equiv w(p, p)=\frac{1}{2 \pi \hbar} \iint d x d x^{\prime} w\left(x, x^{\prime}\right) \exp \left\{-\frac{i p\left(x-x^{\prime}\right)}{\hbar}\right\} . \tag{7.56}
\end{equation*}
$$

Using Eq. (29) and then Eq. (5.60), this function may be presented as

$$
\begin{equation*}
w(p)=\frac{1}{2 \pi \hbar} \sum_{j} W_{j} \iint d x d x^{\prime} \psi_{j}(x) \psi_{j}^{*}(x) \exp \left\{-\frac{i p\left(x-x^{\prime}\right)}{\hbar}\right\}=\sum_{j} W_{j} \varphi_{j}(p) \varphi_{j}^{*}(p), \tag{7.57}
\end{equation*}
$$

and hence interpreted as the probability density of the particle's momentum at point $p$. Now, in variables (51), Eq. (56) has the form

$$
\begin{equation*}
w(p)=\frac{1}{2 \pi \hbar} \iint w\left(X+\frac{\widetilde{X}}{2}, X-\frac{\tilde{X}}{2}\right) \exp \left\{-\frac{i p \tilde{X}}{\hbar}\right\} d \widetilde{X} d X \tag{7.58}
\end{equation*}
$$

Comparing this equality with definition (50) of the Wigner function, we see that

$$
\begin{equation*}
w(P)=\int W(X, P) d X . \tag{7.59}
\end{equation*}
$$

Thus, according to Eqs. (53) and (59), the integrals of the Wigner function over either the coordinate or momentum give the probability densities to find them at certain values of these variables. This is of course the main requirement to any candidate joint probability density, $\rho(X, P)$, to find a classical representation point of a stochastic system on the phase plane $[X, P] .{ }^{22}$

Let us look how does the Wigner function look for the simplest systems in the thermodynamic equilibrium. For a free 1D particle, we can use Eq. (34), ignoring for simplicity the normalization issues:

$$
\begin{equation*}
W(X, P) \propto \int_{-\infty}^{+\infty} \exp \left\{-\frac{m k_{B} T \widetilde{X}^{2}}{2 \hbar^{2}}\right\} \exp \left\{-\frac{i P \tilde{X}}{\hbar}\right\} d \widetilde{X} \tag{7.60}
\end{equation*}
$$

The usual Gaussian integration yields:

$$
\begin{equation*}
W(X, P)=\text { const } \times \exp \left\{-\frac{P^{2}}{2 m k_{B} T}\right\} \tag{7.61}
\end{equation*}
$$

We see that the function is independent of $X$ (as it should be for this translational-invariant system), and coincides with the Gibbs distribution (23). We could get the same result directly from classical statistics. This is natural, because as we know from Sec. 2.2, the free motion is essentially not quantized - at least in terms of its energy and momentum.

Now let us consider a substantially quantum system, the harmonic oscillator. Plugging Eq. (44) into Eq. (50), for that system in thermal equilibrium it is easy to show (and hence is left for reader's exercise) that the Wigner function is also Gaussian, but now in both its arguments:

[^672]Thermal equilibrium: harmonic oscillator

$$
\begin{equation*}
W(X, P)=\text { const } \times \exp \left\{-C\left[\frac{m \omega_{0}^{2} X^{2}}{2}+\frac{P^{2}}{2 m}\right]\right\}, \tag{7.62}
\end{equation*}
$$

though coefficient $C$ is now different from $1 / k_{\mathrm{B}} T$, and tends to that limit only at high temperatures, $k_{B} T$ $\gg \hbar \omega_{0}$. Moreover, for the Glauber state it also gives a very plausible result - a Gaussian distribution similar to Eq. (62), but shifted to the central point of the state - see Sec. 5.5.23

Unfortunately, for some other possible states of the harmonic oscillator, e.g., any pure Fock state with $n>0$, the Wigner function takes negative values in some regions of the [ $X, P$ ] plane - Fig. 3. ${ }^{24}$


Fig. 7.3. The Wigner function of several Fock states of a harmonic oscillator: (a) $n=0$, (b) $n=1$; (c) $n=5$. Adapted from http://en.wikipedia.org/wiki/Wigner_function.

The same is true for most other quantum systems. Indeed, this fact could be predicted just by looking at definition (50) applied to a pure quantum state, in which the density function may be factored - see Eq. (31):

[^673]\[

$$
\begin{equation*}
W(X, P)=\frac{1}{2 \pi \hbar} \int \psi\left(X+\frac{\tilde{X}}{2}\right) \psi^{*}\left(X-\frac{\tilde{X}}{2}\right) \exp \left\{-\frac{i P \tilde{X}}{\hbar}\right\} d \widetilde{X} . \tag{7.63}
\end{equation*}
$$

\]

Changing argument $P$ (say, at fixed $X$ ), we are essentially changing the spatial "frequency" (wavenumber) of the wavefunction product's Fourier component we are calculating, and we know that Fourier images typically change sign as the frequency is changed. Hence the wavefunctions should have some high-symmetry properties to avoid this effect. Indeed, the Gaussian functions (describing, for example, the Glauber states, and as the particular case, the ground state of the harmonic oscillator) have such a symmetry, but many other functions do not.

Hence the Wigner function cannot be used in the role of classical probability density $\rho(X, P)$, otherwise we would get a negative probability for measurement in certain intervals $d X d P$ - the notion hard to interpret. However, the Wigner function is still used for a semi-quantitative interpretation of states of open quantum systems.

### 7.3. Open system dynamics: Dephasing

So far we have discussed the density matrix as something given. Now let us discuss the evolution of the matrix in time, starting from the simplest case when the system is in state (15) with time-independent probabilities $W_{j}$. In the Schrödinger picture we can rewrite Eq. (15) as

$$
\begin{equation*}
\hat{w}(t)=\sum_{j}\left|w_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right| . \tag{7.64}
\end{equation*}
$$

Differentiating this equation by parts, and using Eqs. (4.157)-(4.158), with the account of the Hermitian nature of the Hamiltonian operator, we get

$$
\begin{align*}
i \hbar \dot{\hat{w}} & \left.=i \hbar \sum_{j}\left[\dot{w}_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right|+\left|w_{j}(t)\right\rangle W_{j}\left\langle\dot{w}_{j}(t)\right|\right]=\sum_{j}\left[\hat{H}\left|w_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right|-\left|w_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right| \hat{H}\right] \\
& =\hat{H} \sum_{j}\left|w_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right|-\sum_{j}\left|w_{j}(t)\right\rangle W_{j}\left\langle w_{j}(t)\right| \hat{H} . \tag{7.65}
\end{align*}
$$

Now using Eq. (64) again (twice), we get the so-called von Neumann equation ${ }^{25}$

$$
\begin{equation*}
i \hbar \dot{\hat{w}}=[\hat{H}, \hat{w}] . \tag{7.66}
\end{equation*}
$$

This equation is similar in structure to Eq. (4.199) describing the time evolution of the Heisenbergpicture operators:

$$
\begin{equation*}
i \hbar \dot{\hat{A}}=[\hat{A}, \hat{H}] \tag{7.67}
\end{equation*}
$$

besides the operator order in the commutator, i.e., the sign of the right-hand part. This is quite natural, because Eq. (66) belongs to the Schrödinger picture, while Eq. (67) to the Heisenberg picture of the quantum dynamics.

[^674]In the general case when a system, initially out of equilibrium, comes into a contact with the environment, probabilities $W_{j}$ change, and dynamics is described by equations more complex than Eq. (66). However, we still can use this equation to discuss, using a simple model, the second (after the energy relaxation) major effect of the environment, dephasing (also called "decoherence"). ${ }^{26}$ Let us consider the following model of a system interacting (weakly!) with environment: ${ }^{27}$

System's interaction with
environment

$$
\begin{equation*}
\hat{H}=\hat{H}_{s}+\hat{H}_{e}\{\lambda\}+\hat{H}_{\mathrm{int}} \tag{7.68}
\end{equation*}
$$

Let us consider the simplest, two-level system, taking its Hamiltonian in the simplest form,

$$
\begin{equation*}
\hat{H}_{s}=a_{z} \hat{\sigma}_{z}, \tag{7.69}
\end{equation*}
$$

(as we know from Sec. 4.6, such Hamiltonian is sufficient to avoid the energy level degeneracy), and a factorable (bilinear) interaction - cf. Eq. (6.148) and its discussion:

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=-\hat{f}\{\lambda\} \hat{\sigma}_{z} . \tag{7.70}
\end{equation*}
$$

Here $\hat{f}$ is a Hermitian operator depending only on the set $\{\lambda\}$ of environmental degrees of freedom ("coordinates"). These coordinates belong to the Hilbert space different from that of the two-level system, and hence operators $\hat{f}\{\lambda\}$ and $\hat{H}_{e}\{\lambda\}$ (that describes the environment) commute with $\hat{\sigma}_{z}$ - and any other intrinsic operator of the two-level system. Of course, any realistic $\hat{H}_{e}\{\lambda\}$ is very complex, so that it may be surprising how much we will be able to achieve without specifying it.

Before we proceed to solution, let me remind the reader of the important two-level systems that may be described by this model. The first example is an electron in an external magnetic field of a fixed direction (taken for axis $z$ ), which includes both an average component $\left\langle\mathcal{B}_{z}\right\rangle$ and a random (fluctuating) component $\widetilde{\mathcal{B}}_{z}$. As it follows from the discussion in Chapter 4, it may be described by Hamiltonian (68)(70) with

$$
\begin{equation*}
a_{z}=\mu_{\mathrm{B}}\left\langle\mathcal{B}_{z}\right\rangle, \quad-\hat{f}=\mu_{\mathrm{B}} \hat{\tilde{B}}_{z} . \tag{7.71}
\end{equation*}
$$

The second important example is a particle in a double-quantum-well potential (Fig. 4), with a barrier between them sufficiently high to be impenetrable, and an additional force $F(t)$ exerted by the environment. If the force is sufficiently weak, we can neglect its effects on the shape of quantum wells and hence on the localized wavefunctions $\psi_{L, R}$, so that the force effect is reduced to the variation of the difference $E_{L}-E_{R}=F(t) \Delta x$ between well eigenenergies. As a result, it may described by Eqs. (608)(70) with

$$
\begin{equation*}
a_{z} \approx\langle F\rangle \Delta x / 2 ; \quad-\hat{f} \approx \hat{\tilde{F}} \Delta x / 2 \tag{7.72}
\end{equation*}
$$

[^675]

Fig. 7.4. Dephasing in a double quantum well system.

Returning to the general model (68)-(70), let us start its analysis from writing the usual equation of motion for the Heisenberg operator $\hat{\sigma}_{z}: 28$

$$
\begin{equation*}
i \hbar \dot{\hat{\sigma}}_{z}=\left[\hat{\sigma}_{z}, \hat{H}\right]=\left(a_{z}-\hat{f}\right)\left[\hat{\sigma}_{z}, \hat{\sigma}_{z}\right]=0, \tag{7.73}
\end{equation*}
$$

so that operator $\hat{\sigma}_{z}$ does not evolve in time. What does this mean for the observables? For an arbitrary density matrix of the two-level system,

$$
w=\left(\begin{array}{ll}
w_{11} & w_{12}  \tag{7.74}\\
w_{21} & w_{22}
\end{array}\right)
$$

we can readily calculate the trace of operator $\hat{\sigma}_{z}$ (since operator traces are basis - independent, we can do this in any basis, in particular in the usual $z$-basis):

$$
\operatorname{Tr}\left(\hat{\sigma}_{z} \hat{w}\right)=\operatorname{Tr}\left(\sigma_{z} \mathrm{w}\right)=\operatorname{Tr}\left[\left(\begin{array}{cc}
1 & 0  \tag{7.75}\\
0 & -1
\end{array}\right)\left(\begin{array}{ll}
w_{11} & w_{12} \\
w_{21} & w_{22}
\end{array}\right)\right]=w_{11}-w_{22}=W_{1}-W_{2} .
$$

Hence, according to Eq. (5), $\hat{\sigma}_{z}$ may be considered the operator for observable $W_{1}-W_{2}$, so that in the case (73), the difference $W_{1}-W_{2}$ does not depend on time, and since the sum of the probabilities is also fixed, $W_{1}+W_{2}=1$, both of them are constant. (The physics of this result is especially clear for the model shown in Fig. 4: since the potential barrier separating the quantum wells is so high that tunneling through it is negligible, the interaction with environment cannot move the system from well into another one. It may look like nothing interesting may happen in such situation, but in a minute we will see this is not true.) Hence, we may use the von Neumann equation (66) for the density matrix evolution (in the Schrödinger picture). In the usual $z$-basis:

$$
\begin{align*}
i \hbar \dot{\mathrm{w}} & \equiv i \hbar\left(\begin{array}{cc}
\dot{w}_{11} & \dot{w}_{12} \\
\dot{w}_{21} & \dot{w}_{22}
\end{array}\right)=[\mathrm{H}, \mathrm{w}]=\left(a_{z}-\hat{f}\right)\left[\sigma_{z}, \mathrm{w}\right] \\
& =\left(a_{z}-\hat{f}\right)\left\{\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\left(\begin{array}{ll}
w_{11} & w_{12} \\
w_{21} & w_{22}
\end{array}\right)-\left(\begin{array}{ll}
w_{11} & w_{12} \\
w_{21} & w_{22}
\end{array}\right)\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\right\}=\left(a_{z}-\hat{f}\right)\left(\begin{array}{cc}
0 & 2 w_{12} \\
-2 w_{21} & 0
\end{array}\right) . \tag{7.76}
\end{align*}
$$

[^676]This means that though the diagonal elements, i.e., the probabilities of the states, do not evolve in time (as we already know), the off-diagonal coefficients do change; for example,

$$
\begin{equation*}
i \hbar \dot{w}_{12}=2\left(a_{z}-\hat{f}\right) w_{12} \tag{7.77}
\end{equation*}
$$

with a similar but complex-conjugate equation for $w_{21}$. The solution of the linear differential equation (77) is straightforward, and yields

$$
\begin{equation*}
w_{12}(t)=w_{12}(0) \exp \left\{-i \frac{2 a_{z}}{\hbar} t\right\} \exp \left\{i \frac{2}{\hbar} \int_{0}^{t} \hat{f}\left(t^{\prime}\right) d t^{\prime}\right\} . \tag{7.78}
\end{equation*}
$$

The first exponent is a deterministic $c$-number factor, while in the second one $\hat{f}(t) \equiv \hat{f}\{\lambda(t)\}$ is still an operator in the Hilbert space of the environment, and, from the point of view of the system of our interest, a random function of time.

Let us start from the limit when the environment behaves classically. ${ }^{29}$ In this case, the operator in Eq. (78) may be considered as a classical random function of time $f(t)$, provided that we average the result over the ensemble of many functions $f(t)$ describing many (macroscopically similar) experiments. For a small time interval $t=d t \rightarrow 0$, we can use the Taylor expansion of the exponent, truncating it after the quadratic term:

$$
\begin{align*}
\left\langle\exp \left\{-i \frac{2}{\hbar} \int_{0}^{d t} f\left(t^{\prime}\right) d t^{\prime}\right\}\right. & =1+\left\langle-i \frac{2}{\hbar} \int_{0}^{d t} f\left(t^{\prime}\right) d t^{\prime}\right\rangle+\left\langle\frac{1}{2}\left(-i \frac{2}{\hbar} \int_{0}^{d t} f\left(t^{\prime}\right) d t^{\prime}\right)\left(-i \frac{2}{\hbar} \int_{0}^{d t} f\left(t^{\prime \prime}\right) d t^{\prime \prime}\right)\right\rangle  \tag{7.79}\\
& =1-i \frac{2}{\hbar} \int_{0}^{d t}\left\langle f\left(t^{\prime}\right)\right\rangle d t^{\prime}-\frac{2}{\hbar^{2}} \int_{0}^{d t} d t^{\prime} \int_{0}^{d t} d t^{\prime \prime}\left\langle f\left(t^{\prime}\right) f\left(t^{\prime \prime}\right)\right\rangle=1-\frac{2}{\hbar^{2}} \int_{0}^{d t} d t^{\prime} \int_{0}^{d t} d t^{\prime \prime} K_{f}\left(t^{\prime}-t^{\prime \prime}\right) .
\end{align*}
$$ classical variable only depend on the time difference $\tau \equiv t^{\prime}-t^{\prime \prime}$ :

$$
\begin{equation*}
\left\langle f\left(t^{\prime}\right) f\left(t^{\prime \prime}\right)\right\rangle \equiv K_{f}\left(t^{\prime}-t^{\prime \prime}\right)=K_{f}(\tau) \tag{7.80}
\end{equation*}
$$

If this difference is much larger than some time scale $\tau_{c}$, called the correlation time of the random force, the values $f\left(t^{\prime}\right)$ and $f\left(t^{\prime \prime}\right)$ are completely independent (uncorrelated), as illustrated in Fig. 5a, so that the correlation function has to tend to zero. On the other hand, at $\tau=0$, i.e. $t^{\prime}=t^{\prime \prime}$, the correlation function is just the variance of $f$ :

$$
\begin{equation*}
K_{f}(0)=\left\langle f^{2}\right\rangle \tag{7.81}
\end{equation*}
$$

and has to be positive. As a result, the function looks (qualitatively) like the sketch in Fig. 5b.

[^677]

Fig. 7.5. (a) Typical random process and (b) its correlation function - schematically.

Hence, if we are only interested in time differences $\tau$ much longer than $\tau_{c}$, we may approximate $K_{f}(\tau)$ with a delta-function. Let us take it in the following convenient form

$$
\begin{equation*}
K_{f}(\tau) \approx \hbar^{2} D_{\varphi} \delta(\tau) \tag{7.82}
\end{equation*}
$$

Phase diffusion coefficient
where $D_{\varphi}$ is a positive constant called the phase diffusion coefficient. The origin of this term stems from the very similar effect of diffusion of atoms or small solid particles in real space - the so-called (the Brownian motion. ${ }^{30}$ Indeed, if a small classical particle moves in a highly viscous medium, its velocity is approximately proportional to the external force. Hence, if the random hits of a 1D particle by the molecules may be described by a force which obeys a law similar to Eq. (82), the velocity (along any Cartesian coordinate) is also delta-correlated:

$$
\begin{equation*}
\langle v(t)\rangle=0, \quad\left\langle v\left(t^{\prime}\right) v\left(t^{\prime \prime}\right)\right\rangle=2 D \delta\left(t^{\prime}-t^{\prime \prime}\right) . \tag{7.83}
\end{equation*}
$$

Now we can integrate the kinematic equation $\dot{x}=v$, to calculate particle's deviation from the initial position,

$$
\begin{equation*}
x(t)-x(0)=\int_{0}^{t} v\left(t^{\prime}\right) d t^{\prime} \tag{7.84}
\end{equation*}
$$

and its the variance:

$$
\begin{equation*}
\left\langle(x(t)-x(0))^{2}\right\rangle=\left\langle\int_{0}^{t} v\left(t^{\prime}\right) d t^{\prime} \int_{0}^{t} v\left(t^{\prime \prime}\right) d t^{\prime \prime}\right\rangle=\int_{0}^{t} d t^{\prime} \int_{0}^{t} d t^{\prime \prime}\left\langle v\left(t^{\prime}\right) v\left(t^{\prime \prime}\right)\right\rangle=\int_{0}^{t} d t^{\prime} \int_{0}^{t} d t^{\prime \prime} 2 D \delta\left(t^{\prime}-t^{\prime \prime}\right)=2 D t \tag{7.85}
\end{equation*}
$$

This is the famous law of diffusion, showing that the r.m.s. deviation of the particle from the initial point grows with time as $(2 D t)^{1 / 2}$, where constant $D$ is called the diffusion coefficient.

Returning to the diffusion of the quantum-mechanical phase, using Eq. (82), the last double integral in Eq. (79) yields $\hbar^{2} D_{\varphi} d t$, so that

$$
\begin{equation*}
\left\langle w_{12}(d t)\right\rangle=w_{12}(0) \exp \left\{-i \frac{2 a_{z}}{\hbar} d t\right\}\left(1-2 D_{\varphi} d t\right) \tag{7.86}
\end{equation*}
$$

Applying this formula to sequential time intervals,

[^678]\[

$$
\begin{equation*}
\left\langle w_{12}(2 d t)\right\rangle=\left\langle w_{12}(d t)\right\rangle \exp \left\{-i \frac{2 a_{z}}{\hbar} d t\right\}\left(1-2 D_{\varphi} d t\right)=w_{12}(0) \exp \left\{-i \frac{2 a_{z}}{\hbar} 2 d t\right\}\left(1-2 D_{\varphi} d t\right)^{2}, \tag{7.87}
\end{equation*}
$$

\]

etc., for a finite time $t=N d t$, in the limit $N \rightarrow \infty$ and $d t \rightarrow 0$ (at fixed $t$ ) we get, ${ }^{31}$

$$
\begin{equation*}
\left\langle w_{12}(t)\right\rangle=\left.w_{12}(0) \exp \left\{-i \frac{2 a_{z}}{\hbar} t\right\} \lim \right|_{N \rightarrow \infty}\left(1-2 D_{\varphi} t \frac{1}{N}\right)^{N} . \tag{7.88a}
\end{equation*}
$$

By the definition of the natural logarithm base $e,{ }^{32}$ this limit is just $\exp \left\{-2 D_{\varphi} t\right\}$, so that, finally:

$$
\begin{equation*}
\left\langle w_{12}(t)\right\rangle=w_{12}(0) \exp \left\{-i \frac{2 a}{\hbar} t\right\} \exp \left\{-2 D_{\phi} t\right\} \equiv w_{12}(0) \exp \left\{-i \frac{2 a}{\hbar} t\right\} \exp \left\{-\frac{t}{T_{2}}\right\} . \tag{7.88b}
\end{equation*}
$$

So, due to coupling to environment, the off-diagonal elements of the density matrix decay with the characteristic dephasing time $T_{2}=1 / 2 D_{\varphi}$, providing a natural evolution from the density matrix (22) of a pure state, to the diagonal matrix,

$$
\mathrm{w}=\left(\begin{array}{cc}
W_{1} & 0  \tag{7.89}\\
0 & W_{2}
\end{array}\right)
$$

with the same probabilities $W_{1,2}$, describing a fully dephased (incoherent) classical mixture.
Our simple model offers a very clear look at the nature of decoherence: "force" $f(t)$, exerted by the environment, "shakes" the energy difference between two eigenstates of the system and hence the instant velocities $2\left(a_{z}-f\right) / \hbar$ of their mutual phase shift $\varphi(t)-\mathrm{cf}$. Eq. (24). Due to randomness of the force, $\varphi(t)$ performs a random walk around the trigonometric circle, so that eventually, averaging of its trigonometric functions $\exp \{ \pm i \varphi\}$ over the possible states of environment yields zero, killing the offdiagonal elements of the density matrix. Our analysis, however, has left open two important issues:
(i) Is it approach valid for a quantum description of a typical environment?
(ii) If yes, what is $D_{\varphi}$ ?

### 7.4. Fluctuation-dissipation theorem

Similar questions may be asked about a more general situation, when the Hamiltonian $\hat{H}_{s}$ of the system of interest ( $s$ ), in the composite Hamiltonian (68), is not specified at all, but the interaction between that system its environment still has the bilinear form similar to Eqs. (70) and (6.130):

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=-\hat{F}\{\lambda\} \hat{x}, \tag{7.90}
\end{equation*}
$$

[^679]where $x$ is some observable of the subsystem $s$ (say, a generalized coordinate or a generalized momentum). It may look incredible that in this very general situation one may make a very simple and powerful statement about the statistical properties of the generalized external force $F$, under only two (interrelated) conditions - which are satisfied in a huge number of cases of interest:
(i) the coupling of system $s$ of interest to environment $e$ is weak - in the sense of the perturbation theory (see Chapter 6), and
(ii) the environment may be considered as staying in thermodynamic equilibrium, with certain temperature $T$, regardless of the process in the system of interest. ${ }^{33}$

This famous statement is called the fluctuation-dissipation theorem (FDT). ${ }^{34}$ Due to the importance of this fundamental result, let me derive it. ${ }^{35}$

Since by writing Eq. (68) we treat the whole system $(s+e)$ as a Hamiltonian one, ${ }^{36}$ we may use the Heisenberg equation (4.199) to write

$$
\begin{equation*}
i \hbar \dot{\hat{F}}=[\hat{F}, \hat{H}]=\left[\hat{F}, \hat{H}_{e}\right] \tag{7.91}
\end{equation*}
$$

because, as was discussed in the last section, operator $\hat{F}\{\lambda\}$ commutes with operators $\hat{H}_{s}$ and $\hat{x}$. Generally, very little may be done with this equation, because the time evolution of the environment's Hamiltonian depends, in turn, on that of the force. This is where the perturbation theory becomes indispensable. Let us decompose the external force's operator into the following sum:

$$
\begin{equation*}
\hat{F}\{\lambda\}=\langle\hat{F}\rangle+\hat{\tilde{F}}(t), \quad \text { with }\langle\hat{\tilde{F}}(t)\rangle=0 \tag{7.92}
\end{equation*}
$$

where (until further notice) sign $\langle\ldots\rangle$ means the statistical averaging over the environment alone. ${ }^{37}$ From the point of view of system $s$, the first term of the sum (still an operator!) describes the average response

[^680]of the environment to the system dynamics (possibly, including such irreversible effects as friction), and has to be calculated with account of their interaction - as will do later in this section. On the other hand, the second term in Eq. (92) presents fluctuations of the environment, which exist even in the absence of system $s$. Hence, in the first nonvanishing approximation in the interaction strength, the fluctuation part may be calculated ignoring the interaction, i.e. treating the environment as being in the thermodynamic equilibrium: ${ }^{38}$
\[

$$
\begin{equation*}
i \hbar \dot{\tilde{F}}=\left[\hat{\widetilde{F}},\left.\hat{H}_{e}\right|_{\mathrm{eq}}\right] \tag{7.93}
\end{equation*}
$$

\]

Since in this approximation the environment's Hamiltonian does not have an explicit dependence of time, the solution of this equation may be written combining Eqs. (4.175) and (4.190):

$$
\begin{equation*}
\hat{F}(t)=\exp \left\{\left.\frac{i}{\hbar} \hat{H}_{e}\right|_{\mathrm{eq}} t\right\} \hat{F}(0) \exp \left\{-\left.\frac{i}{\hbar} \hat{H}_{e}\right|_{\mathrm{eq}} t\right\} . \tag{7.94}
\end{equation*}
$$

Let us use this relation to calculate the correlation function of fluctuations, defined similarly to Eq. (80), but paying close attention to the order of the time arguments (very soon we will see why):

$$
\begin{equation*}
\left\langle\widetilde{F}(t) \widetilde{F}\left(t^{\prime}\right)\right\rangle=\left\langle\exp \left\{\frac{i}{\hbar} \hat{H}_{e} t\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t\right\} \exp \left\{\frac{i}{\hbar} \hat{H}_{e} t^{\prime}\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e^{\prime}} t^{\prime}\right\}\right\rangle, \tag{7.95}
\end{equation*}
$$

where the thermal equilibrium of environment is implied. We are at will to calculate this expectation value in any basis, and the best choice is evident, because in the environment's stationary state basis, its Hamiltonian, the exponents in Eq. (95), and the density operator of the environment are all represented by diagonal matrices. Using Eq. (5), the correlation function becomes

$$
\begin{align*}
\left\langle\widetilde{F}(t) \widetilde{F}\left(t^{\prime}\right)\right\rangle & =\operatorname{Tr}\left[\hat{w} \exp \left\{\frac{i}{\hbar} \hat{H}_{e} t\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t\right\} \exp \left\{\frac{i}{\hbar} \hat{H}_{e} t^{\prime}\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t^{\prime}\right\}\right] \\
& =\sum_{n}\left[\hat{w} \exp \left\{\frac{i}{\hbar} \hat{H}_{e} t\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t\right\} \exp \left\{\frac{i}{\hbar} \hat{H}_{e} t^{\prime}\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t^{\prime}\right\}\right]_{n n}  \tag{7.96}\\
& =\sum_{n, n^{\prime}} W_{n} \exp \left\{\frac{i}{\hbar} E_{n} t\right\} \hat{F}_{n n^{\prime}} \exp \left\{-\frac{i}{\hbar} E_{n^{\prime}} t\right\} \exp \left\{\frac{i}{\hbar} E_{n^{\prime}, t^{\prime}}\right\} \hat{F}_{n^{\prime} n} \exp \left\{-\frac{i}{\hbar} E_{n} t^{\prime}\right\} \\
& =\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \exp \left\{i \frac{\left(E_{n}-E_{n^{\prime}}\right)\left(t-t^{\prime}\right)}{\hbar}\right\}, \quad \text { where } \widetilde{E} \equiv E_{n}-E_{n^{\prime}} .
\end{align*}
$$

Here $W_{n}$ are the Gibbs distribution probabilities, given by Eq. (23) with environment's temperature $T$, and $F_{n n}$, are the Schrödinger-picture matrix elements of the interaction force operator.

We see that correlator (96) is a function of the difference $\tau \equiv t-t^{\prime}$ only (as it should be for fluctuations in a macroscopically stationary system), but may depend on the order of the operands. This is why let us denote this particular correlation function by upper index "+",

$$
\begin{equation*}
K_{F}^{+}(\tau) \equiv\left\langle\widetilde{F}(t) \widetilde{F}\left(t^{\prime}\right)\right\rangle=\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \exp \left\{i \frac{\widetilde{E} \tau}{\hbar}\right\}, \quad \text { where } \widetilde{E} \equiv E_{n}-E_{n^{\prime}} \tag{7.97}
\end{equation*}
$$

[^681]and its counterpart by upper index "-":
\[

$$
\begin{equation*}
K_{F}^{-}(\tau) \equiv K_{F}^{+}(-\tau)=\left\langle\widetilde{F}\left(t^{\prime}\right) \widetilde{F}(t)\right\rangle=\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \exp \left\{-i \frac{\widetilde{E} \tau}{\hbar}\right\} . \tag{7.98}
\end{equation*}
$$

\]

So, in contrast with classical processes, in quantum mechanics the correlation function of fluctuations $\widetilde{F}$ is not necessarily time-symmetric:

$$
\begin{equation*}
K_{F}^{+}(\tau)-K_{F}^{-}(\tau) \equiv K_{F}^{+}(\tau)-K_{F}^{+}(-\tau)=\left\langle\widetilde{F}(t) \widetilde{F}\left(t^{\prime}\right)-\widetilde{F}\left(t^{\prime}\right) \widetilde{F}(t)\right\rangle=2 i \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \sin \frac{\widetilde{E} \tau}{\hbar} \neq 0 \tag{7.99}
\end{equation*}
$$

so that $\hat{F}(t)$ gives a good example of a Heisenberg-picture operator whose "values", taken in different moments of time, generally do not commute - the opportunity already mentioned in Sec. 4.6. ${ }^{39}$

Now let us return to the force decomposition (92), and calculate the first (average) component of the force. In order to do that, let us write the formal solution of Eq. (91) as follows:

$$
\begin{equation*}
\hat{F}(t)=\frac{1}{i \hbar} \int_{-\infty}^{t}\left[\hat{F}\left(t^{\prime}\right), \hat{H}_{e}\left(t^{\prime}\right)\right] d t^{\prime} \tag{7.100}
\end{equation*}
$$

In the right-hand part of this relation, we cannot treat the Hamiltonian of the environment as an unperturbed (equilibrium) one, because the result would have zero statistical average. Hence, we should make one more step in our perturbative treatment, and take into account (in the first nonvanishing approximation) the effect of our system of interest ( $s$ ) on the environment. To do this, let us write the (so far, exact) Heisenberg equation of motion for the environment's Hamiltonian,

$$
\begin{equation*}
i \hbar \dot{\hat{H}}_{e}=\left[\hat{H}_{e}, \hat{H}\right]=-\hat{x}\left[\hat{H}_{e}, \hat{F}\right] \tag{7.101}
\end{equation*}
$$

and its formal solution, similar to Eq. (100), but for an arbitrary time $t^{\prime}$ rather than $t$ :

$$
\begin{equation*}
\hat{H}_{e}\left(t^{\prime}\right)=-\frac{1}{i \hbar} \int_{-\infty}^{t} \hat{x}\left(t^{\prime \prime}\right)\left[\hat{H}_{e}\left(t^{\prime \prime}\right), \hat{F}\left(t^{\prime \prime}\right)\right] d t^{\prime \prime} \tag{7.102}
\end{equation*}
$$

Plugging this equality into the right-hand part of Eq. (100), and averaging the result (again, over the environment only!), we get

$$
\begin{equation*}
\langle\hat{F}(t)\rangle=\frac{1}{\hbar^{2}} \int_{-\infty}^{t} d t^{\prime} \int_{-\infty}^{t^{\prime}} d t^{\prime \prime} \hat{x}\left(t^{\prime \prime}\right)\left\langle\left[\hat{F}\left(t^{\prime}\right),\left[\hat{H}_{e}\left(t^{\prime \prime}\right), \hat{F}\left(t^{\prime \prime}\right)\right]\right\rfloor\right\rangle . \tag{7.103}
\end{equation*}
$$

As we will see imminently, this expression gives a nonvanishing result even if the right-handpart averaging is carried over the unperturbed (thermal-equilibrium) environment, so that unless we are interested in higher-order corrections, there is no need to refine the result any further. This fact enables us to calculate the average in the right-hand part of Eq. (103) absolutely similarly to that in Eq. (96), using Eq. (94):

[^682]\[

$$
\begin{align*}
& \left\langle\left[\hat{F}\left(t^{\prime}\right),\left[\left.\hat{H}_{e}\left(t^{\prime \prime}\right)\right|_{\mathrm{eq}}, \hat{F}\left(t^{\prime \prime}\right)\right]\right]\right\rangle=\operatorname{Tr}\left\{\mathrm{w}\left[\mathrm{~F}\left(t^{\prime}\right),\left[\mathrm{H}_{e} \mathrm{~F}\left(t^{\prime \prime}\right)\right]\right]\right\} \\
& =\operatorname{Tr}\left\{\mathrm{w}\left[\mathrm{~F}\left(t^{\prime}\right) \mathrm{H}_{e} \mathrm{~F}\left(t^{\prime \prime}\right)-\mathrm{F}\left(t^{\prime}\right) \mathrm{F}\left(t^{\prime \prime}\right) \mathrm{H}_{e}-\mathrm{H}_{e} \mathrm{~F}\left(t^{\prime \prime}\right) \mathrm{F}\left(t^{\prime}\right)+\mathrm{F}\left(t^{\prime \prime}\right) \mathrm{H}_{e} \mathrm{~F}\left(t^{\prime}\right)\right]\right\} \\
& =\sum_{n, n^{\prime}} W_{n}\left[F_{n n^{\prime}}\left(t^{\prime}\right) E_{n^{\prime}} F_{n^{\prime} n}\left(t^{\prime \prime}\right)-F_{n n^{\prime}}\left(t^{\prime}\right) F_{n^{\prime} n}\left(t^{\prime \prime}\right) E_{n}-E_{n} F_{n n^{\prime}}\left(t^{\prime \prime}\right) F_{n^{\prime} n}\left(t^{\prime}\right)+F_{n n^{\prime}}\left(t^{\prime \prime}\right) E_{n^{\prime}} F_{n^{\prime} n}\left(t^{\prime \prime}\right)\right] \\
& =-\sum_{n, n^{\prime}} W_{n} \widetilde{E}\left|F_{n n^{\prime}}\right|^{2}\left[\exp \left\{i \frac{\widetilde{E}}{\hbar}\left(t^{\prime}-t^{\prime \prime}\right)\right\}+\text { c.c. }\right] . \tag{7.104}
\end{align*}
$$
\]

Now, if we try to integrate each term of this sum, as Eq. (103) seems to require, we will see that the lower-limit substitution (at $t^{\prime}, t^{\prime \prime} \rightarrow-\infty$ ) is uncertain, because the exponents oscillate without decay. This technical difficulty may be overcome by the following reasoning. As illustrated by the example considered in the previous section, coupling to a disordered environment makes the "memory horizon" of the subsystem of our interest ( $s$ ) finite: its current state does not depend on its history beyond certain time scale - in that example, the dephasing time $T_{2}$. (Actually, this is true for virtually all real physical systems, in contrast to the idealized models such as a dissipation-free pendulum that swings for ever and ever with the same amplitude.) As a result, the functions under integrals of Eq. (103), i.e. the sum (104), should self-average at a certain finite time. One simple technique for expressing this fact mathematically is just dropping the lower-limit substitution; this would give the correct result for Eq. (103). However, a better (mathematically more acceptable) trick is to first multiply the function under each integral by, respectively, $\exp \left\{\varepsilon\left(t-t^{\prime}\right)\right\}$ and $\exp \left\{\varepsilon\left(t-t^{\prime}\right)\right\}$, where $\varepsilon$ is a very small positive constant, then carry out the integration, and after that take the limit $\varepsilon \rightarrow 0$. The physical justification of this procedure may be provided by saying that system's behavior should not be affected if its interaction with the environment was not kept constant but was turned on gradually - say, exponentially with an infinitesimal rate $\varepsilon$. With this modification, Eq. (103) becomes

$$
\begin{equation*}
\langle\hat{F}(t)\rangle=-\frac{1}{\hbar^{2}} \sum_{n, n^{\prime}} W_{n} \widetilde{E}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0} \int_{-\infty}^{t} d t^{\prime} \int_{-\infty}^{t^{\prime}} d t^{\prime \prime} \hat{x}\left(t^{\prime \prime}\right)\left[\exp \left\{i \frac{\widetilde{E}}{\hbar}\left(t^{\prime}-t^{\prime \prime}\right)+\varepsilon\left(t^{\prime \prime}-t\right)\right\}+\text { c.c. }\right] . \tag{7.105}
\end{equation*}
$$

This double integration is over the area shaded in Fig. 6, so that the order of integration may be changed to the opposite one as

$$
\begin{equation*}
\int_{-\infty}^{t} d t^{\prime} \int_{-\infty}^{t^{\prime}} d t^{\prime \prime} \ldots=\int_{-\infty}^{t} d t^{\prime \prime} \int_{t^{\prime \prime}}^{t} d t^{\prime} \ldots=\int_{-\infty}^{t} d t^{\prime \prime} \int_{0}^{\tau} d \tau^{\prime} \ldots \tag{7.106}
\end{equation*}
$$

where $\tau^{\prime} \equiv t-t^{\prime}$, and $\tau \equiv t-t^{\prime \prime}$.


Fig. 7.6. 2D integration area in Eqs. (105) and (106).

As a result, Eq. (105) may be rewritten as a single integral,

$$
\langle\hat{F}(t)\rangle=\int_{-\infty}^{t} G\left(t-t^{\prime \prime}\right) \hat{x}\left(t^{\prime \prime}\right) d t^{\prime \prime}=\int_{0}^{\infty} G(\tau) \hat{x}(t-\tau) d \tau
$$

$$
\begin{align*}
G(\tau>0) & =-\frac{1}{\hbar^{2}} \sum_{n, n^{\prime}} W_{n} \widetilde{E}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0} \int_{0}^{\tau}\left[\exp \left\{i \frac{\widetilde{E}}{\hbar}\left(\tau-\tau^{\prime}\right)-\varepsilon \tau\right\}+\text { c.c. }\right] d \tau^{\prime}  \tag{7.108}\\
& =\lim _{\varepsilon \rightarrow 0} \frac{2}{\hbar} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \sin \frac{\widetilde{E} \tau}{\hbar} e^{-\varepsilon \tau}=\frac{2}{\hbar} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \sin \frac{\widetilde{E} \tau}{\hbar},
\end{align*}
$$

does not depend on the particular law of evolution of the subsystem ( $s$ ) under study, i.e. provides a general characterization of its coupling to the environment.

In Eq. (107) we may readily recognize the most general form of the linear response of a system (in our case, the environment), taking into account the causality principle, where $G(\tau)$ is the response function (also called the "temporal Green's function") of the environment. ${ }^{40}$ Comparing Eq. (108) with Eq. (99), we get a wonderfully simple universal relation, ${ }^{41}$

$$
\begin{equation*}
\langle[\tilde{\tilde{F}}(\tau), \hat{\tilde{F}}(0)]\rangle=i \hbar G(\tau) . \tag{7.109}
\end{equation*}
$$

that emphasizes once again the quantum nature of the correlation function's time asymmetry. However, the relation between $G(\tau)$ and the force anti-commutator,

$$
\begin{equation*}
\langle\{\hat{\vec{F}}(t+\tau), \hat{\widetilde{F}}(t)\}\rangle \equiv\langle\hat{\tilde{F}}(t+\tau) \hat{\tilde{F}}(t)+\hat{\tilde{F}}(t) \hat{\widetilde{F}}(t+\tau)\rangle=K_{F}^{+}(\tau)+K_{F}^{-}(\tau) \tag{7.110}
\end{equation*}
$$

is much more important because of the following reason. Relations (97)-(98) show that the so-called symmetrized correlation function,

$$
\begin{align*}
K_{F}(\tau) & \equiv \frac{K_{F}^{+}(\tau)+K_{F}^{-}(\tau)}{2}=\frac{1}{2}\langle\langle\hat{\tilde{F}}(\tau), \tilde{\tilde{F}}(0)\}\rangle=\lim _{\varepsilon \rightarrow 0} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \cos \frac{\widetilde{E} \tau}{\hbar} e^{-2 \varepsilon|\tau|} \\
& =\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \cos \frac{\widetilde{E} \tau}{\hbar}, \tag{7.111}
\end{align*}
$$

Fluctuation commutator via Green's function

Symmetrized correlation function

[^683]\[

$$
\begin{equation*}
K_{F}(\tau)=\int_{-\infty}^{+\infty} S_{F}(\omega) e^{-i \omega \tau} d \omega=2 \int_{0}^{+\infty} S_{F}(\omega) \cos \omega \tau d \omega \tag{7.112}
\end{equation*}
$$

\]

with the reciprocal transform

$$
\begin{equation*}
S_{F}(\omega)=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} K_{F}(\tau) e^{i \omega \tau} d \tau=\frac{1}{\pi} \int_{0}^{+\infty} K_{F}(\tau) \cos \omega \tau d \tau \tag{7.113}
\end{equation*}
$$

via the symmetrized spectral density of variable $F$, defined as

$$
\begin{equation*}
S_{F}(\omega) \delta\left(\omega-\omega^{\prime}\right) \equiv \frac{1}{2}\left\langle\hat{F}_{\omega} \hat{F}_{-\omega^{\prime}}+\hat{F}_{-\omega^{\prime}} \hat{F}_{\omega}\right\rangle=\frac{1}{2}\left\langle\left\{\hat{F}_{\omega}, \hat{F}_{-\omega^{\prime}}\right\}\right\rangle, \tag{7.114}
\end{equation*}
$$

where $\hat{F}_{\omega}$ (also an operator rather than a $c$-number!) is defined as

$$
\begin{equation*}
\hat{F}_{\omega} \equiv \frac{1}{2 \pi} \int_{-\infty}^{+\infty} \hat{\tilde{F}}(t) e^{i \omega t} d t, \quad \text { so that } \hat{\tilde{F}}(t)=\int_{-\infty}^{+\infty} \hat{F}_{\omega} e^{-i \omega t} d \omega \tag{7.115}
\end{equation*}
$$

The physical meaning of function $S_{F}(\omega)$ becomes evident if we write Eq. (112) for the particular case $\tau=0$ :

$$
\begin{equation*}
K_{F}(0) \equiv\left\langle\hat{\widetilde{F}}^{2}\right\rangle=\int_{-\infty}^{+\infty} S_{F}(\omega) d \omega=2 \int_{0}^{+\infty} S_{F}(\omega) d \omega \tag{7.116}
\end{equation*}
$$

This formula implies that if we pass function $F(t)$ through a linear filter cutting from its frequency spectrum a narrow band $d \omega$ of real (positive) frequencies, then variance $\left\langle F_{f}^{2}\right\rangle$ of the filtered signal $F_{f}(t)$ would be equal to $2 S_{F}(\omega) d \omega$ - hence the name "spectral density". ${ }^{43}$

Let us use Eqs. (111) and (113) to calculate the spectral density for our model:

$$
\begin{align*}
S_{F}(\omega) & =\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \frac{1}{2 \pi} \lim _{\varepsilon \rightarrow 0} \int_{-\infty}^{+\infty} \cos \frac{\widetilde{E} \tau}{\hbar} e^{-\varepsilon \mid \tau} e^{i \omega \tau} d \tau \\
& =\frac{1}{2 \pi} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0} \int_{0}^{+\infty}\left[\exp \left\{i \frac{\widetilde{E} \tau}{\hbar}\right\}+\text { c.c. }\right] e^{-\varepsilon \tau} e^{i \omega \tau} d \tau  \tag{7.117}\\
& =\frac{1}{2 \pi} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0}\left[\frac{1}{i(\widetilde{E} / \hbar+\omega)-\varepsilon}+\frac{1}{i(-\widetilde{E} / \hbar+\omega)-\varepsilon}\right] .
\end{align*}
$$

Now it is a convenient time to recall that each of the two summations here is over the eigenenergy spectrum of the environment whose spectrum is virtually continuous because of its large size, so that we may transform each sum into an integral just as this was done in Sec. 6.6:

$$
\begin{equation*}
\sum_{n} \ldots \rightarrow \int \ldots d n=\int \ldots \rho\left(E_{n}\right) d E_{n} \tag{7.118}
\end{equation*}
$$

${ }^{43}$ An alternative popular measure of spectral density is $S_{F}(v) \equiv\left\langle F_{f}^{2}\right\rangle / d \nu=4 \pi S_{F}(\omega)$, where $v=\omega / 2 \pi$ is the "cyclic" frequency (measured in Hz ).
where $\rho(E)$ is the density of environment's states at a given energy. This transformation yields

$$
\begin{equation*}
S_{F}(\omega)=\frac{1}{2 \pi} \lim _{\varepsilon \rightarrow 0} \int d E_{n} W\left(E_{n}\right) \rho\left(E_{n}\right) \int d E_{n^{\prime}} \rho\left(E_{n^{\prime}}\right)\left|F_{n n^{\prime}}\right|^{2}\left[\frac{1}{i(\widetilde{E} / \hbar-\omega)-\varepsilon}+\frac{1}{i(-\widetilde{E} / \hbar-\omega)-\varepsilon}\right] \tag{7.119}
\end{equation*}
$$

Since the square bracket depends only on a specific linear combination of two energies, $\widetilde{E} \equiv E_{n}-E_{n^{\prime}}$, it is convenient to introduce also another, linearly-independent combination of the energies, for example, the average energy $\bar{E}=\left(E_{n}+E_{n^{\prime}}\right) / 2$, so that the state energies may be presented as

$$
\begin{equation*}
E_{n}=\bar{E}+\frac{\widetilde{E}}{2}, \quad E_{n^{\prime}}=\bar{E}-\frac{\widetilde{E}}{2} . \tag{7.120}
\end{equation*}
$$

With this notation, Eq. (119) becomes

$$
\begin{align*}
S_{F}(\omega)=-\frac{\hbar}{2 \pi} \lim _{\varepsilon \rightarrow 0} \int d \bar{E} & {\left[\int W\left(\bar{E}+\frac{\widetilde{E}}{2}\right)\left|F_{n n^{\prime}}\right|^{2} \rho\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}-\frac{\widetilde{E}}{2}\right) \frac{d \widetilde{E}}{i(\widetilde{E}-\hbar \omega)-\hbar \varepsilon}\right.}  \tag{7.121}\\
& \left.+\int W\left(\bar{E}+\frac{\widetilde{E}}{2}\right)\left|F_{n n^{\prime}}\right|^{2} \rho\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}-\frac{\widetilde{E}}{2}\right) \frac{d \widetilde{E}}{i(-\widetilde{E}-\hbar \omega)-\hbar \varepsilon}\right]
\end{align*}
$$

Due to the smallness of parameter $\hbar \varepsilon$ (which should be much less than all real energies, including $k_{\mathrm{B}} T$, $\hbar \omega, E_{n}$, and $E_{n}$ '), each of the internal integrals is dominated by an infinitesimal vicinity of one point, $\widetilde{E}_{ \pm}= \pm \hbar \omega$, in which the spectral density, matrix elements, and the Gibbs probabilities do not change considerably, and may be taken out of the integrals, so that they may be worked out explicitly: ${ }^{44}$

$$
\begin{align*}
& S_{F}(\omega)=-\frac{\hbar}{2 \pi} \lim _{\varepsilon \rightarrow 0} \int d \bar{E} \rho_{+} \rho_{-}\left[W_{+}\left|F_{+}\right|^{2} \int_{-\infty}^{+\infty} \frac{d \widetilde{E}}{i(\widetilde{E}-\hbar \omega)-\hbar \varepsilon}+W_{-}\left|F_{-}\right|^{2} \int_{-\infty}^{+\infty} \frac{d \widetilde{E}}{i(-\widetilde{E}-\hbar \omega)-\hbar \varepsilon}\right] \\
& =-\frac{\hbar}{2 \pi} \lim _{\varepsilon \rightarrow 0} \int d \bar{E} \rho_{+} \rho_{-}\left[W_{+}\left|F_{+}\right|^{2} \int_{-\infty}^{+\infty} \frac{-i(\widetilde{E}-\hbar \omega)-\hbar \varepsilon}{(\widetilde{E}-\hbar \omega)^{2}+(\hbar \varepsilon)^{2}} d \widetilde{E}+W_{-}\left|F_{-}\right|^{2} \int_{-\infty}^{+\infty} \frac{i(\widetilde{E}+\hbar \omega)-\hbar \varepsilon}{(\widetilde{E}+\hbar \omega)^{2}+(\hbar \varepsilon)^{2}} d \widetilde{E}\right]  \tag{7.122}\\
& =\frac{\hbar}{2} \int \rho_{+} \rho_{-}\left[W_{+}\left|F_{+}\right|^{2}+W_{-}\left|F_{-}\right|^{2}\right] d \bar{E}
\end{align*}
$$

where indices $\pm$ mark function values at the special points $\widetilde{E}_{ \pm}= \pm \hbar \omega$, i.e. $E_{n}=E_{n}{ }^{\prime} \pm \hbar \omega$. The physics of these points becomes simple if we interpret state $n$, that is the argument of the equilibrium Gibbs distribution function $W_{n}$, as the initial state of the environment, and $n$ ' as its final state. Then the topsign point corresponds to $E_{n}{ }^{\prime}=E_{n}-\hbar \omega$, i.e. to the emission of one energy quantum $\hbar \omega$ of the "observation" frequency $\omega$ by the environment into subsystem $s$ of interest, while the bottom-sign point $E_{n^{\prime}}=E_{n}+\hbar \omega$, corresponds to the absorption of such quantum by the environment. As Eq. (122) shows, both processes give similar positive contributions into force fluctuations.

[^684]The situation is different for the Fourier image of the response function $G(\tau),{ }^{45}$

$$
\begin{equation*}
\chi(\omega) \equiv \int_{0}^{+\infty} G(\tau) e^{i \omega \tau} d \tau \tag{7.123}
\end{equation*}
$$

Generalized susceptibility
that is frequently called either the generalized susceptibility or the response function - in our case, of the environment. Its physical meaning is that the complex function $\chi(\omega)=\chi^{\prime}(\omega)+i \chi$ '" $(\omega)$ relates the Fourier amplitudes of the generalized coordinate and generalized force:46

$$
\begin{equation*}
\left\langle\hat{F}_{\omega}\right\rangle=\chi(\omega) \hat{x}_{\omega} \tag{7.124}
\end{equation*}
$$

The physics of its imaginary part $\chi$ " $(\omega)$ is especially clear. Indeed, if both $F_{\omega}$ and $x_{\omega}$ represent a sinusoidal classical process, say

$$
\begin{equation*}
x(t)=x_{0} \cos \omega t=\frac{x_{0}}{2} e^{-i \omega t}+\frac{x_{0}}{2} e^{+i \omega t}, \text { i.e. } x_{\omega}=x_{-\omega}=\frac{x_{0}}{2} \tag{7.125}
\end{equation*}
$$

Then, in accordance with the correspondence principle, Eq. (124) should hold for the $c$-number complex amplitudes $F_{\omega}$ and $x_{\omega}$, enabling us to calculate the time dependence of force,

$$
\begin{align*}
F(t) & =F_{\omega} e^{-i \omega t}+F_{-\omega} e^{+i \omega t}=\chi(\omega) x_{\omega} e^{-i \omega t}+\chi(-\omega) x_{-\omega} e^{+i \omega t}=\frac{x_{0}}{2}\left[\chi(\omega) e^{-i \omega t}+\chi(-\omega) e^{+i \omega t}\right]  \tag{7.126}\\
& =\frac{x_{0}}{2}\left[\left(\chi^{\prime}+i \chi^{\prime \prime}\right) e^{-i \omega t}+\left(\chi^{\prime}-i \chi^{\prime \prime}\right) e^{+i \omega t}\right]=x_{0}\left[\chi^{\prime}(\omega) \cos \omega t+\chi^{\prime \prime}(\omega) \sin \omega t\right]
\end{align*}
$$

We see that $\chi^{\prime \prime}(\omega)$ scales the part of the force that is $\pi / 2$-shifted from the coordinate oscillations, i.e. is in phase with those of velocity, and hence characterizes the time-average power flow from the system into the environment, i.e. the energy dissipation rate: ${ }^{47}$

$$
\begin{equation*}
\bar{P}=\overline{-F(t) \dot{x}(t)}=\overline{-x_{0}\left[\chi^{\prime}(\omega) \cos \omega t+\chi^{\prime \prime}(\omega) \sin \omega t\right]\left(-\omega x_{0} \sin \omega t\right)}=\frac{x_{0}^{2}}{2} \omega \chi^{\prime \prime}(\omega) \tag{7.127}
\end{equation*}
$$

Let us calculate this function from Eqs. (108) and (123), just as we have done for the spectral density of fluctuations:

$$
\begin{aligned}
\chi^{\prime \prime}(\omega) & =\operatorname{Im} \int_{0}^{+\infty} G(\tau) e^{i \omega \tau} d \tau=\frac{2}{\hbar} \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0} \operatorname{Im} \int_{0}^{+\infty} \frac{1}{2 i}\left(\exp \left\{i \frac{\widetilde{E} \tau}{\hbar}\right\}-\text { c.c. }\right) e^{i \omega \tau} e^{-\varepsilon \tau} d \tau \\
& =\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0} \operatorname{Im}\left(\frac{1}{-\widetilde{E}-\hbar \omega-i \hbar \varepsilon}-\frac{1}{\widetilde{E}-\hbar \omega-i \hbar \varepsilon}\right)
\end{aligned}
$$

[^685]\[

$$
\begin{equation*}
=\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \lim _{\varepsilon \rightarrow 0}\left(\frac{\hbar \varepsilon}{(\widetilde{E}+\hbar \omega)^{2}+(\hbar \varepsilon)^{2}}-\frac{\hbar \varepsilon}{(\widetilde{E}-\hbar \omega)^{2}+(\hbar \varepsilon)^{2}}\right) . \tag{7.128}
\end{equation*}
$$

\]

Making the transfer (118) from the double sum to the double integral, and then the integration variable transfer (120), we get

$$
\begin{align*}
\chi^{\prime \prime}(\omega)=\lim _{\varepsilon \rightarrow 0} \int d \bar{E} & {\left[\int_{-\infty}^{+\infty} W\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}-\frac{\widetilde{E}}{2}\right)\left|F_{n n^{\prime}}\right|^{2} \frac{\hbar \varepsilon}{(\widetilde{E}+\hbar \omega)^{2}+(\hbar \varepsilon)^{2}} d \widetilde{E}\right.} \\
& \left.-\int_{-\infty}^{+\infty} W\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}+\frac{\widetilde{E}}{2}\right) \rho\left(\bar{E}-\frac{\widetilde{E}}{2}\right)\left|F_{n n^{\prime}}\right|^{2} \frac{\hbar \varepsilon}{(\widetilde{E}-\hbar \omega)^{2}+(\hbar \varepsilon)^{2}} d \widetilde{E}\right] . \tag{7.129}
\end{align*}
$$

Now using the same argument about the smallness of parameter $\varepsilon$ as above, we may take the spectral densities, matrix elements of force, and the Gibbs probabilities out of the integrals, and work out the integrals, getting a result very similar to Eq. (122):

$$
\begin{equation*}
\chi^{\prime \prime}(\omega)=\pi \int \rho_{+} \rho_{-}\left[W_{-}\left|F_{-}\right|^{2}-W_{+}\left|F_{+}\right|^{2}\right] d \bar{E} \tag{7.130}
\end{equation*}
$$

In order to relate these results, it is sufficient to notice that according to Eq. (23), the Gibbs probabilities $W_{ \pm}$are related by coefficients dependent on only the temperature $T$ and observation frequency $\omega$ :

$$
\begin{equation*}
W_{ \pm} \equiv W\left(\bar{E}+\frac{\widetilde{E}_{ \pm}}{2}\right) \equiv W\left(\bar{E} \pm \frac{\hbar \omega}{2}\right)=\frac{1}{Z} \exp \left\{-\frac{\bar{E} \pm \hbar \omega / 2}{k_{\mathrm{B}} T}\right\}=W(\bar{E}) \exp \left\{\mp \frac{\hbar \omega}{2 k_{\mathrm{B}} T}\right\} \tag{7.131}
\end{equation*}
$$

so that both the spectral density and the dissipative part of susceptibility may expressed via the same integral over environment energies:

$$
\begin{align*}
& S_{F}(\omega)=\hbar \cosh \left(\frac{\hbar \omega}{2 k_{\mathrm{B}} T}\right) \int \rho_{+} \rho_{-} W(\bar{E})\left[\left|F_{+}\right|^{2}+\left|F_{-}\right|^{2}\right] d \bar{E},  \tag{7.132}\\
& \chi^{\prime \prime}(\omega)=2 \pi \sinh \left(\frac{\hbar \omega}{2 k_{\mathrm{B}} T}\right) \int \rho_{+} \rho_{-} W(\bar{E})\left[\left|F_{+}\right|^{2}+\left|F_{-}\right|^{2}\right] d \bar{E} \tag{7.133}
\end{align*}
$$

and hence are universally related as

$$
\begin{equation*}
S_{F}(\omega)=\frac{\hbar}{2 \pi} \chi^{\prime \prime}(\omega) \operatorname{coth} \frac{\hbar \omega}{2 k_{\mathrm{B}} T} \tag{7.134}
\end{equation*}
$$

This is the Callen-Welton's fluctuation-dissipation theorem (FDT). It reveals the fundamental, intimate relation between dissipation and fluctuations induced by environment ("no dissipation without fluctuations") - hence the name. ${ }^{48}$ In the classical limit, $\hbar \omega \ll k_{\mathrm{B}} T$, the FDT is reduced to

[^686]\[

$$
\begin{equation*}
S_{F}(\omega)=\frac{\hbar}{2 \pi} \chi^{\prime \prime}(\omega) \frac{2 k_{\mathrm{B}} T}{\hbar \omega}=\frac{k_{\mathrm{B}} T}{\pi} \frac{\operatorname{Im} \chi(\omega)}{\omega} . \tag{7.135}
\end{equation*}
$$

\]

In most systems of interest the last fraction tends to a finite (positive) constant in a substantial range of relatively low frequencies. Indeed, expanding Eq. (123) in the Taylor series in small $\omega$, we get

$$
\begin{equation*}
\chi(\omega)=\chi(0)+i \omega \eta+\ldots, \quad \text { with } \quad \chi(0)=\int_{0}^{\infty} G(\tau) d \tau, \quad \text { and } \eta \equiv \int_{0}^{\infty} G(\tau) \tau d \tau \tag{7.136}
\end{equation*}
$$

Since the temporal Green's function is real by definition, the Taylor expansion of $\chi$ " $(\omega) \equiv \operatorname{Im} \chi(\omega)$ starts with the linear term $i \omega \eta$, where $\eta$ is a certain real coefficient, and unless $\eta=0$, is dominated by this term at small $\omega$. (The physical sense of constant $\eta$ becomes clear if we consider an environment that provides viscous friction with the simple law

$$
\begin{equation*}
\langle\hat{F}\rangle=-\eta \dot{\hat{x}}, \quad \eta \geq 0 . \tag{7.137}
\end{equation*}
$$

| Drag |
| :--- |

For the Fourier images of coordinate and force this gives the relation $F_{\omega}=i \omega x_{\omega}$, so that according to Eq. (124),

$$
\begin{equation*}
\chi(\omega)=i \omega \eta \text {, i.e. } \frac{\chi^{\prime \prime}(\omega)}{\omega} \equiv \frac{\operatorname{Im} \chi(\omega)}{\omega}=\eta \geq 0 \tag{7.138}
\end{equation*}
$$

Hence, even in the general case, coefficient $\eta$ describes an effective low-speed drag (kinematic friction) provided by the environment.)

In this case Eq. (134) turns into the Nyquist formula:49
Nyquist
formula

$$
\begin{equation*}
S_{F}(\omega)=\frac{k_{\mathrm{B}} T}{\pi} \eta, \quad \text { i.e. }\left\langle F_{f}^{2}\right\rangle=4 k_{\mathrm{B}} T \eta d v . \tag{7.139}
\end{equation*}
$$

According to Eq. (112), if such a constant spectral density ${ }^{50}$ persisted at all frequencies, it would correspond to a delta-correlated process $F(t)$, with

$$
\begin{equation*}
K_{F}(\tau)=2 \pi S_{F}(0) \delta(\tau)=2 k_{\mathrm{B}} T \eta \delta(\tau), \tag{7.140}
\end{equation*}
$$

similar to already discussed above - see Eq. (82).
oscillator was by no means used in its derivation. As will see in the next section, this fact leads to rather interesting consequences and even conceptual opportunities.
${ }^{49}$ Actually, the 1928 work by H. Nyquist was about electronic noise in resistors, just discovered experimentally by his Bell Labs colleague J. Johnson. For an Ohmic resistor, as a dissipative "environment" of the electric circuit it is connected with, Eq. (137) is just the Ohm's law, and may be recast as either $\langle V\rangle=-R(d Q / d t)=R I$, or $\langle I\rangle=-$ $G(d \Phi / d t)=G V$. Thus for voltage $V$ in an open circuit, $\eta$ corresponds to resistance $R$, while for current $I$ in the short circuit, to conductance $G=1 / R$. In this case, the fluctuations described by Eq. (139) are referred to as the Johnson-Nyquist noise. (Because of this important application, any model leading to Eqs. (136)-(137) is frequently referred to as Ohmic dissipation, even if the physical nature of variables $x$ and $F$ is quite different.) Another note: the Nyquist formula (139) should not be confused with the Nyquist-Shannon theorem describing the minimum sampling rate of an analog signal.
${ }^{50}$ A random process whose properties may be reasonably approximated by constant spectral density is frequently called the white noise, because then it is a random mixture of all possible sinusoidal components with equal weights, reminding natural white light's composition.

Since in the classical limit the right-hand part of Eq. (109) is negligible, and the correlation function may be considered an even function of time, the symmetrized function under the integral in Eq. (113) may be rewritten just as $\langle F(\tau) F(0)\rangle$. In the limit of low observation frequencies (in the sense that $\omega$ is much smaller than not only the quantum frontier $k_{\mathrm{B}} T / \hbar$, but also the frequency scale of function $\left.\chi^{\prime \prime}(\omega) / \omega\right)$, Eq. (138) may be used to recast Eq. (135) in the form ${ }^{51}$

$$
\begin{equation*}
\eta \equiv \lim _{\omega \rightarrow 0} \frac{\chi^{\prime \prime}(\omega)}{\omega}=\frac{1}{k_{\mathrm{B}} T} \int_{0}^{\infty}\langle F(\tau) F(0)\rangle d \tau . \tag{7.141}
\end{equation*}
$$

To conclude this section, let me return for a minute to the questions formulated in our earlier discussion of dephasing in the two-level model. In that problem, the dephasing time scale is $T_{2}=1 / 2 D_{\varphi}$. Hence the classical approach to the environment, used in Sec. 3, is adequate if $\hbar D_{\varphi} \ll k_{\mathrm{B}} T$. Next, we may identify operators $\hat{f}$ and $\hat{\sigma}_{z}$ participating in Eq. (70) with, respectively, operators $\hat{F}$ and $\hat{x}$ of the general Eq. (90). Then the comparison of Eqs. (82), (88) and (140) yields

$$
\begin{equation*}
\frac{1}{T_{2}}=2 D_{\varphi}=\frac{4 k_{\mathrm{B}} T}{\hbar^{2}} \eta, \tag{7.142}
\end{equation*}
$$

so that, for the model described by Eq. (137) with temperature-independent drag coefficient $\eta$, the dephasing rate is proportional to temperature.

### 7.5. The Heisenberg-Langevin approach

The fluctuation-dissipation theorem opens a very simple and efficient way for analysis of the system of interest ( $s$ in Fig. 1). It is to write its Heisenberg equations (4.199) of motion for relevant operators, which would now include the environmental force operator, and explore these equations using the Fourier transform and the Wiener-Khinchin theorem (112)-(113). Such approach to classical equations of motion is commonly associated with the name of Langevin, ${ }^{52}$ so that its extension to dynamics of Heisenberg-picture operators is frequently referred to as the Heisenberg-Langevin (or "quantum Langevin") approach to open system analysis. ${ }^{53}$

Perhaps the best way to describe this method is to demonstrate how it works for the very important case of a 1D harmonic oscillator, so that the generalized coordinate $x$ of Sec. 4 is just the oscillator's coordinate. For the sake of simplicity, let us assume that the environment provides the simple Ohmic dissipation described by Eq. (137) - which is a good approximation in many cases. As we already know from Chapter 5, the Heisenberg equations of motion for operators of coordinate and momentum of the oscillator, in the presence of external force, are
${ }^{51}$ In some fields (especially in physical kinetics and chemical physics), this particular limit of the Nyquist formula, is called the Green-Kubo (or just "Kubo") formula. As was discussed above, these names may be more reasonably associated with Eq. (109).
${ }^{52}$ After P. Langevin, whose 1908 work was the first systematic development of Einstein's ideas (1905) of the Brownian motion theory in the random force language, as an alternative to M. Smoluchowski's approach using the probability density language - see Sec. 6 below.
${ }^{53}$ Perhaps the largest credit for this extension belongs to M. Lax whose work, in the early 1960s, was motivated mostly by quantum electronics applications - see, e.g., his monograph M. Lax, Fluctuation and Coherent Phenomena in Classical and Quantum Physics, Gordon and Breach, 1968, and references therein.

$$
\begin{equation*}
\dot{\hat{x}}=\frac{\hat{p}}{m}, \quad \dot{\hat{p}}=-m \omega_{0}^{2} \hat{x}+\hat{F}, \tag{7.143}
\end{equation*}
$$

so that using Eqs. (92) and (137), we get

$$
\begin{equation*}
\dot{\hat{x}}=\frac{\hat{p}}{m}, \quad \dot{\hat{p}}=-m \omega_{0}^{2} \hat{x}-\eta \dot{\hat{x}}+\hat{\tilde{F}}(t) . \tag{7.144}
\end{equation*}
$$

Combining Eqs. (144), we may write their system as a singe differential equation

$$
\begin{equation*}
m \ddot{\hat{x}}+\eta \dot{\hat{x}}+m \omega_{0}^{2} \hat{x}=\hat{\widetilde{F}}(t) \tag{7.145}
\end{equation*}
$$

that is absolutely similar to the classical equation of motion. ${ }^{54}$ (In the view of Eqs. (5.42) and (5.48), whose corollary the Ehrenfest theorem (5.49) is, this should be by no means surprising.) For the Fourier images of the operators, defined similarly to Eq. (115), Eq. (145) gives the following relation,

$$
\begin{equation*}
\hat{x}_{\omega}=\frac{\hat{F}_{\omega}}{m\left(\omega_{0}^{2}-\omega^{2}\right)-i \eta \omega} \tag{7.146}
\end{equation*}
$$

that should be also well known to the reader from the classical theory of forced oscillations. However, since the Fourier components are still Heisenberg-picture operators, and their "values" for different $\omega$ do not commute, we have to tread carefully. The best way to proceed is to write a copy of Eq. (146) for frequency ( $-\omega^{\prime}$ ), and then combine these equations to form a symmetrical combination similar that used in Eq. (114). The result is

$$
\begin{equation*}
\frac{1}{2}\left\langle\hat{x}_{\omega} \hat{x}_{-\omega^{\prime}}+\hat{x}_{-\omega^{\prime}} \hat{x}_{\omega}\right\rangle=\frac{1}{\left|m\left(\omega_{0}^{2}-\omega^{2}\right)-i \eta \omega\right|^{2}} \frac{1}{2}\left\langle\hat{F}_{\omega} \hat{F}_{-\omega^{\prime}}+\hat{F}_{-\omega^{\prime}} \hat{F}_{\omega}\right\rangle . \tag{7.147}
\end{equation*}
$$

Since the spectral density definition similar to Eq. (114) is valid for any observable, in particular for $x$, Eq. (147) allows us to relate the symmetrized spectral densities of coordinate and force:

$$
\begin{equation*}
S_{x}(\omega)=\frac{S_{F}(\omega)}{\left|m\left(\omega_{0}^{2}-\omega^{2}\right)-i \eta \omega\right|^{2}}=\frac{S_{F}(\omega)}{m^{2}\left(\omega_{0}^{2}-\omega^{2}\right)^{2}+(\eta \omega)^{2}} . \tag{7.148}
\end{equation*}
$$

Now using an analog of Eq. (116) for $x$, we can calculate coordinate's variance:

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=K_{x}(0)=\int_{-\infty}^{+\infty} S_{x}(\omega) d \omega=2 \int_{0}^{+\infty} \frac{S_{F}(\omega) d \omega}{m^{2}\left(\omega_{0}^{2}-\omega^{2}\right)^{2}+(\eta \omega)^{2}}, \tag{7.149}
\end{equation*}
$$

where now, in contrast to the notation used in Sec. 4, sign $\langle\ldots\rangle$ means the averaging over the usual statistical ensemble of many systems of interest - in our current case, of many harmonic oscillators.

If the coupling to environment is so weak that drag coefficient $\eta$ is small (in the sense that the oscillator's dimensionless $Q$-factor ${ }^{48}$ is large, $Q \equiv m \omega_{0} / \eta \gg 1$ ), this integral is dominated by the resonance peak in a narrow vicinity, $\left|\omega-\omega_{0}\right| \equiv|\xi| \ll \omega_{0}$, of its resonance frequency, and we can take the relatively smooth function $S_{F}(\omega)$ out of the integral, thus reducing it to a table integral:55

[^687]\[

$$
\begin{align*}
\left\langle x^{2}\right\rangle & \approx 2 S_{F}\left(\omega_{0}\right) \int_{0}^{+\infty} \frac{d \omega}{m^{2}\left(\omega_{0}^{2}-\omega^{2}\right)^{2}+(\eta \omega)^{2}} \approx 2 S_{F}\left(\omega_{0}\right) \int_{-\infty}^{+\infty} \frac{d \xi}{\left(2 m \omega_{0} \xi\right)^{2}+\left(\eta \omega_{0}\right)^{2}}  \tag{7.150}\\
& =2 S_{F}\left(\omega_{0}\right) \frac{1}{\left(\eta \omega_{0}\right)^{2}} \int_{-\infty}^{+\infty} \frac{d \xi}{(2 m \xi / \eta)^{2}+1}=2 S_{F}\left(\omega_{0}\right) \frac{1}{\left(\eta \omega_{0}\right)^{2}} \frac{\pi \eta}{2 m}=\frac{\pi}{\eta m \omega_{0}^{2}} S_{F}\left(\omega_{0}\right) .
\end{align*}
$$
\]

With the account of the FDT (134) and Eq. (138), this gives

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=\frac{\pi}{\eta m \omega_{0}^{2}} \frac{\hbar}{2 \pi} \eta \omega_{0} \operatorname{coth} \frac{\hbar \omega_{0}}{2 k_{B} T}=\frac{\hbar}{2 m \omega_{0}} \operatorname{coth} \frac{\hbar \omega_{0}}{2 k_{B} T} \tag{7.151}
\end{equation*}
$$

But this is exactly Eq. (48) that was obtained from the Gibbs distribution, without any explicit account of the environment - though keeping it in mind by using the notion of the thermally-equilibrium ensemble. ${ }^{56}$ (Notice that the drag coefficient $\eta$, which characterizes the oscillator-to-environment interaction strength, has cancelled!) Does this mean that we have toiled in vain?

By no means. First of all, the FDT result has an important conceptual value. For example, let us consider the low-temperature limit $k_{\mathrm{B}} T \ll \hbar \omega_{0}$, when Eq. (151) is reduced to

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=\frac{x_{0}^{2}}{2}=\frac{\hbar}{2 m \omega_{0}} . \tag{7.152}
\end{equation*}
$$

Let us ask a naïve question: What exactly is the origin of this coordinate uncertainty? From the point of view of the usual quantum mechanics of closed (Hamiltonian) systems, there is no doubt: this nonvanishing variance of coordinate is the result of the final spatial extension of the ground-state wavefunction, reflecting the Heisenberg's uncertainty relation (that in turn results from the fact that the operators of coordinate and momentum do not commute) - see Eq. (2.271). However, from the point of view of the Heisenberg-Langevin equation (145), variance (152) is an unalienable part of the oscillator's response to the fluctuation force $\widetilde{F}(t)$ exerted by the environment at frequencies $\omega \approx \omega_{0}$. Though it is impossible to refute the former, absolutely legitimate point of view, in many applications it is much easier to subscribe to the latter standpoint, and treat the coordinate uncertainty as the result of the socalled quantum noise of the environment. This notion has received numerous confirmations in experiments that did not include any oscillators with the eigenfrequencies $\omega_{0}$ close to the noise measurement frequency $\omega .{ }^{57}$

The advantage of the Heisenberg-Langevin approach is that for any $\eta>0$ it is possible to calculate the (experimentally measurable!) distribution $S_{x}(\omega)$, i.e. decompose the fluctuations into spectral components. This procedure is not restricted to the limit of small $\eta$ (large $Q$ factors); for any damping we may just plug the FDT (134) into Eq. (149) and integrate. As an example, let us have a look at the so-called quantum diffusion. A free 1D particle may be considered as the particular case of a 1D harmonic oscillator with $\omega_{0}=0$, so that combining Eqs. (134) and (149), we get

[^688]\[

$$
\begin{equation*}
\left\langle x^{2}\right\rangle=2 \int_{0}^{+\infty} \frac{S_{F}(\omega) d \omega}{\left(m \omega^{2}\right)^{2}+(\eta \omega)^{2}}=2 \eta \int_{0}^{+\infty} \frac{1}{\left(m \omega^{2}\right)^{2}+(\eta \omega)^{2}} \frac{\hbar \omega}{2 \pi} \operatorname{coth} \frac{\hbar \omega}{2 k_{B} T} d \omega . \tag{7.153}
\end{equation*}
$$

\]

This integral has two divergences. The first one, of the type $\int d \omega / \omega^{2}$ at the lower limit, is just a classical effect: according to Eq. (85), particle's displacement variance grows with time, so it cannot have a finite time-independent value that Eq. (153) tries to calculate. However, we still can use that result to single out the quantum noise effect on diffusion - say, by comparing it with a similar but purely classical case. These effects are prominent at high frequencies, especially if the quantum noise overcomes the thermal noise before the dynamic cut-off, i.e. if

$$
\begin{equation*}
\frac{k_{\mathrm{B}} T}{\hbar} \ll \frac{\eta}{m} . \tag{7.154}
\end{equation*}
$$

In this case there is a broad range of frequencies where the quantum noise gives a substantial contribution to the integral:

$$
\begin{equation*}
\left\langle x^{2}\right\rangle_{Q} \approx 2 \eta \int_{k_{\mathrm{B}} T / \hbar}^{\eta / m} \frac{1}{(\eta \omega)^{2}} \frac{\hbar \omega}{2 \pi} d \omega=\frac{\hbar}{\pi \eta} \int_{k_{\mathrm{B}} T / \hbar}^{\eta / m} \frac{d \omega}{\omega}=\frac{\hbar}{\pi \eta} \ln \frac{\hbar \eta}{m k_{\mathrm{B}} T} \sim \frac{\hbar}{\eta} \tag{7.155}
\end{equation*}
$$

Formally, this contribution diverges at either $m \rightarrow 0$ or $T \rightarrow 0$, but this logarithmic (i.e. extremely weak) divergence is readily quenched by an almost any change of the environment model at very high frequencies, where the "Ohmic" approximation given by Eq. (136) becomes unrealistic.

The Heisenberg-Langevin approach is extremely simple and powerful, ${ }^{58}$ but is has its limitations. The main one is that if the equations of motion for the Heisenberg operators are not linear, there is no linear relation, such as Eq. (146), between the Fourier images of the generalized force and generalized coordinate, and as the result there is no simple relation, such as Eq. (148), between their spectral densities. In other words, if the Heisenberg equation of motion are nonlinear, there is no regular simple way to use them to calculate statistical properties of the observables. For example, let us return to the dephasing problem described by Eqs. (68)-(70), and assume that the generalized force is characterized by relations similar to (93) and (134). Now writing the Heisenberg equations of motion for the two remaining spin operators, and using the commutation relations between them, we get

$$
\begin{equation*}
\dot{\hat{\sigma}}_{x}=-2 \frac{a-\hat{\tilde{f}}(t)}{\hbar} \hat{\sigma}_{y}, \quad \dot{\hat{\sigma}}_{y}=2 \frac{a-\hat{\tilde{f}}(t)}{\hbar} \hat{\sigma}_{x} \tag{7.156}
\end{equation*}
$$

These equations do not provide a linear relation between the Pauli operators and the fluctuation force, so even if we know spectral properties of the latter from the FDT, this does not help too much - unless we return to the approximate, classical approach described in Sec. 3 above. ${ }^{59}$

[^689]
### 7.6. Density matrix approach

The main alternative approach, that is essentially a generalization of that used in Sec. 2, is to extract the final results from the dynamics of the density matrix of our subsystem $s$ of interest (which, from this point on, will be called $w_{s}$ ). I will discuss this approach in detail, ${ }^{60}$ cutting just a few technical corners, in each case referring the reader to special literature.

We already know that the density matrix allows the calculation of the expectation value of any observable of system $s$ - see Eq. (5). However, our initial recipe (6) for the density matrix calculation, which requires the knowledge of the exact state (2) of the whole Universe, is not too practicable, while the von Neumann equation (66) for the density matrix evolution is limited to cases in which probabilities $W_{j}$ of the system states are fixed - thus excluding such important effects as the energy relaxation. However, such effects may be analyzed using a different assumption - that the system of interest interacts only with some local environment (say, with the lab room) that is in the thermallyequilibrium state described by a diagonal density matrix - see Eqs. (15) and (23).

This calculation is facilitated by the following observation. Let us number the basis states of the full local system (the system of our interest plus its local environment) by index $l$, and apply Eq. (5) to write

$$
\begin{equation*}
\langle A\rangle=\operatorname{Tr}(\hat{A} \hat{w})=\sum_{l, l^{\prime}} A_{l l^{\prime}} w_{l l^{\prime}}=\sum_{l, l^{\prime}}\langle l| \hat{A}\left|l^{\prime}\right\rangle\left\langle l^{\prime}\right| \hat{w}|l\rangle, \tag{7.157}
\end{equation*}
$$

where $\hat{w}$ is the statistical operator of this full composite system. At weak interaction between the system $s$ and local environment $e$, their variables reside in different Hilbert spaces, so that we can write

$$
\begin{equation*}
|l\rangle=\left|s_{j}\right\rangle \otimes\left|e_{k}\right\rangle . \tag{7.158}
\end{equation*}
$$

and if observable $A$ depends only on the coordinates of system $s$, Eq. (157) yields

$$
\begin{align*}
& \langle A\rangle=\sum_{\substack{j, j^{\prime} \\
k, k^{\prime}}}\left\langle e_{k}\right| \otimes\left\langle s_{j}\right| \hat{A}\left|s_{j^{\prime}}\right\rangle \otimes\left|e_{k^{\prime}}\right\rangle\left\langle e_{k^{\prime}}\right| \otimes\left\langle s_{j^{\prime}}\right| \hat{w}\left|s_{j}\right\rangle \otimes\left|e_{k}\right\rangle  \tag{7.159}\\
& =\sum_{\substack{i, j^{\prime} \\
k, k^{\prime}}}\left\langle s_{j}\right| \hat{A}\left|s_{j^{\prime}}\right\rangle \delta_{k k^{\prime}}\left\langle e_{k^{\prime}}\right| \otimes\left\langle s_{j^{\prime}}\right| \hat{w}\left|s_{j}\right\rangle \otimes\left|e_{k}\right\rangle=\sum_{j, j^{\prime}} A_{i j^{\prime}}\left\langle s_{j^{\prime}}\left(\sum_{k} \otimes\left\langle e_{k}\right| \hat{w}\left|e_{k}\right\rangle \otimes\right) \mid s_{j}\right\rangle=\operatorname{Tr}_{j}\left(\hat{A} \hat{w}_{s}\right),
\end{align*}
$$

where $\hat{w}_{s}$ is defined as

$$
\begin{equation*}
\hat{w}_{s} \equiv \sum_{k}\left\langle e_{k}\right| \hat{w}\left|e_{k}\right\rangle=\operatorname{Tr}_{k} \hat{w} . \tag{7.160}
\end{equation*}
$$

Since Eq. (159) is similar to Eq. (5), $\hat{w}_{s}$ may serve as the statistical operator defined in the Hilbert space of the system of our interest. The huge advantage of Eqs. (159)-(160) is that they are valid for an arbitrary state of the local environment, including the case when it is in the thermodynamic equilibrium. By the way, the similarity of Eqs. (5) and (159) may serve as the strong argument, promised in Sec. 1, for the validity of the former relation even if the Universe as a whole is not in a pure state. (The argument is, however, imperfect, because the latter relation has been derived from the former one.)

[^690]Now, since at a sufficiently large size of the local environment $e$, the composite system $(s+e)$ may be considered Hamiltonian, with fixed probabilities of its states, for the description of time evolution of its statistical operator $\hat{w}$ (again, in contrast to that, $\hat{w}_{s}$, of the system of our interest) we may use the von Neumann equation (66). Partitioning its right-hand part in accordance with Eq. (68), we get:

$$
\begin{equation*}
i \hbar \dot{\hat{w}}=\left[\hat{H}_{s}, \hat{w}\right]+\left[\hat{H}_{e}, \hat{w}\right]+\left[\hat{H}_{\mathrm{int}}, \hat{w}\right] . \tag{7.161}
\end{equation*}
$$

The next step is to use the perturbation theory to solve this equation in the lowest order in $\hat{H}_{\text {int }}$ that yields nonvanishing results due to the interaction. For that, Eq. (161) is not very convenient, because its right-hand part contains two other terms, which are much larger than the interaction Hamiltonian. To mitigate this technical difficulty, the interaction picture (which was discussed in the end of Sec. 4.6), is very handy - though not absolutely necessary.

As a reminder, in that picture (whose entities will be marked with index $I$, with the unmarked operators assumed to be in the Schrödinger picture), both the operators and the state vectors (and hence the density matrix) depend on time. However, the time evolution of the operator of any observable $A$ is described by Eq. (67) with the unperturbed part of the Hamiltonian only - see Eq. (4.214). In our current case (68), this means

$$
\begin{equation*}
i \hbar \dot{\hat{A}}_{I}=\left[\hat{A}_{I}, \hat{H}_{0}\right] \tag{7.162}
\end{equation*}
$$

where the unperturbed Hamiltonian consists of two independent parts:

$$
\begin{equation*}
\hat{H}_{0} \equiv \hat{H}_{s}+\hat{H}_{e} \tag{7.163}
\end{equation*}
$$

On the other hand, the state vector evolution is governed by the interaction evolution operator $\hat{u}_{I}$ that obeys Eqs. (4.215). Since this equation, using the interaction-picture Hamiltonian (4.216),

$$
\begin{equation*}
\hat{H}_{I} \equiv \hat{u}_{0}^{\dagger} \hat{H}_{\mathrm{int}} \hat{u}_{0} \tag{7.164}
\end{equation*}
$$

is absolutely similar to the ordinary Schrödinger equation using the full Hamiltonian, we may repeat all arguments given in the beginning of Sec. 3 to conclude that the dynamics of the density matrix in the interaction picture of a Hamiltonian system is governed by the following analog of the von Neumann equation (66):

$$
\begin{equation*}
i \hbar \dot{\hat{w}}_{I}=\left[\hat{H}_{I}, \hat{w}_{I}\right] . \tag{7.165}
\end{equation*}
$$

Since this equation is similar in structure (with the opposite sign) to the Heisenberg equation (66), we may use solution Eq. (4.190) of the latter equation to write its analog: ${ }^{61}$

$$
\begin{equation*}
\hat{w}_{I}(t)=\hat{u}_{I}(t, 0) \hat{w}(0) \hat{u}_{I}^{\dagger}(t .0) . \tag{7.166}
\end{equation*}
$$

It is also straightforward to verify that in this picture, the expectation value of any observable $A$ may be found from the expression similar to the basic Eq. (5):
${ }^{61}$ Notice the opposite order of the unitary operators, which results from the already mentioned sign difference. Note also that we could write a similar expression in the Schrödinger picture: $\hat{w}(t)=\hat{u} \hat{w}(0) \hat{u}^{\dagger}$, where $\hat{u}$ is the full time-evolution operator.

$$
\begin{equation*}
\langle A\rangle=\operatorname{Tr}\left(\hat{A}_{I} \hat{w}_{I}\right), \tag{7.167}
\end{equation*}
$$

so that the interaction and Schrödinger pictures give the same final results.
In the most frequent case of bilinear interaction (90), ${ }^{62}$ Eq. (162) is readily simplified, in different ways, for the both operators participating in the product. In particular, for $\hat{A}=\hat{x}$, it yields

$$
\begin{equation*}
i \hbar \dot{\hat{x}}_{I}=\left[\hat{x}_{I}, \hat{H}_{0}\right]=\left[\hat{x}_{I}, \hat{H}_{s}\right]+\left[\hat{x}_{I}, \hat{H}_{e}\right] . \tag{7.168}
\end{equation*}
$$

Since operator of coordinate is defined in the Hilbert space of system $s$, it commutes with the Hamiltonian of the environment, so that we finally get

$$
\begin{equation*}
i \hbar \dot{\hat{x}}_{I}=\left[\hat{x}_{I}, \hat{H}_{s}\right] \tag{7.169}
\end{equation*}
$$

On the other hand, taking $\hat{A}=\hat{F}$, we should take into account that the last operator is defined in the Hilbert space of the environment, and commutes with the Hamiltonian of the unperturbed system $s$. As a result, we get

$$
\begin{equation*}
i \hbar \dot{\hat{F}}_{I}=\left[\hat{F}_{I}, \hat{H}_{e}\right] \tag{7.170}
\end{equation*}
$$

This means that with our time-independent unperturbed Hamiltonians $\hat{H}_{s}$ and $\hat{H}_{e}$, the time evolution of the interaction-picture operators is rather simple. In particular, the analogy between Eq. (170) and Eq. (93) allows us to immediately write the following analog of Eq. (94):

$$
\begin{equation*}
\hat{F}_{I}(t)=\exp \left\{\frac{i}{\hbar} \hat{H}_{e} t\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t\right\}, \tag{7.171}
\end{equation*}
$$

so that in the stationary (eigenstate) basis of the environment,

$$
\begin{equation*}
\left(\hat{F}_{I}\right)_{n n^{\prime}}(t)=\exp \left\{\frac{i}{\hbar} E_{n} t\right\} F_{n n^{\prime}}(0) \exp \left\{-\frac{i}{\hbar} E_{n^{\prime}} t\right\}=F_{n n^{\prime}}(0) \exp \left\{-i \frac{E_{n}-E_{n^{\prime}}}{\hbar} t\right\} \tag{7.172}
\end{equation*}
$$

and similarly (but in the basis of the eigenstates of system $s$ ) for operator $\hat{x}$. As a result, Eq. (164) may be also factored:

$$
\begin{align*}
\hat{H}_{I}(t) & \equiv \hat{u}_{0}^{\dagger}(t, 0) \hat{H}_{\mathrm{int}} \hat{u}_{0}(t, 0)=\exp \left\{\frac{i}{\hbar}\left(\hat{H}_{s}+\hat{H}_{e}\right) t\right\}(-\hat{x} \hat{F}) \exp \left\{-\frac{i}{\hbar}\left(\hat{H}_{s}+\hat{H}_{e}\right) t\right\} \\
& =-\left(\exp \left\{\frac{i}{\hbar} \hat{H}_{s} t\right\} \hat{x} \exp \left\{-\frac{i}{\hbar} \hat{H}_{s} t\right\}\right)\left(\exp \left\{\frac{i}{\hbar} \hat{H}_{e} t\right\} \hat{F}(0) \exp \left\{-\frac{i}{\hbar} \hat{H}_{e} t\right\}\right)=-\hat{x}_{I}(t) \hat{F}_{I}(t) \tag{7.173}
\end{align*}
$$

Now, as in Sec. 4, we may rewrite Eq. (165) in the integral form:

$$
\begin{equation*}
\hat{w}_{I}(t)=\frac{1}{i \hbar} \int_{-\infty}^{t}\left[\hat{H}_{I}\left(t^{\prime}\right), \hat{w}_{I}\left(t^{\prime}\right)\right] d t^{\prime} \tag{7.174}
\end{equation*}
$$

[^691]plugging this result, for time $t^{\prime}$, into the right-hand part of Eq. (174) again, we get
\[

$$
\begin{equation*}
\dot{\hat{w}}_{I}(t)=-\frac{1}{\hbar^{2}} \int_{-\infty}^{t}\left[\hat{H}_{I}(t),\left[\hat{H}_{I}\left(t^{\prime}\right), \hat{w}_{I}\left(t^{\prime}\right)\right]\right] d t^{\prime}=-\frac{1}{\hbar^{2}} \int_{-\infty}^{t}\left[\hat{x}(t) \hat{F}(t),\left[\hat{x}\left(t^{\prime}\right) \hat{F}\left(t^{\prime}\right), \hat{w}_{I}\left(t^{\prime}\right)\right]\right] d t^{\prime} \tag{7.175}
\end{equation*}
$$

\]

where, for the notation brevity, from this point on I will strip operators $\hat{x}$ and $\hat{F}$ of their index $I$. (Their time dependence indicates the interaction picture clearly enough.)

So far, this equation is exact (and cannot be solved analytically), but this is the right time to notice that even if we take the density matrix in its right-hand part equal to its unperturbed value (corresponding to no interaction between system $s$ and its thermally-equilibrium environment $e$ ),

$$
\begin{equation*}
\hat{w}_{I}\left(t^{\prime}\right) \rightarrow \hat{w}_{s}\left(t^{\prime}\right) \hat{w}_{e}, \quad \text { with }\left\langle e_{n}\right| \hat{w}_{e}\left|e_{n^{\prime}}\right\rangle=W_{n} \delta_{n n^{\prime}}, \tag{7.176}
\end{equation*}
$$

where $e_{n}$ are the stationary states of the environment and $W_{n}$ are the Gibbs probabilities (23), Eq. (175) would still provide some nonvanishing time evolution of the density operator. This is exactly the first nonvanishing perturbation we have been looking for. Now using Eq. (160), we find the equation of evolution of the density operator of our system of interest:

$$
\begin{equation*}
\dot{\hat{w}}_{s}(t)=-\frac{1}{\hbar^{2}} \int_{-\infty}^{t} \operatorname{Tr}_{n}\left[\hat{x}(t) \hat{F}(t),\left[\hat{x}\left(t^{\prime}\right) \hat{F}\left(t^{\prime}\right), \hat{w}_{s}\left(t^{\prime}\right) \hat{w}_{e}\right]\right] d t^{\prime} \tag{7.177}
\end{equation*}
$$

where the trace is over the stationary states of the environment. In order to spell out the right-hand part of Eq. (177), note again that the coordinate and force operators commute with each other (but not with themselves at different time moments!) and hence may be swapped, so that we may write

$$
\begin{align*}
\operatorname{Tr}_{n}[\ldots,[\ldots, \ldots]]= & \hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}_{s}\left(t^{\prime}\right) \operatorname{Tr}_{n}\left[\hat{F}(t) \hat{F}\left(t^{\prime}\right) \hat{w}_{e}\right]-\hat{x}(t) \hat{w}_{s}\left(t^{\prime}\right) \hat{x}\left(t^{\prime}\right) \operatorname{Tr}_{n}\left[\hat{F}(t) \hat{w}_{e} \hat{F}\left(t^{\prime}\right)\right] \\
& -\hat{x}\left(t^{\prime}\right) \hat{w}_{s}\left(t^{\prime}\right) \hat{x}(t) \operatorname{Tr}_{n}\left[\hat{F}\left(t^{\prime}\right) \hat{w}_{e} \hat{F}(t)\right]+\hat{w}_{s}\left(t^{\prime}\right) \hat{x}\left(t^{\prime}\right) \hat{x}(t) \operatorname{Tr}_{n}\left[\hat{w}_{e} \hat{F}\left(t^{\prime}\right) \hat{F}(t)\right] \\
= & \hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}_{s}\left(t^{\prime}\right) \sum_{n, n^{\prime}} F_{n n^{\prime}}(t) F_{n^{\prime} n}\left(t^{\prime}\right) W_{n}-\hat{x}(t) \hat{w}_{s}\left(t^{\prime}\right) \hat{x}\left(t^{\prime}\right) \sum_{n, n^{\prime}} F_{n n^{\prime}}(t) W_{n^{\prime}} F_{n^{\prime} n}\left(t^{\prime}\right)  \tag{7.178}\\
& -\hat{x}\left(t^{\prime}\right) \hat{w}_{s} \hat{x}(t) \sum_{n, n^{\prime}} F_{n n^{\prime}}\left(t^{\prime}\right) W_{n^{\prime}} F_{n^{\prime} n}(t)+\hat{w}_{s} \hat{x}\left(t^{\prime}\right) \hat{x}(t) \sum_{n, n^{\prime}} W_{n} F_{n n^{\prime}}\left(t^{\prime}\right) F_{n^{\prime} n}(t) .
\end{align*}
$$

Since the summation on both indices $n$ and $n$ ' in this expression is over the same energy level set (of all eigenstates of the environment), we may swap the indices in any of the sums. Doing that in the terms with factors $W_{n}$, we turn them into $W_{n}$, so that this factor becomes common:

$$
\begin{align*}
\operatorname{Tr}_{n}[\ldots,[\ldots, \ldots]]= & \sum_{n, n^{\prime}} W_{n}\left[\hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}_{s}\left(t^{\prime}\right) F_{n n^{\prime}}(t) F_{n^{\prime} n}\left(t^{\prime}\right)-\hat{x}(t) \hat{w}_{s}\left(t^{\prime}\right) \hat{x}\left(t^{\prime}\right) F_{n^{\prime} n}(t) F_{n n^{\prime}}\left(t^{\prime}\right)\right.  \tag{7.179}\\
& \left.-\hat{x}\left(t^{\prime}\right) \hat{w}_{s} \hat{x}(t) F_{n^{\prime} n}\left(t^{\prime}\right) F_{n n^{\prime}}(t)+\hat{w}_{s} \hat{x}\left(t^{\prime}\right) \hat{x}(t) F_{n n^{\prime}}\left(t^{\prime}\right) F_{n^{\prime} n}(t)\right] .
\end{align*}
$$

Now using Eq. (172), we get

$$
\begin{array}{r}
\begin{array}{r}
\operatorname{Tr}_{n}[\ldots,[\ldots, \ldots]]=\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2}\left[\hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}_{s}\left(t^{\prime}\right) \exp \left\{i \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\right\}-\hat{x}(t) \hat{w}_{s}\left(t^{\prime}\right) \hat{x}\left(t^{\prime}\right) \exp \left\{-i \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\right\}\right. \\
\left.-\hat{x}\left(t^{\prime}\right) \hat{w}_{s} \hat{x}(t) \exp \left\{i \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\right\}+\hat{w}_{s} \hat{x}\left(t^{\prime}\right) \hat{x}(t) \exp \left\{-i \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\right\}\right] \\
=\sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \cos \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\left[\hat{x}(t),\left[\hat{x}\left(t^{\prime}\right), \hat{w}_{s}\left(t^{\prime}\right)\right]\right]+i \sum_{n, n^{\prime}} W_{n}\left|F_{n n^{\prime}}\right|^{2} \sin \frac{\widetilde{E}\left(t-t^{\prime}\right)}{\hbar}\left[\hat{x}(t),\left\{\hat{x}\left(t^{\prime}\right), \hat{w}_{s}\left(t^{\prime}\right)\right\}\right],
\end{array}
\end{array}
$$

where $\{\ldots, \ldots\}$ means the anticommutator - see Eq. (4.34). Comparing the two double sums participating in this expression with Eqs. (108) and (111), we see that they are nothing else than, respectively, the symmetrized correlation function and the Green's function (multiplied by $\hbar / 2$ ) of the time-difference argument $\tau=t-t^{\prime} \geq 0$. As the result, Eq. (177) takes a very simple form:

$$
\begin{equation*}
\dot{\hat{w}}_{s}(t)=-\frac{1}{\hbar^{2}} \int_{-\infty}^{t} K_{F}\left(t-t^{\prime}\right)\left[\hat{x}(t),\left[\hat{x}\left(t^{\prime}\right), \hat{w}_{s}\left(t^{\prime}\right)\right]\right] d t^{\prime}-\frac{i}{2 \hbar} \int_{-\infty}^{t} G\left(t-t^{\prime}\right)\left[\hat{x}(t),\left\{\hat{x}\left(t^{\prime}\right), \hat{w}_{s}\left(t^{\prime}\right)\right\}\right] d t^{\prime} \tag{7.181}
\end{equation*}
$$

Let me hope that the reader enjoys this beautiful result as much as I do, and that it is a sufficient intellectual award for his or her effort of following its derivation. It gives a self-sufficient equation for time evolution of the density matrix of the system of our interest ( $s$ ), with the effects of its environment represented only by two real algebraic functions of $\tau$ - one ( $K_{F}$ ) describing environment's fluctuations and another one $(G)$ representing its the average response to system's dynamics. And most spectacularly, these are exactly the same functions as participate in the Heisenberg-Langevin approach to the problem, and hence related to each other by the fluctuation-dissipation theorem (134).

After a short celebration, let us acknowledge that Eq. (181) is still an integro-differential equation that needs to be solved together with Eq. (169). Such equations do not allow explicit analytical solutions except for very simple (and not very interesting) cases. For most applications, further simplifications should be made. One of them is based on the fact (which was already discussed in Sec. 3) that both environmental functions participating in Eq. (181) tend to zero when their argument $\tau$ becomes larger that certain environment correlation time $\tau_{c}$, which is frequently much shorter that the time scales $T_{n n}$ ' of the evolution of the density matrix elements. Moreover, the characteristic time scale of the coordinate operator evolution may be also short on the scale of $T_{n n^{\prime}}$. In this limit, all arguments $t^{\prime}$ of the density operator giving substantial contributions to the right-hand part of Eq. (172) are so close to $t$ that it does not matter whether its argument is $t^{\prime}$ or just $t$. This simplification $\left(t^{\prime} \rightarrow t\right)$ is known as the Markov approximation. ${ }^{63}$ However, this approximation alone is still insufficient for finding the general solution of Eq. (181). Substantial further progress is possible in two important cases.

The most important of them is when the intrinsic Hamiltonian $\hat{H}_{s}$ of our system of interest is time-independent and has a very discrete eigenenergy spectrum $E_{n}{ }^{64}$ with well-separated levels:

[^692]\[

$$
\begin{equation*}
\left|E_{n}-E_{n^{\prime}}\right| \gg \frac{\hbar}{T_{n n^{\prime}}} . \tag{7.182}
\end{equation*}
$$

\]

Let us see what does this condition yield for Eq. (181) rewritten for the matrix elements in the stationary state basis (from this point on, I will drop index $s$ for brevity):

$$
\begin{equation*}
\dot{w}_{n n^{\prime}}=-\frac{1}{\hbar^{2}} \int_{-\infty}^{t} K_{F}\left(t-t^{\prime}\right)\left[\hat{x}(t),\left[\hat{x}\left(t^{\prime}\right), \hat{w}\right]\right]_{n n^{\prime}} d t^{\prime}-\frac{i}{2 \hbar} \int_{-\infty}^{t} G\left(t-t^{\prime}\right)\left[\hat{x}(t),\left\{\hat{x}\left(t^{\prime}\right), \hat{w}\right\}\right]_{n n^{\prime}} d t^{\prime} ; \tag{7.183}
\end{equation*}
$$

after spelling out the commutators, it includes 4 operator products, which differ "only" by the operator order. Let us have a good look at the first product,

$$
\begin{equation*}
\left(\hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}\right)_{n n^{\prime}}=\sum_{m, m^{\prime}} x_{n m}(t) x_{m m^{\prime}}\left(t^{\prime}\right) w_{m^{\prime} n^{\prime}} \tag{7.184}
\end{equation*}
$$

where indices $m$ and $m$ ' run over the same set of eigenenergies of the system $s$ of our interest as indices $n$ and $n^{\prime}$. According to Eq. (169) with a time-independent $H_{s}$, matrix elements $x_{n n}$ ' (in the stationary state basis) oscillate in time as $\exp \left\{i \omega_{n n} \cdot t\right\}$, so that

$$
\begin{equation*}
\left(\hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}\right)_{n n^{\prime}}=\sum_{m, m^{\prime}} x_{n m} x_{m m^{\prime}} \exp \left\{i\left(\omega_{n m} t+\omega_{m m^{\prime}} \cdot t^{\prime}\right)\right\} w_{m^{\prime} n^{\prime}}, \tag{7.185}
\end{equation*}
$$

where the coordinate matrix elements are in the Schrödinger picture now, and I have used the natural notation (6.85) for the quantum transition frequencies:

$$
\begin{equation*}
\hbar \omega_{n n^{\prime}} \equiv E_{n}-E_{n^{\prime}} . \tag{7.186}
\end{equation*}
$$

According to condition (182), frequencies $\omega_{n n^{\prime}}$ with $n \neq n^{\prime}$ are much higher than the speed of evolution of the density matrix elements (in the interaction picture!) - in both the left-hand and right-hand parts of Eq. (183). As we already know from Sec. 6.5, this means that in the right-hand part of Eq. (183) we may keep only the terms that do not oscillate with frequencies $\omega_{n n}$, because they would give negligible contribution to the density matrix dynamics. ${ }^{65}$ For that, in the double sum (185) we may keep only the terms proportional to difference ( $t-t^{\prime}$ ), because they will give (after integration over $t^{\prime}$ ) a slowly changing contribution to the right-hand part. ${ }^{66}$ These terms should have $\omega_{n m}+\omega_{m m^{\prime}}=0$, i.e. $\left(E_{n}-E_{m}\right)+$ $\left(E_{m}-E_{m^{\prime}}\right) \equiv E_{n}-E_{m^{\prime}}=0$. For a non-degenerate energy spectrum, this requirement means $m^{\prime}=n$; as a result, the double sum is reduced to a single one:

$$
\begin{equation*}
\left(\hat{x}(t) \hat{x}\left(t^{\prime}\right) \hat{w}\right)_{n n^{\prime}} \approx \sum_{m} x_{n m} x_{m n} \exp \left\{i \omega_{n m}\left(t-t^{\prime}\right)\right\} w_{n n^{\prime}}=\sum_{m}\left|x_{n m}\right|^{2} \exp \left\{i \omega_{n m}\left(t-t^{\prime}\right)\right\} w_{n n^{\prime}} \tag{7.187}
\end{equation*}
$$

Another product, $\left(\hat{w} \hat{x}\left(t^{\prime}\right) \hat{x}(t)\right)_{n n^{\prime}}$, that appears in the right-hand part of Eq. (183), may be simplified absolutely similarly, giving

$$
\begin{equation*}
\left(\hat{w} \hat{x}\left(t^{\prime}\right) \hat{x}(t)\right)_{n n^{\prime}} \approx \sum_{m}\left|x_{n^{\prime} m}\right|^{2} \exp \left\{i \omega_{n^{\prime} m}\left(t^{\prime}-t\right)\right\} w_{n n^{\prime}} \tag{7.188}
\end{equation*}
$$

[^693]These expressions hold true whether $n$ and $n$ ' are equal or not. The situation is different for two other products in the right-hand part of Eq. (183), with $w$ sandwiched between $x$ and $x$ '. For example,

$$
\begin{equation*}
\left(\hat{x}(t) \hat{w} \hat{x}\left(t^{\prime}\right)\right)_{n n^{\prime}}=\sum_{m, m^{\prime}} x_{n m}(t) w_{m m^{\prime}} x_{m^{\prime} n^{\prime}}\left(t^{\prime}\right)=\sum_{m, m^{\prime}} x_{n m} w_{m m^{\prime}} x_{m^{\prime} n^{\prime}} \exp \left\{i\left(\omega_{n m} t+\omega_{m^{\prime} n^{\prime}}, t^{\prime}\right)\right\} \tag{7.189}
\end{equation*}
$$

For this term, the same requirement of having a fast oscillating function of $\left(t-t^{\prime}\right)$ only yields a different condition: $\omega_{n m}+\omega_{m^{\prime} n^{\prime}}=0$, i.e.

$$
\begin{equation*}
\left(E_{n}-E_{m}\right)+\left(E_{m^{\prime}}-E_{n^{\prime}}\right)=0 . \tag{7.190}
\end{equation*}
$$

Here the double sum reduction is possible only if we make an additional assumption that all interlevel energy distances are unique, i.e. our system of interest has no equidistant levels (such as in the harmonic oscillator). For diagonal elements ( $n=n^{\prime}$ ), the RWA requirement is reduced to $m=m^{\prime}$, giving sums over all diagonal elements of the density matrix:

$$
\begin{equation*}
\left(\hat{x}(t) \hat{w} \hat{x}\left(t^{\prime}\right)\right)_{n n}=\sum_{m}\left|x_{n m}\right|^{2} \exp \left\{i \omega_{n m}\left(t-t^{\prime}\right)\right\} w_{m m} . \tag{7.191}
\end{equation*}
$$

(Another similar term $\left(\hat{x}\left(t^{\prime}\right) \hat{w} \hat{x}(t)\right)_{n n}$, is just a complex conjugate of Eq. (191).) However, for offdiagonal matrix elements $\left(n \neq n^{\prime}\right)$, the situation is different: Eq. (190) may be satisfied only if $m=n$ and also $m^{\prime}=n^{\prime}$, so that the double sum is reduced to just one, non-oscillating term:

$$
\begin{equation*}
\left(\hat{x}(t) \hat{w} \hat{x}\left(t^{\prime}\right)\right)_{n n^{\prime}}=x_{n n} w_{n n^{\prime}} x_{n^{\prime} n^{\prime}}, \quad \text { for } n \neq n^{\prime} . \tag{7.192}
\end{equation*}
$$

The second similar term, $\left(\hat{x}\left(t^{\prime}\right) \hat{w} \hat{x}(t)\right)_{n n}$, is exactly the same, so that in one of the integrals of Eq. (183), these terms add up, while in the second one, they cancel.

This is why the final equations of evolution look differently for diagonal and off-diagonal elements of the density matrix. For the former case ( $n=n^{\prime}$ ), Eq. (183) is reduced to the so-called master equation ${ }^{67}$ relating diagonal elements $w_{n n}$ of the density matrix, i.e. the energy level occupancies $W_{n}$ : ${ }^{68}$

$$
\begin{align*}
\dot{W}_{n}=\sum_{m \neq n}\left|x_{n m}\right|^{2} \int_{0}^{\infty} & {\left[-\frac{1}{\hbar^{2}} K_{F}(\tau)\left(W_{n}-W_{m}\right)\left(\exp \left\{i \omega_{n m} \tau\right\}+\exp \left\{-i \omega_{n m} \tau\right\}\right)\right.}  \tag{7.193}\\
& \left.-\frac{i}{2 \hbar} G(\tau)\left(-W_{n}-W_{m}\right)\left(\exp \left\{i \omega_{n m} \tau\right\}-\exp \left\{-i \omega_{n m} \tau\right\}\right)\right] d \tau
\end{align*}
$$

where $\tau \equiv t-t^{\prime}$. Changing the summation index notation from $m$ to $n$ ', we may rewrite the master equation in its canonical form

$$
\begin{equation*}
\dot{W}_{n}=\sum_{n^{\prime} \neq n}\left(\Gamma_{n^{\prime} \rightarrow n} W_{n^{\prime}}-\Gamma_{n \rightarrow n^{\prime}} W_{n}\right), \tag{7.194}
\end{equation*}
$$

where coefficients

$$
\begin{equation*}
\Gamma_{n^{\prime} \rightarrow n} \equiv\left|x_{n n^{\prime}}\right|^{2} \int_{0}^{\infty}\left[\frac{2}{\hbar^{2}} K_{F}(\tau) \cos \omega_{n n^{\prime}} \tau-\frac{1}{\hbar} G(\tau) \sin \omega_{n n^{\prime}} \tau\right] d t^{\prime} \tag{7.195}
\end{equation*}
$$

[^694]Master equations and interlevel transition rates
are called the interlevel transition rates. ${ }^{69}$ Equation (194) has a very clear physical meaning of the level occupancy dynamics (i.e. the balance of probability flows $\Gamma W$ ) due to the quantum transitions between the energy levels (Fig. 6), in our current case caused by the interaction between the system of our interest and its environment. ${ }^{70}$


Fig. 7.6. Probability flows between the energy levels, described by the master equation (186).

The Fourier transforms (113) and (123) enable us to express two integrals in Eq. (195) via, respectively, the symmetrized spectral density $S_{F}(\omega)$ of environment force fluctuations and the imaginary part $\chi$ " $(\omega)$ of the generalized susceptibility, both at frequency $\omega=\omega_{n n}$. After that we may use the fluctuation-dissipation theorem (134) to exclude the former function, getting finally

Transition
rates via generalized susceptibility

$$
\begin{equation*}
\Gamma_{n^{\prime} \rightarrow n}=\frac{1}{\hbar}\left|x_{n n^{\prime}}\right|^{2} \chi^{\prime \prime}\left(\omega_{n n^{\prime}}\right)\left(\operatorname{coth} \frac{\hbar \omega_{n n^{\prime}}}{2 k_{\mathrm{B}} T}-1\right)=\frac{2}{\hbar}\left|x_{n n^{\prime}}\right|^{2} \frac{\chi^{\prime \prime}\left(\omega_{n n^{\prime}}\right)}{\exp \left\{\left(E_{n}-E_{n^{\prime}}\right) / k_{\mathrm{B}} T\right\}-1} . \tag{7.196}
\end{equation*}
$$

Note that since the imaginary part of the generalized susceptibility is an odd function of frequency, Eq. (196) is in compliance with the Gibbs distribution for arbitrary temperature. Indeed, according to this equation, the ratio of "up" and "down" rates for each pair of levels equals

$$
\begin{equation*}
\frac{\Gamma_{n^{\prime} \rightarrow n}}{\Gamma_{n \rightarrow n^{\prime}}}=\frac{\chi^{\prime \prime}\left(\omega_{n n^{\prime}}\right)}{\exp \left\{\left(E_{n}-E_{n^{\prime}}\right) / k_{\mathrm{B}} T\right\}-1} / \frac{\chi^{\prime \prime}\left(\omega_{n^{\prime}}\right)}{\exp \left\{\left(E_{n^{\prime}}-E_{n}\right) / k_{\mathrm{B}} T\right\}-1}=\exp \left\{-\frac{E_{n}-E_{n^{\prime}}}{k_{\mathrm{B}} T}\right\} . \tag{7.197}
\end{equation*}
$$

On the other hand, according to the Gibbs distribution (23), in thermal equilibrium the level populations should be in the same proportion, satisfying the so-called detailed balance equations,

Detailed balance equations

$$
\begin{equation*}
W_{n} \Gamma_{n \rightarrow n^{\prime}}=W_{n^{\prime}} \Gamma_{n^{\prime} \rightarrow n}, \tag{7.198}
\end{equation*}
$$

for each pair $\left\{n, n^{\prime}\right\}$, so that all right-hand parts of all Eqs. (194) could vanish - as they should. Thus, the stationary solution of the master equations indeed describes the thermal equilibrium.

The closed system of master equations (194), sometimes complemented by additional right-hand-part terms that describe interlevel transitions due to other factors (e.g., by an external ac force with a frequency close to one of $\omega_{n n}$ ), is the key starting point for practical analyses of many quantum

[^695]systems including quantum generators (masers and lasers). It is important to remember that it is strictly valid only in the rotating-wave approximation, i.e. if Eq. (182) is well satisfied for all $n$ and $n$ '.

For a particular but very important case of a two-level system (with, say, $E_{1}>E_{2}$ ), the rate $\Gamma_{1 \rightarrow 2}$ may be interpreted (especially in the low-temperature limit $k_{\mathrm{B}} T \ll \hbar \omega_{12}=E_{1}-E_{2}$, when $\Gamma_{1 \rightarrow 2} \gg \Gamma_{2 \rightarrow 1}$ ) as the reciprocal characteristic time $1 / T_{1} \equiv \Gamma_{1 \rightarrow 2}$ of the energy relaxation process that brings the diagonal elements of the density matrix to their thermally-equilibrium values (24). For the Ohmic dissipation described by Eqs. (137)-(138), Eq. (196) yields

$$
\frac{1}{T_{1}} \equiv \Gamma_{1 \rightarrow 2}=\frac{2}{\hbar^{2}}\left|x_{12}\right|^{2} \eta \times \begin{cases}\hbar \omega_{12}, & \text { for } k_{\mathrm{B}} T \ll \hbar \omega_{12},  \tag{7.199}\\ k_{\mathrm{B}} T, & \text { for } \hbar \omega_{12} \ll k_{\mathrm{B}} T\end{cases}
$$

Of course, time $T_{1}$ should not be confused with the characteristic time $T_{2}$ of relaxation of the offdiagonal elements, i.e. dephasing, which was already discussed in Sec. 3. By the way, let us see what do Eqs. (183) say about the dephasing rate. Taking into account our intermediate results (187)-(192), and merging the non-oscillating components (with $m=n$ and $m=n$ ') of sums Eq. (187) and (188) with the terms (192), that also do not oscillate in time, we get the following equation: ${ }^{71}$

$$
\begin{align*}
\dot{w}_{n n^{\prime}}=-\left\{\int_{0}^{\infty}\right. & {\left[\frac{1}{\hbar^{2}} K_{F}(\tau)\left(\sum_{m \neq n}\left|x_{n m}\right|^{2} \exp \left\{i \omega_{n m} \tau\right\}+\sum_{m \neq n^{\prime}}\left|x_{n^{\prime} m}\right|^{2} \exp \left\{-i \omega_{n^{\prime} m} \tau\right\}+\left(x_{n n}-x_{n^{\prime} n^{\prime}}\right)^{2}\right)\right.} \\
& \left.\left.+\frac{i}{2 \hbar} G(\tau)\left(\sum_{m \neq n}\left|x_{n m}\right|^{2} \exp \left\{i \omega_{n m} \tau\right\}-\sum_{m \neq n^{\prime}}\left|x_{n^{\prime} m}\right|^{2} \exp \left\{-i \omega_{n^{\prime} m} \tau\right\}\right)\right] d \tau\right\} w_{n n^{\prime}}, \text { for } n \neq n^{\prime} . \tag{7.200}
\end{align*}
$$

In contrast with Eq. (194), the right-hand part of this equation includes both a real and an imaginary part, and hence it may be presented as

$$
\begin{equation*}
\dot{w}_{n n^{\prime}}=-\left(1 / T_{n n^{\prime}}+i \Delta_{n n^{\prime}}\right) w_{n n^{\prime}} \tag{7.201}
\end{equation*}
$$

where both factors $1 / T_{n n}$, and $\Delta_{n n^{\prime}}$ are real. ${ }^{72}$ As should be clear from Eq. (201), the second term in the right-hand part of this equation causes slow oscillations of the matrix elements $w_{n n}$, that, after returning to the Schrödinger picture, add just small corrections ${ }^{73}$ to the unperturbed frequencies (186) of their oscillations, and are hence are not important for most applications. More important is the first term,

[^696]\[

$$
\begin{align*}
\frac{1}{T_{n n^{\prime}}}=\int_{0}^{\infty} & \frac{1}{\hbar^{2}} K_{F}(\tau)\left(\sum_{m \neq n}\left|x_{n m}\right|^{2} \cos \omega_{n m} \tau+\sum_{m \neq n^{\prime}}\left|x_{n^{\prime} m}\right|^{2} \cos \omega_{n^{\prime} m} \tau+\left(x_{n n}-x_{n^{\prime} n^{\prime}}\right)^{2}\right)  \tag{7.202}\\
& \left.-\frac{1}{2 \hbar} G(\tau)\left(\sum_{m \neq n}\left|x_{n m}\right|^{2} \sin \omega_{n m} \tau+\sum_{m \neq n^{\prime}}\left|x_{n^{\prime} m}\right|^{2} \sin \omega_{n^{\prime} m} \tau\right)\right] d \tau, \quad \text { for } n \neq n^{\prime},
\end{align*}
$$
\]

because it describes the effect absent without the environment: an exponential decay of the off-diagonal matrix elements, i.e. dephasing. Comparing the first 2 terms of Eq. (202) with Eq. (195), we see that the dephasing rates may be described by a very simple formula: r

$$
\begin{align*}
\frac{1}{T_{n n^{\prime}}} & =\frac{1}{2}\left(\sum_{m \neq n} \Gamma_{n \rightarrow m}+\sum_{m \neq n^{\prime}} \Gamma_{n^{\prime} \rightarrow m}\right)+\frac{\pi}{\hbar^{2}}\left(x_{n n}-x_{n^{\prime} n^{\prime}}\right)^{2} S_{F}(0) \\
& =\frac{1}{2}\left(\sum_{m \neq n} \Gamma_{n \rightarrow m}+\sum_{m \neq n^{\prime}} \Gamma_{n^{\prime} \rightarrow m}\right)+\frac{k_{\mathrm{B}} T}{\hbar^{2}} \eta\left(x_{n n}-x_{n^{\prime} n^{\prime}}\right)^{2}, \quad \text { for } n \neq n^{\prime} \tag{7.203}
\end{align*}
$$

where the low-frequency drag coefficient $\eta$ is again defined as $\lim _{\omega \rightarrow 0} \chi$ " $(\omega) / \omega$ - see Eq. (138).
This result shows that two effects yield independent contributions into dephasing. The first of them may be interpreted as a result of the "virtual" transitions of the system to other energy levels $m$; according to Eq. (187), it is proportional to the strength of coupling to environment at relatively high frequencies $\omega_{n m}$ and $\omega_{n^{\prime} m}$. (If the energy quanta $\hbar \omega$ of these frequencies are much larger than the thermal fluctuation scale $k_{\mathrm{B}} T$, only the lower levels, with $E_{m}<\max \left[E_{n}, E_{n}\right]$ are important.) On the contrary, the second contribution is due to low-frequency, essentially classical fluctuations of the environment, and hence to the low-frequency dissipative susceptibility. If the susceptibility (more exactly, the ratio $\eta=$ $\left.\chi^{\prime \prime}(\omega) / \omega\right)$ is frequency-independent, both contributions are of the same order, but their exact relation depends on the relation between the matrix elements $x_{n n}$ ' of a particular system.

Returning again to the two-level system discussed in Sec. 3, the high-frequency contributions vanish because of the absence of transitions between its energy levels, while the low-frequency contribution yields

$$
\begin{equation*}
\frac{1}{T_{2}} \equiv \frac{1}{T_{12}}=\frac{k_{\mathrm{B}} T}{\hbar^{2}} \eta\left(x_{n n}-x_{n^{\prime} n^{\prime}}\right)^{2} \rightarrow \frac{k_{\mathrm{B}} T}{\hbar^{2}} \eta\left[\left(\sigma_{z}\right)_{11}-\left(\sigma_{z}\right)_{22}\right]^{2}=\frac{4 k_{\mathrm{B}} T}{\hbar^{2}} \eta, \tag{7.204}
\end{equation*}
$$

thus exactly reproducing the result (142) of the Heisenberg-Langevin approach. ${ }^{74}$ Note also that Eq. (204) for $T_{2}$ is very close in structure to Eq. (199) for $T_{1}$. For our simple interaction model (70), the offdiagonal elements of operator $\hat{x}=\hat{\sigma}_{z}$ in the stationary-state $z$-basis vanish, so that $T_{1} \rightarrow \infty$. For the twowell implementation of the model (see Fig. 4 and its discussion), this result corresponds to a very high energy barrier between the wells, that inhibits tunneling, and hence any change of well occupancies $W_{L}$
electromagnetic environment is ignored.) The explanation of the shift, by H. Bethe in the same 1947, has launched the whole field of quantum electrodynamics - to be briefly discussed in Chapter 9.
${ }^{74}$ The first form of Eq. (203), as well as the analysis of Sec. 3, imply that low-frequency fluctuations of any other origin, not taken into account in own current calculations (say, unintentional noise from experimental equipment), may also cause dephasing; such "technical fluctuations" are indeed a serious challenge at the experimental implementation of coherent qubit systems - see Sec. 8.5 below.
and $W_{R}$. However, $T_{1}$ may become finite, and comparable with $T_{2}$, if tunneling between the wells is substantial. ${ }^{75}$

Now let us briefly discuss dissipative systems with continuous spectrum. Unfortunately, for them the only (relatively :-) simple results that may be obtained from Eq. (181) are essentially classical in nature. As an illustration, let us consider the simplest example of a 1D particle that interacts with a thermally-equilibrium environment, but otherwise is free to move (unconfined). As we know from Chapters 2 and 5, in this case the most convenient basis is that of momentum eigenstates $p$. In the momentum representation, the density matrix is just the $c$-number function $w\left(p, p^{\prime}\right)$, defined by Eq. (54), that has already been discussed in brief in Sec. 2. On the other hand, the coordinate operator, that also participates in the right-hand part of Eq. (181), has the form given by the first of Eqs. (5.64),

$$
\begin{equation*}
\hat{x}=i \hbar \frac{\partial}{\partial p} \tag{7.205}
\end{equation*}
$$

dual to the coordinate representation formula (5.29). As we already know, such operators are local - see, e.g., Eq. (5.28b). Due to this locality, the whole right-hand part of Eq. (181) is local as well, and hence (within the framework of our perturbative treatment) the interaction with environment affects essentially only the diagonal values $w(p, p)$ of the density matrix, i.e. the momentum probability density $w(p)$. Let us find the equation governing the evolution of this function in time.

Generally, in the interaction picture, matrix elements of operators $\hat{x}$ and $\hat{w}$ acquire some time dependence, but in the limit $p^{\prime} \rightarrow p$, this dynamics lacks the high frequencies (186) that have been so helpful for the derivation of master equations. As a result, the only serious simplification of Eq. (181) is possible in the Markov approximation, when the time scale of the density matrix evolution is much longer than the correlation time $\tau_{c}$ of the environment, i.e. the time scale of functions $K_{F}(\tau)$ and $G(\tau)$. In this approximation, we may take the matrix elements out of the first integral of Eq. (181),

$$
\begin{align*}
& -\frac{1}{\hbar^{2}} \int_{-\infty}^{t} K_{F}\left(t-t^{\prime}\right) d t^{\prime}\left[\hat{x}(t),\left[\hat{x}\left(t^{\prime}\right), \hat{w}\left(t^{\prime}\right)\right]\right] \approx-\frac{1}{\hbar^{2}} \int_{0}^{\infty} K_{F}(\tau) d \tau[\hat{x},[\hat{x}, \hat{w}]]  \tag{7.206}\\
& =-\frac{\pi}{\hbar^{2}} S_{F}(0)[\hat{x},[\hat{x}, \hat{w}]]=-\frac{k_{\mathrm{B}} T}{\hbar^{2}} \eta[\hat{x},[\hat{x}, \hat{w}]]
\end{align*}
$$

and calculate the double commutator in the Schrödinger picture. This may be done either using an explicit expression for the matrix elements of the coordinate operator, dual to Eq. (5.28b), or in a simpler way, using the same trick as at the derivation of the Ehrenfest theorem in Sec. 5.2. Namely, expanding an arbitrary function $f(p)$ into the Taylor series in one of its arguments (say, $p$ ),

$$
\begin{equation*}
f(p)=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} f}{\partial p^{k}} p^{k} \tag{7.207}
\end{equation*}
$$

and applying Eq. (205) to each term, we can prove the following simple commutation relation:

[^697]\[

$$
\begin{equation*}
[\hat{x}, f]=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} f}{\partial p^{k}}\left[\hat{x}, p^{k}\right]=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^{k} f}{\partial p^{k}}\left(i \hbar k p^{k-1}\right)=i \hbar \sum_{k=1}^{\infty} \frac{1}{(k-1)!} \frac{\partial^{k-1}}{\partial p^{k-1}}\left(\frac{\partial f}{\partial p}\right) p^{k-1}=i \hbar \frac{\partial f}{\partial p} . \tag{7.208}
\end{equation*}
$$

\]

Now applying this result sequentially, first to $w\left(p, p^{\prime}\right)$ and then to the resulting commutator, we get

$$
\begin{equation*}
[\hat{x},[\hat{x}, w]]=\left[\hat{x}, i \hbar \frac{\partial w}{\partial p}\right]=i \hbar \frac{\partial}{\partial p}\left(i \hbar \frac{\partial w}{\partial p}\right)=-\hbar^{2} \frac{\partial^{2} w}{\partial p^{2}} . \tag{7.209}
\end{equation*}
$$

It may look like the second integral in Eq. (181) might be simplified similarly. However, it vanishes at $p^{\prime} \rightarrow p$, and $t^{\prime} \rightarrow t$, so that in order to calculate the first nonvanishing contribution from that integral for $p=p$, we have to take into account the small difference $\tau \equiv t-t^{\prime} \sim \tau_{c}$ between the arguments of the coordinate operators under that integral. This may be done using Eq. (169) with the free-particle Hamiltonian consisting of the kinetic-energy contribution alone:

$$
\begin{equation*}
\hat{x}\left(t^{\prime}\right)-\hat{x}(t) \approx-\tau \dot{\hat{x}}=-\tau \frac{1}{i \hbar}\left[\hat{x}, \hat{H}_{s}\right]=-\tau \frac{1}{i \hbar}\left[\hat{x}, \frac{\hat{p}^{2}}{2 m}\right]=-\tau \frac{\hat{p}}{m}, \tag{7.210}
\end{equation*}
$$

where the exact argument of the operator in the right-hand part is already unimportant, and may be taken for $t$. As a result, we may use the last of Eqs. (136) to reduce the second term in the right-hand part of Eq. (181) to

$$
\begin{equation*}
-\frac{i}{2 \hbar} \int_{-\infty}^{t} G\left(t-t^{\prime}\right)\left[\hat{x}(t),\left\{\hat{x}\left(t^{\prime}\right), \hat{w}\left(t^{\prime}\right)\right\}\right] d t^{\prime} \approx \frac{i}{2 \hbar} \int_{0}^{\infty} G(\tau) \tau d \tau\left[\hat{x},\left\{\frac{\hat{p}}{m}, \hat{w}\right\}\right]=\frac{\eta}{2 i \hbar}\left[\hat{x},\left\{\frac{\hat{p}}{m}, \hat{w}\right\}\right] . \tag{7.211}
\end{equation*}
$$

In the momentum representation, the momentum operator and the density matrix $w$ are just $c$-numbers and commute, so that, applying Eq. (208) to product $p w$, we get

$$
\begin{equation*}
\left[\hat{x},\left\{\frac{\hat{p}}{m}, \hat{w}\right\}\right]=\left[\hat{x}, 2 \frac{p}{m} w\right]=2 i \hbar \frac{\partial}{\partial p}\left(\frac{p}{m} w\right), \tag{7.212}
\end{equation*}
$$

and may finally reduce the integro-differential equation Eq. (181) to a partial differential equation: Equation: free 1D particle

$$
\begin{equation*}
\frac{\partial w}{\partial t}=\frac{\partial}{\partial p}\left(\eta \frac{p}{m} w\right)+k_{\mathrm{B}} T \eta \frac{\partial^{2} w}{\partial p^{2}} \tag{7.213}
\end{equation*}
$$

This is the 1D form of the famous Fokker-Planck equation describing the classical statistics of motion of a free 1D particle in a medium with a linear drag characterized by the coefficient $\eta$. The first, drift term in the right-hand part of Eq. (213) describes particle's deceleration due to the average viscous force (137), $\langle F\rangle=-\eta v=-\eta p / m$, provided by the environment, while the second, diffusion term describes the effect of fluctuations: particle's random walk that obeys Eq. (85) with the diffusion coefficient

Einstein relation

$$
\begin{equation*}
D=\eta k_{\mathrm{B}} T \tag{7.214}
\end{equation*}
$$

This fundamental Einstein relation, ${ }^{76}$ shows again the intimate connection between the dissipation (friction) and fluctuations, in this classical limit represented by their thermal energy scale $k_{\mathrm{B}} T .{ }^{.77}$

[^698]Just for reader's reference, let me note that the Fokker-Planck equation (213) may be readily generalized to the 3D motion of a particle under the effect of an additional external force $F_{\text {ext }}(\mathbf{r}, t):{ }^{78}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}=-\nabla\left(\frac{\mathbf{p}}{m} w\right)-\nabla_{p} \cdot(\mathbf{F} w)+D \nabla_{p}^{2} w, \quad \text { with } \mathbf{F}=\mathbf{F}_{\mathrm{ext}}-\eta \frac{\mathbf{p}}{m} \tag{7.215}
\end{equation*}
$$

where $w=w(\mathbf{r}, \mathbf{p}, t)$ is the time-dependent probability density in the 6 D phase space, and $\nabla_{p}$ is the nabla/del operator of differentiation over the momentum components, defined similarly to its coordinate counterpart $\nabla$. The Fokker-Planck equation in this form is the basis for many important applications; however, due to its classical character, its discussion is left for the SM part of my lecture notes. ${ }^{79}$

To summarize our discussion of the two alternative approaches to the analysis of quantum systems interacting with a thermally-equilibrium environment, described in the last three sections, let me emphasize that they give descriptions of the same phenomena, and are characterized by the same two functions $G(\tau)$ and $K_{F}(\tau)$, but from two different points of view. Namely, in the Heisenberg-Langevin approach we describe the system by operators that change (fluctuate) in time, even in thermal equilibrium, while in the density-matrix approach the system is described by non-fluctuating probability functions, such as $W_{n}(t)$ or $w(p)$, that are stationary in equilibrium. In the (relatively rare) cases when a problem may be solved by either method, they give identical results for all observables.

### 7.7. Quantum measurements

Now we have got a sufficient quantum mechanics background for a brief discussion of quantum measurements. ${ }^{80}$ Let me start with reminding the reader the only postulate of quantum mechanics that relates this theory with experiment. In Chapter 4 it was formulated for a pure state described with ketvector

$$
\begin{equation*}
|\alpha\rangle=\sum_{j} \alpha_{j}\left|a_{j}\right\rangle, \tag{7.216}
\end{equation*}
$$

${ }^{77}$ This classical relation may be derived using several other ways - including those much simpler than used above. For example, since the Brownian particle's motion may be described by a linear Langevin equation, Eq. (214) may be readily obtained from the Nyquist formula (139) - see, e.g., SM Sec. 5.5.
${ }^{78}$ Moreover, Eq. (213) may be generalized to the motion in an additional periodic potential $U(\mathbf{r})$. In this case, an analog of Eq. (215) for the probability density of quasi-momentum $\hbar \mathbf{q}$ (rather than the genuine momentum $\mathbf{p}$ ) includes an additional energy band index (say, $n$ ), an additional force $\mathbf{F}_{n}=-\nabla E_{n}$ (where $E_{n}(\mathbf{q})$ is the energy band structure that was discussed in Secs. 2.7 and 3.4), and an additional term similar to the right-hand part of Eq. (194), describing interband transitions with quasi-momentum-dependent rates $\Gamma_{n \rightarrow n}(\mathbf{q})$. These rates are still expressed by Eq. (196), but with the matrix elements $x_{n n}$, replaced by those of the vector operator $\hat{\boldsymbol{\Omega}} \equiv \hat{\mathbf{r}}-i \nabla_{q}$ of interband transitions, which was discussed in Chapter 5. For details and a particular example of a sinusoidal potential see, e.g., K. Likharev and A. Zorin, J. Low Temp. Phys. 59, 347 (1985).
${ }^{79}$ For a more detailed analysis and several examples of quantum effects in dissipative systems with continuous spectra see, e. g., U. Weiss, Quantum Dissipative Systems, $2^{\text {nd }}$ ed., World Scientific, 1999, or H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems, Oxford U. Press, 2007.
80 "Quantum measurements" is a very unfortunate term; it would be more sensible to speak about "measurements of quantum mechanical observables". However, the former term is so common and compact that I will use it.
where $a_{j}$ and $A_{j}$ are, respectively, the eigenstates of the operator of observable $A$, defined by Eq. (4.68). According to the postulate, the outcome of each particular measurement of observable $A$ may be uncertain, ${ }^{81}$ but is restricted to the set of eigenstates $A_{j}$, with the probability of outcome $A_{j}$ equal to

$$
\begin{equation*}
W_{j}=\left|\alpha_{j}\right|^{2} \tag{7.217}
\end{equation*}
$$

Since we know now that the state of the system (or rather of the statistical ensemble of similar systems we are using for measurements) is generally not pure, this postulate should be re-worded as follows: even if the system is in the least uncertain state (216), the measurement outcomes are still probabilistic, and obey Eq. (133). ${ }^{82}$

Quantum measurement may be understood as a procedure of transferring the "microscopic" information contained in coefficients $\alpha_{j}$ into "macroscopically" available information about the outcomes of particular experiments, that may be recorded and reliably stored - say, on paper, or in a computer, or in our minds. If we believe that such transfer may be always done well enough, and do not worry too much how exactly, we are subscribing to the mathematical notion of measurement, that was (rather reluctantly) used in these notes - up to this point. However, every physicist should understand that measurements are performed by physical devices that also should obey the laws of quantum mechanics, and it is important to understand the basic laws of their operation.

The founding fathers of quantum mechanics have not paid much attention to these issues, probably because of the following two reasons. First, at that time it looked like the experimental instruments (at least the best of them :-) were doing exactly what postulate (217) was telling. For example, had not the $z$-oriented Stern-Gerlach experiment turned two complex coefficients $\alpha \uparrow$ and $\alpha \downarrow$, describing the incoming electron beam, into particle counter clicks with rates proportional to, respectively, $|\alpha \uparrow|^{2}$ and $|\alpha \downarrow|^{2}$ ? Also, the crude internal nature of these instruments made more detailed questions unnatural. For example, the electron rate counting with a Geiger counter involves an effective disappearance of each incoming electron inside a zillion-particle electric discharge avalanche. Thinking about such devices, it was hard to even imagine measurements that would not disturb the quantum state of the particle being measured.

However, since that time the experimental techniques, notably including high vacuum, low temperatures, and low-noise electronics, have much improved, and eventually more inquisitive questions started to look not so hopeless. In my scheme of things, these questions may be grouped as follows:
(i) What are the main laws of a quantum measurement as a physical process? In particular, should it always involve time irreversibility? a human/intelligent observer? (The last question is not as laughable as it may look - see below.)
(ii) What is the state of the measured system just after a single-shot measurement - meaning the measurement process limited to a time interval much shorter that the time scale of measured system's evolution? This question is naturally related to the issues of repeated measurements and continuous monitoring of system's state.

[^699](iii) If a measurement of observable $A$ produced a certain outcome $A_{j}$, can we believe that the system had been in the corresponding state $\alpha_{j}$ just before the measurement?

The last question is most closely related to various interpretations of quantum mechanics, and will be discussed in the concluding Chapter 10, and now let me provide some input on the first two groups of issues.

First of all, I am happy to report that these is a virtual consensus of physicists on the two first questions of series (i). According to this consensus, any quantum measurement needs to result in a certain, distinguishable state of a macroscopic output component of the measurement instrument - see Fig. 7. (Traditionally, its component is called a pointer, though its role may be played by a printer or a plotter, an electronic circuit sending out the result as a number, etc.).

This requirement implies that the measurement process should have the following features:

- be time-irreversible,
- provide large "signal gain", i.e. mapping the quantum process with its $\hbar$-scale of action (i.e. of the energy-by-time product) onto a macroscopic motion of the pointer with a much larger action scale, and
- if we want high measurement fidelity, the process should introduce as little additional uncertainty as permitted by the law of physics.


Fig.7.7. General scheme of quantum measurement.

All these requirements are fulfilled in a good Stern-Gerlach experiment. However, since the internal physics of the particle detector at this measurement is rather complex, let me give an example of a different, more simple single-shot scheme ${ }^{83}$ capable of measuring the instant state of a typical twolevel system, for example, a particle in a double quantum well potential (Fig. 8). ${ }^{84}$ Let the system be, at $t$ $=0$, in a pure quantum state described by ket-vector

$$
\begin{equation*}
|\alpha\rangle=\alpha_{\rightarrow}|\rightarrow\rangle+\alpha_{\leftarrow}|\leftarrow\rangle, \tag{7.218}
\end{equation*}
$$

[^700]where the component states $\rightarrow$ and $\leftarrow$ may be described by wavefunctions localized near the potential well bottoms at $x_{s} \sim \pm x_{0}$ - see the blue lines in Fig. 8b. Let us rapidly change the potential profile of the system at $t=0$, so that at $t>0$, and near the origin, it may be well approximated by an inverted parabola (see the red line in Fig. 8b):
\[

$$
\begin{equation*}
U\left(x_{s}\right) \approx-\frac{m \lambda^{2}}{2} x_{s}^{2}, \quad \text { at } t>0,\left|x_{s}\right| \ll x_{f} . \tag{7.219}
\end{equation*}
$$

\]



Fig. 7.8. Potential inversion on (a) "macroscopic" and (b) "microscopic" scales of coordinate $x$.

It is straightforward to verify that the Heisenberg equations of motion in such inverted potential describe an exponential growth of operator $\hat{x}_{s}$ in time (proportional to $\exp \{\lambda t\}$ and hence a similar growth of the expectation value $\left\langle x_{s}\right\rangle$ and its r.m.s. uncertainty $\delta x_{s} .{ }^{85}$ At this "inflation" stage, the coherence between the two component states $\rightarrow$ and $\leftarrow$ is still preserved, i.e. the time evolution is reversible.

Now let the system be weakly coupled to a dissipative (e.g., Ohmic) environment. As we already know, the environment performs two functions. First, it provides motion with the drag coefficient $\eta$ (141), so that the system would eventually come to rest at one of the relatively distant minima, $\pm x_{f}$, of the inverted potential (Fig. 8a). Second, the dissipative environment ensures state's dephasing on some time scale $T_{2}$. If we select the measurement system parameters in such a way that

$$
\begin{equation*}
x_{0} \ll x_{0} \exp \left\{\lambda T_{2}\right\} \ll x_{f}, \tag{7.220}
\end{equation*}
$$

then the process, after the potential inversion, consists of the following stages, well separated in time:

- the "inflation" stage, preserving the component state coherence but providing an exponential increase of its energy,

[^701]- the dephasing stage, at which the coherence is suppressed, and the density matrix of the system is reduced to a diagonal form describing the classical mixture of the probability packets propagating to the left and to the right, and
- the stage of settling to a new stationary state - a classical mixture of two states located near points $x_{s}= \pm x_{f}$, with probabilities (217) equal to, respectively, $W_{\rightarrow}=\left|\alpha_{\rightarrow}\right|^{2}$ and $W_{\leftarrow}=\left|\alpha_{\leftarrow}\right|^{2}=1-\left|\alpha_{\rightarrow}\right|^{2}$.

If the final states are macroscopically distinguishable (i.e. may play the role of a bistable pointer), as they are in the balanced-comparator implementation, there is absolutely no need, at any of these stages, to involve any mysterious "another mechanism of wavefunction change" (different from the regular, Schrödinger evolution) for the measurement process description.

This may be the only appropriate time to mention, very briefly, the famous - or rather infamous Schrödinger cat paradox so much overplayed in popular press. (The only good aspect of this popularity is that the formulation of this paradox is certainly so well known to the reader, that I do not need to repeat it.) In this thought experiment, there is no need to discuss the (rather complex :-) physics of the cat. As soon as the charged particle, produced at the radioactive decay, reaches the Geiger counter, the process rapidly becomes irreversible, so that the coherent state of the system is reduced to a classical mixture of two possible states: "decay" - "no decay", leading, correspondingly, to the "cat alive" - "cat dead" states. So, despite attempts by numerous authors, typically without proper physics background, to present this situation as a mystery whose discussion needs the involvement of professional philosophers, hopefully by this point the reader knows enough about dephasing to pay any attention. Let me, however, note the two non-trivial features of this gedanken experiment, that are met in most real experiments as well, including that with the potential inversion (Fig. 8).

First, the role of the measured coordinate of the system under observation ( $s$ ) may be played not by a coordinate of a single fundamental particle, but a certain combination of coordinates of many microscopic components of a macroscopic body. In particular, in Josephson junction systems such as the balanced comparator we essentially measure the persistent electric current ("supercurrent") - a certain linear combination of Cartesian components of the momenta of the electrons that constitute the BoseEinstein condensate of Cooper pairs. At that, the role of the local environment (that contributes significantly to dissipative phenomena) is played by the same electrons, with other linear combinations of electron momenta playing the role of environmental degrees of freedom - which were called $\{\lambda\}$ in the last few sections. This makes the coupling to environment somewhat less apparent (at least for the people who do not know what a linear combination is :-).

Second, one may argue that even after the balanced comparator (in our first example) or the cat (in the second example) has reached its final macroscopic state, human observer's realization that in this particular experiment the bistable pointer is in a certain state instantly decreases the probability (for the same observer!) of its being in the opposite state to zero. However, as was already discussed in Sec. 2.5, this is a very classical problem of the statistical ensemble redefinition that may be (or may be not) performed at observer's will. Such redefinition, if performed, is the only possible role of a human (or otherwise intelligent :-) observer in the measurement process; if we are only interested in an objective recording of results of a pre-fixed sequence of experiments, there is no need to include such observer into any discussion.

The ensemble redefinition at measurement leads to several other paradoxes, of which the socalled quantum Zeno paradox is perhaps most spectacular. ${ }^{86}$ Let us return to a two-level system with the unperturbed Hamiltonian given by Eq. (4.166), with $2 \pi / \Omega$ much longer than the single-shot measurement time, in which the system initially (at $t=0$ ) is in a certain quantum well. Then, as we know from Secs. 2.6 and 4.6, before the first measurement, the probability to find state in the initial state at time $t$ is

$$
\begin{equation*}
W(t)=\cos ^{2} \frac{\Omega t}{2} . \tag{7.221}
\end{equation*}
$$

If the time is small enough $(t=d t \ll 1 / \Omega)$, we may use the Taylor expansion to write

$$
\begin{equation*}
W(d t) \approx 1-\frac{\Omega^{2} d t^{2}}{4} . \tag{7.222}
\end{equation*}
$$

Now, let us return the two-level system, after its measurement, into the same quantum well, and let it evolve with the same Hamiltonian. Since the occupation of the opposite state is very small, the evolution of $W$ will closely follow the same law as in Eq. (221), but with the initial value given by Eq. (222) Thus, when the system is measured again at time $2 d t$,

$$
\begin{equation*}
W(2 d t) \approx W(d t)\left(1-\frac{\Omega^{2} d t^{2}}{4}\right)=\left(1-\frac{\Omega^{2} d t^{2}}{4}\right)^{2} \tag{7.223}
\end{equation*}
$$

After repeating this cycle $N$ times (with the total time $t=N d t$ still much less than $N^{1 / 2} / \Omega$ ), the probability that the system is still in the initial state is

$$
\begin{equation*}
W(N d t) \equiv W(t) \approx\left(1-\frac{\Omega^{2} d t^{2}}{4}\right)^{N}=\left(1-\frac{\Omega^{2} t^{2}}{4 N^{2}}\right)^{N} \approx 1-\frac{\Omega^{2} t^{2}}{4 N} \tag{7.224}
\end{equation*}
$$

Comparing this result with Eq. (222), we see that the process of system transfer to the opposite quantum well has been slowed down rather dramatically, and in the limit $N \rightarrow \infty$ (at fixed $t$ ), its evolution is completely stopped by the measurement process. There is of course nothing mysterious here; the evolution slowdown is due to statistical ensemble's redefinition.

Now let me proceed to question group (ii), in particular to the general issue of the back action of the instrument upon the system under measurement (symbolized with the back arrow in Fig. 7). In instruments like the Geiger counter or the balanced comparator, such back action is very large, because the instrument essentially destroys ("demolishes") the initial state of the system under measurement.

[^702]However, in the 1970s it was realized that this is not really necessary. In Sec. 3, we have already discussed an example of a two-level system coupled with environment (in our current context, with measurement instrument) and described by Hamiltonian

$$
\begin{equation*}
\hat{H}=\hat{H}_{s}+\hat{H}_{\mathrm{int}}+\hat{H}_{e}\{\lambda\}, \quad \text { with } \hat{H}_{s}=a \hat{\sigma}_{z}, \quad \hat{H}_{\mathrm{int}}=-f\{\lambda\} \hat{\sigma}_{z}, \tag{7.225}
\end{equation*}
$$

so that

$$
\begin{equation*}
\left[\hat{H}_{s}, \hat{H}_{\mathrm{int}}\right]=0 \tag{7.226}
\end{equation*}
$$

Comparing this equality with Eq. (67) we see that in the Heisenberg picture, the Hamiltonian operator (and hence the energy) of the system of our interest does not change with time. On the other hand, the interaction can change the state of the instrument, so it may be used to measure its energy - or another observable whose operator commutes with the interaction Hamiltonian. Such trick is called either the quantum non-demolition (QND) or back-action-evading (BAE) measurements. ${ }^{87}$ Let me present a fine example of a real measurement of this kind - see Fig. $9 .{ }^{88}$

(b)

Fig. 7.9. QND measurement of single electron's energy by Peil and Gabrielse: (a) the core of experimental setup, and (b) a record of the thermal excitation and spontaneous relaxation of Fock states. © 1999 APS.

In this experiment, a single electron is captured in a Penning trap - a combination of a (virtually) uniform magnetic field $\mathbf{B}$ and a quadrupole electric field. ${ }^{89}$ Such electric field stabilizes cyclotron orbits but does not have any noticeable effect on electron motion in the plane perpendicular to the magnetic field, and hence on its Landau level energies (see Sec. 3.2):

[^703]\[

$$
\begin{equation*}
E_{n}=\hbar \omega_{c}\left(n+\frac{1}{2}\right), \quad \text { with } \omega_{c}=\frac{e B}{m_{e}} \tag{7.227}
\end{equation*}
$$

\]

(In the cited work, at $B \approx 5.3 \mathrm{~T}$, the cyclic frequency $\omega_{c} / 2 \pi$ was about 147 GHz , so that the level splitting $\hbar \omega_{c}$ was close to $10^{-22} \mathrm{~J}$, i.e. corresponded to temperature $\sim 10 \mathrm{~K}$, while the physical temperature of the system might be reduced well below that, down to $\sim 80 \mathrm{mK}$ ). Now note that the analogy between a particle on a Landau levels and a harmonic oscillator goes beyond the energy spectrum. Indeed, since the Hamiltonian of a 2D particle in a perpendicular magnetic field may be reduced to that of a 1D oscillator, we may repeat all procedures of Sec. 5.4 and rewrite it in the terms of creation-annihilation operators:

$$
\begin{equation*}
\hat{H}_{s}=\hbar \omega_{c}\left(\hat{a}^{\dagger} \hat{a}+\frac{1}{2}\right) \tag{7.228}
\end{equation*}
$$

In the Peil and Gabrielse experiment, the electron had one more degree of freedom - along the magnetic field. The electric field of the Penning trap creates a soft confining potential along this direction (vertical in Fig. 9a; let us take it for axis $z$ ), so that small electron oscillations along that axis could be well described as a 1D harmonic oscillator of much lower eigenfrequency, in that particular experiment with $\omega_{z} / 2 \pi \approx 64 \mathrm{MHz}$. This frequency could be measured very accurately (with error $\sim 1 \mathrm{~Hz}$ ) by sensitive electronics whose electric field affects $z$-motion of the electron, but not its motion in the perpendicular plane. In an exactly uniform magnetic field, the two modes of electron motion would be completely uncoupled. However, the experimental setup included two special superconducting rings made of niobium (Fig. 9a), which slightly distorted the magnetic field and created an interaction between the modes, which might be well approximated by Hamiltonian ${ }^{90}$

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=\operatorname{const} \times\left(\hat{a}^{\dagger} \hat{a}+\frac{1}{2}\right) \hat{z}^{2} \tag{7.228}
\end{equation*}
$$

so that the main condition (226) of a QND measurement was well satisfied. At the same time, coupling (228) ensured that a change of the Fock state number $n$ by 1 changed the $z$-oscillation eigenfrequency by $\sim 12.4 \mathrm{~Hz}$. Since this shift was substantially larger than electronics noise, spontaneous changes of $n$ (due to an uncontrolled coupling of the electron to environment) could be readily observed - moreover, continuously monitored - see Fig. 9b. (These data imply that there is virtually no effect of the measuring instrument on the statistics on $n-$ at least on the scale of minutes, i.e. as many as $\sim 10^{13}$ cyclotron orbit periods.) Of course, any measurement - QND or not - cannot avoid the Heisenberg uncertainty relations; in this particular case, a permanent monitoring of the Fock state number $n$ keeps its quantum phase fully uncertain.

It is natural to wonder whether the QND measurement concept may be extended from quadratic forms like the energy to "usual" observables such as coordinates and momenta whose uncertainties are bound by the fundamental Heisenberg's relation. The answer is yes, but the required methods are a bit more tricky. For example, let us place an electrically charged particle into a uniform electric field $\boldsymbol{\varepsilon}=$ $\mathbf{n}_{x} \mathcal{E}(t)$ of the instrument, so that their interaction Hamiltonian is

[^704]\[

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=-q \hat{\varepsilon}(t) \hat{x} \tag{7.229}
\end{equation*}
$$

\]

Such interaction certainly passes the information on the time evolution of coordinate $x$ to the instrument. However, since Eq. (226) is not satisfied - at least for the kinetic-energy part of system's Hamiltonian; as a result the interaction simultaneously distorts the time evolution of particle's momentum. Indeed, writing the Heisenberg equation of motion (4.199) for the $x$-component of momentum, we get

$$
\begin{equation*}
\dot{\hat{p}}-\left.\dot{\hat{p}}\right|_{\varepsilon=0}=q \hat{\varepsilon}(t) \tag{7.230}
\end{equation*}
$$

Integrating Eq. (5.139) for the coordinate operator evolution, ${ }^{91}$ we get expression,

$$
\begin{equation*}
\hat{x}(t)=\hat{x}(0)+\frac{1}{m} \int_{0}^{t} \hat{p}\left(t^{\prime}\right) d t^{\prime} \tag{7.231}
\end{equation*}
$$

that shows that the perturbations (230) of the momentum would eventually find their way to the coordinate evolution.

However, for such an important particular system as a harmonic oscillator, the following trick is possible. For this system, Eqs. (5.170) and (230) may be readily combined to give a second-order differential equation for the coordinate operator, that is absolutely similar to the classical equation of motion, and has a similar solution: ${ }^{92}$

$$
\begin{equation*}
\hat{x}(t)=\hat{x}(0)+\frac{q}{m \omega_{0}} \int_{0}^{t} \hat{\varepsilon}\left(t^{\prime}\right) \sin \omega_{0}\left(t-t^{\prime}\right) d t^{\prime} \tag{7.232}
\end{equation*}
$$

This formula confirms that generally the external field $\mathscr{A} t$ ) (in our case, the sensing field of the measurement instrument) affects the time evolution law. Note, however, that if the field is applied only at moments $t_{n}^{\prime}$ separated by intervals $T / 2$, where $T=2 \pi / \omega_{0}$ is the oscillation period, its effect on coordinate vanishes at similarly spaced observation instants $t_{n}=t_{n}{ }^{\prime}+(m+1 / 2) T$. This the idea of stroboscopic QND measurements. Of course, according to Eq. (230), even such measurement strongly perturbs the oscillator momentum, so that even if values $x_{n}$ are measured with high accuracy, the Heisenberg's uncertainty relation is not violated.

Experimental implementation of such measurements is not simple (and to the best of my knowledge they have never been successfully demonstrated), but this initial idea has opened a way to more practicable solutions. For example, it straightforward to use the Heisenberg equations of motion to show that if coupling of two harmonic oscillators, with coordinates $x$ and $X$, and unperturbed eigenfrequencies $\omega$ and $\Omega$, is modulated in time as

$$
\begin{equation*}
\hat{H}_{\mathrm{int}} \propto \hat{x} \hat{X} \cos \omega t \cos \Omega t \tag{7.233}
\end{equation*}
$$

[^705]then the process in one of oscillators (say, that with frequency $\Omega$ ) does not affect dynamics of one of the quadrature components of another oscillator, defined by relations ${ }^{93}$
\[

$$
\begin{equation*}
\hat{x}_{1} \equiv \hat{x} \cos \omega t-\frac{\hat{p}}{m \omega} \sin \omega t, \quad \hat{x}_{2} \equiv \hat{x} \sin \omega t+\frac{\hat{p}}{m \omega} \cos \omega t, \tag{7.234}
\end{equation*}
$$

\]

while this component's motion does affect the dynamics of one of quadrature components of the counterpart oscillator. (For the counterpart couple of quadrature components, the information transfer goes in the opposite direction.) This scheme has been successfully used for QND measurements in the optical range, with coupling (233) provided by the optical Kerr effect. ${ }^{94}$

Please note that the last two QND measurement examples are based on the idea of modulation of a certain parameter in time - either in a short-pulse or sinusoidal form. So, the reader should not be surprised that if the only role of a QND measurement is a sensitive measurement of a weak classical force acting on a quantum probe system, ${ }^{95}$ i.e. a 1 D oscillator of eigenfrequency $\omega_{0}$, it may be implemented much simpler - just by modulating the oscillator parameter with frequency $\omega \approx 2 \omega_{0}$. From classical dynamics, we know that if the depth of such modulation exceeds a certain threshold value, it results in excitation of the so-called parametric oscillations with frequency $\omega / 2$, and one of two opposite phases. ${ }^{96}$ In the language of Eq. (234), parametric excitation means an exponential growth of one of the quadrature components, with the sign depending on initial conditions, while the counterpart component is suppressed. Close to, but below the excitation threshold, the parameter modulation boosts all perturbations of the almost-excited component (including its quantum-mechanical uncertainty), and suppresses (squeezes) those of the counterpart component. The result is a squeezed state, already discussed in Sec. 5.5 above (see in particular Fig. 5.6), that allows one to notice the effect of external force on the oscillator on the backdrop of a quantum uncertainty smaller that the standard quantum limit (5.138) - see the first of Eqs. (5.174).

In electrical engineering, this fact may be conveniently formulated in terms of noise parameter $\Theta_{N}$ of a linear amplifier - the instrument for continuous monitoring of an input "signal" - e.g., a microwave or optical waveform. ${ }^{97}$ Namely, $\Theta_{N}$ of "usual" (say, transistor or maser) amplifiers which are equally sensitive to both quadrature components of the signal, $\Theta_{N}$ has a minimum value $\hbar \omega / 2$, due to the quantum uncertainty pertinent to the quantum state of the amplifier itself (which therefore plays the role

[^706]of its "quantum noise"). ${ }^{98}$ On the other hand, a degenerate parametric amplifier, sensitive to just one quadrature component, may have $\Theta_{N}$ well below $\hbar \omega / 2$, due to the squeezing of its ground state. ${ }^{99}$

Finally, let me note that the parameter-modulation schemes of the QND measurements are not limited to harmonic oscillators, and may be applied to other important quantum systems, notably including two-level (i.e. spin-1/2-like) systems. ${ }^{100}$

### 7.8. Exercise problems

7.1. Calculate the density matrix of a two-level system described by Hamiltonian with matrix

$$
\mathrm{H}=\mathbf{a} \cdot \boldsymbol{\sigma}=a_{x} \sigma_{x}+a_{y} \sigma_{y}+a_{z} \sigma_{z},
$$

where $\sigma_{k}$ are the Pauli matrices, and $a_{k}$ are $c$-numbers, in thermodynamic equilibrium.
7.2. Find the Wigner function of a harmonic oscillator in:
(i) at the thermodynamic equilibrium at temperature $T$,
(ii) in the ground state, and
(ii) in the Glauber state with dimensionless complex amplitude $\alpha$.

Discuss the relation between the first of the results and the Gibbs distribution.
7.3. Calculate the Wigner function of a harmonic oscillator, with mass $m$ and frequency $\omega_{0}$, in its first excited stationary state $(n=1)$.
7.4. Show that the quantum-mechanical Golden Rule (6.111) and the master equation (196) give the same results for the rate of spontaneous quantum transitions $n^{\prime} \rightarrow n$ in a system with discrete energy spectrum, weakly coupled to a low-temperature the heat bath $\left(k_{\mathrm{B}} T \ll \hbar \omega_{n n}\right)$.

Hint: Try to establish a relation between function $\operatorname{Im} \chi\left(\omega_{n n}\right)$ that participates in Eq. (196), and the density of states $\rho_{n}$ that participates in the Golden Rule formulas, by considering a particular case of sinusoidal oscillations in the system of interest.
7.5.* A harmonic oscillator is weakly coupled to an Ohmic environment.
(i) Use the rotating-wave approximation to write equations of motion for the Heisenberg operators of the complex amplitude of oscillations.
(ii) Calculate the expectation values of the correlators of the fluctuation force operators, participating in these equations, and express them via the average number $\langle n\rangle$ of thermally-induced excitations in equilibrium, given by the second of Eqs. (26b).
7.6. For a harmonic oscillator with weak Ohmic dissipation:
(i) Spell out the system of differential equations for the energy level occupancies $W_{n}$.

[^707](ii) Use this system to find the time evolution of the expectation value $\langle E\rangle$ of oscillator's energy. (iii) Compare the last result with that following from the Heisenberg-Langevin approach.
7.7. Derive Eq. (209) in an alternative way, using an expression dual to Eq. (5.28b).
7.8. ${ }^{*}$ A particle in a system of two coupled quantum wells (see, e.g., Fig. 4) is weakly coupled to an Ohmic environment.
(i) Derive the equations of time evolution of the density matrix elements.
(ii) Solve these equations in the low-temperature limit, when the energy level splitting is much larger than $k_{\mathrm{B}} T$, to calculate the time evolution of the probability $W_{L}(t)$ of finding the particle one of the wells, after it had been placed there at $t=0$.
7.9. ${ }^{*}$ A spin- $-1 / 2$ particle is placed into magnetic field $\mathcal{B}(t)=\mathcal{B}_{0}+\widetilde{\mathcal{B}}(t)$ with an arbitrary but small time-dependent component $\left(|\widetilde{\mathcal{B}}| \ll\left|\mathcal{B}_{0}\right|\right)$, and is also weakly coupled to dissipative environment. Derive the differential equations describing the time evolution of the expectation values ( $\left\langle S_{x}\right\rangle$, etc.) of spin's Cartesian components.


## Chapter 8. Multiparticle Systems

This chapter is a brief introduction to quantum mechanics of systems of similar particles, with a special attention to the case when they are indistinguishable. For such systems, the theory predicts (and experiment confirms) very specific effects even in the case of negligible explicit ("direct") interaction between the particles. The effects notably include the Bose-Einstein condensation of bosons, and the Pauli exclusion principle and exchange interaction for fermions.

### 8.1. Distinguishable and indistinguishable particles

The importance of quantum systems of many similar particles is probably self-evident; just the very fact of that most atoms include several/many electrons is sufficient to attract our attention. There are also important systems where the number of electrons is much higher than in one atom; for example, a cubic centimeter of a typical metal features $\sim 10^{23}$ conduction electrons that cannot be attributed to particular atoms, and have to considered as common (and interacting!) pats of the system as the whole. Though quantum mechanics offers virtually no exact analytical solutions for systems of strongly interacting particles, ${ }^{1}$ it reveals very important new effects even in the simplest case when particles do not interact, and least explicitly (directly).

If non-interacting particles are either different from each other by their nature (say, an electron and a proton), or physically similar but still distinguishable because of other reasons (say, because of their reliable spatial separation) everything is simple - at least, conceptually. Then, as was already discussed in Sec. 6.7, a system of two particles, 1 and 2, each in a pure quantum state, may be described by a ket vector

$$
\begin{equation*}
|\alpha\rangle=|\beta\rangle_{1} \otimes\left|\beta^{\prime}\right\rangle_{2} \tag{8.1a}
\end{equation*}
$$

where the single-particle states $\beta$ and $\beta^{\prime}$ are defined in different Hilbert spaces. (Below, I will frequently use the following convenient shorthand,

$$
\begin{equation*}
|\alpha\rangle=\left|\beta \beta^{\prime}\right\rangle, \tag{8.1b}
\end{equation*}
$$

in which the state position within a vector codes the particle number.) Hence the permuted state

$$
\begin{equation*}
\hat{\mathcal{P}}\left|\beta \beta^{\prime}\right\rangle \equiv\left|\beta^{\prime} \beta\right\rangle=\left|\beta^{\prime}\right\rangle_{1} \otimes|\beta\rangle_{2}, \tag{8.2}
\end{equation*}
$$

where $\hat{P}$ is the permutation operator, is clearly different from the initial one.

[^708]Again, such description is valid even for identical particles if they are still distinguishable by their spatial separation. (The separation does not preclude particles from interacting with each other, e.g., electrostatically.) Such systems of similar but clearly distinguishable particles (or subsystems) are broadly discussed nowadays, for example in the context of quantum computing and encryption - see Sec. 8.5 below. This is why it is unfortunate that term "identical particles" is frequently used in the sense of indistinguishable particles. I will try to avoid this confusion by using the latter term, despite it being rather unpleasant grammatically.

Now comes the most important experimental fact: identical elementary particles, ${ }^{2}$ if they are not reliably separated, are genuinely indistinguishable, i.e. their Hilbert spaces are not separable. Hence, instead of Eq. (1), for a set of two particles, we need to use a linear combination of products like $\left|\beta \beta^{\prime}\right\rangle$ and $\left|\beta^{\prime} \beta\right\rangle$ for the construction of genuine quantum states. ${ }^{3}$ In order to comprehend what exactly linear combinations should be used, it is convenient to discuss properties of the permutation operator defined by the first of Eqs. (2).

Let us consider an observable $A$, and a system of eigenstates of its operator:

$$
\begin{equation*}
\hat{A}\left|a_{j}\right\rangle=A_{j}\left|a_{j}\right\rangle . \tag{8.3}
\end{equation*}
$$

If the particles are indistinguishable indeed, the observable expectation value should not be affected by their permutation. Hence operators $\hat{A}$ and $\hat{P}$ have to commute, and share their eigenstates. This is why eigenstates of operator $\hat{\mathcal{P}}$ are so important: in particular, they are also eigenstates of the Hamiltonian, i.e. the stationary states of the system of particles.

Now let us have a look at the operation described by the square of the permutation operator, on an elementary ket-vector product:

$$
\begin{equation*}
\hat{\mathcal{P}}^{2}\left|\beta \beta^{\prime}\right\rangle=\hat{\mathcal{P}}\left(\hat{\mathcal{P}}\left|\beta \beta^{\prime}\right\rangle\right)=\hat{\mathcal{P}}\left|\beta^{\prime} \beta\right\rangle=\left|\beta \beta^{\prime}\right\rangle, \tag{8.4}
\end{equation*}
$$

[^709]i.e. $\hat{P}^{2}$ brings the state back to its original form. Since any pure state of a two-particle system may be represented as a linear combination of such products, this result does not depend on the state, and may be represented as an operator relation:
\[

$$
\begin{equation*}
\hat{\mathcal{P}}^{2}=\hat{I} . \tag{8.5}
\end{equation*}
$$

\]

Now let us find the possible eigenvalues $\mathcal{P}_{j}$ of the permutation operator. Acting by both sides of Eq. (5) on any of eigenstates $\left|\alpha_{j}\right\rangle$ of the permutation operator, we get a very simple equation for its eigenvalues:

$$
\begin{equation*}
P_{j}^{2}=1, \tag{8.6}
\end{equation*}
$$

with two possible solutions:

$$
\begin{equation*}
P_{j}= \pm 1 . \tag{8.7}
\end{equation*}
$$

Let us find the eigenstates of the permutation operator in the simplest case when each of the component particles can be only in two single-particle states - say, $\beta$ and $\beta$ '. Evidently, none of the simple products $\left|\beta \beta^{\prime}\right\rangle$ and $\left|\beta^{\prime} \beta\right\rangle$, taken alone, does qualify for the eigenstate - unless states $\beta$ and $\beta^{\prime}$ are identical. Let us try their linear combination

$$
\begin{equation*}
\left|\alpha_{j}\right\rangle=a\left|\beta \beta^{\prime}\right\rangle+b\left|\beta^{\prime} \beta\right\rangle, \tag{8.8}
\end{equation*}
$$

so that

$$
\begin{equation*}
\hat{\mathcal{P}}\left|\alpha_{j}\right\rangle=\mathcal{P}_{j}\left|\alpha_{j}\right\rangle=a\left|\beta^{\prime} \beta\right\rangle+b\left|\beta \beta^{\prime}\right\rangle . \tag{8.9}
\end{equation*}
$$

For the case $P_{j}=+1$ we have to require states (8) and (9) to be the same, so that $a=b$. Assuming also that the single-particle states $\beta$ and $\beta$ ' are normalized, and requiring the same for the composite state $\alpha$, we get the so-called symmetric eigenstate ${ }^{4}$

$$
\begin{equation*}
\left|\alpha_{+}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|\beta \beta^{\prime}\right\rangle+\left|\beta^{\prime} \beta\right\rangle\right) \tag{8.10}
\end{equation*}
$$

Symmetric and antisymmetric entangled eigenstates

Similarly, for $\mathcal{P}_{j}=-1$ we get $a=-b$, and the antisymmetric eigenstate

$$
\begin{equation*}
\left|\alpha_{-}\right\rangle=\frac{1}{\sqrt{2}}\left(\left|\beta \beta^{\prime}\right\rangle-\left|\beta^{\prime} \beta\right\rangle\right) \tag{8.11}
\end{equation*}
$$

where the front coefficients guarantee the orthonormality of the two-particle states, provided that the single-particle states are orthonormal. These are typical examples of entangled states, defined as multiparticle states whose state vectors cannot be factored into a product of single-particle vectors.

So far, our math does not preclude either sign of $\mathcal{P}_{j}$, in particular the possibility that the sign depends on the state (i.e. index $j$ ). Here, however, comes in another crucial experimental fact: all elementary particles fall into two groups: ${ }^{5}$

[^710](i) bosons, particles with integer spin $s$, for which $\mathcal{P}_{j}=+1$ for any $j$, and
(ii) fermions, particles with half-integer spin, with $\mathcal{P}_{j}=-1$, also for any $j$.

In the non-relativistic theory we are discussing now, this key fact should be considered as experimental one. (The relativistic quantum theory, to be discussed in Chapter 9, offers a proof that half-integer-spin particles cannot be bosons and integer-spin ones cannot be fermions, but not more than that.) However, our discussion of spin in Sec. 5.7 allows the following interpretation of the fermionboson difference. In free space, the permutation of particles 1 and 2 may be viewed as a result of rotation of this pair by angle $\pm \pi$ about a certain axis. As we have seen in Sec. 5.7, at a rotation by such an angle, the state vector $|\beta\rangle$ of a particle with quantum number $m_{s}$ (that ranges from $-s$ to $+s$, and hence may take only integer values for integer $s$, and only half-integer values for half-integer $s$ ) changes by factor $\exp \left\{ \pm i \pi m_{s}\right\}$, so that the state product $\left|\beta \beta^{\prime}\right\rangle$ changes by $\exp \left\{ \pm i 2 \pi m_{s}\right\}$, i.e. by factor +1 for integer $s$, and by factor (-1) for half-integer $s$.

Since eigenvalues $P_{j}$ do not depend on the particular state of the system, we can write explicit expressions for the permutation operator:

$$
\hat{\mathcal{P}}=\hat{I} \times\left\{\begin{array}{lr}
+1, & \text { for bosons },  \tag{8.12}\\
-1, & \text { for fermions } .
\end{array}\right.
$$

The most impressive corollaries of Eqs. (10) and (11) are for the case when the partial states of the two particles are the same: $\beta=\beta^{\prime}$. The corresponding Bose state $\alpha_{+}$is possible; in particular, at sufficiently low temperatures, a set of non-interacting Bose particles condenses on the ground state of each of them - the so-called Bose-Einstein condensate ("BEC"). ${ }^{6}$ Its examples include superfluid fluids like helium, the Cooper-pair condensate in superconductors, and the BEC of weakly interacting atoms. Perhaps the most fascinating feature of a multiparticle Bose-Einstein condensate is that dynamics of its observables is governed by laws of quantum mechanics, while (for nearly all purposes) may be treated as $c$-numbers - see, e.g., Eqs. (2.54)-(2.55). ${ }^{7}$

On the other hand, if we take $\beta=\beta^{\prime}$ in Eq. (11), we see that state $\alpha$ - vanishes, i.e. cannot exist at all. This is the mathematical expression of the Pauli exclusion principle: two indistinguishable fermions cannot be in the same quantum state. ${ }^{8}$ (As will be discussed below, this is true for systems with more than two fermions as well.) Probably, the key importance of this principle is self-evident: if it was not valid for electrons (that are fermions), all electrons of each atom would condense on its ground ( $1 s$ ) level, and all the usual chemistry (and biochemistry, and biology, including dear us!) would not exist. The Pauli principle effectively makes fermions interacting even if they do not interact directly, in the usual sense of this word.

[^711]
### 8.2. Singlets, triplets, and the exchange interaction

Now let us discuss possible approaches to analysis of identical particles on a simple but very important example of a pair of spin- $1 / 2$ particles (say, electrons) whose interaction with either each other or the external world does not involve spin. Then the ket-vector of a total state is factorable as

$$
\begin{equation*}
\left|\alpha_{-}\right\rangle=\left|o_{12}\right\rangle \otimes\left|s_{12}\right\rangle, \tag{8.13}
\end{equation*}
$$

with the orbital function $\left|o_{12}\right\rangle$ and the spin function $\left|s_{12}\right\rangle$ (that depends on the state of both spins of the pair) belonging to different Hilbert spaces. It is frequently convenient to use the coordinate representation of such state, sometimes called the spinor:

2-particle spinor

$$
\begin{equation*}
\left\langle\mathbf{r}_{1}, \mathbf{r}_{2} \mid \alpha_{-}\right\rangle=\left\langle\mathbf{r}_{1}, \mathbf{r}_{2} \mid o_{12}\right\rangle \otimes\left|s_{12}\right\rangle \equiv \psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)\left|s_{12}\right\rangle . \tag{8.14}
\end{equation*}
$$

Since spin- $1 / 2$ particles are fermions, the particle permutation,

$$
\begin{equation*}
\hat{\mathcal{P}} \psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)\left|s_{12}\right\rangle=\psi\left(\mathbf{r}_{2}, \mathbf{r}_{1}\right)\left|s_{21}\right\rangle=-\psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)\left|s_{12}\right\rangle, \tag{8.15}
\end{equation*}
$$

has to change the sign of either the spin part or the orbital factor of the spinor. In the case of a symmetric orbital factor,

$$
\begin{equation*}
\psi\left(\mathbf{r}_{2}, \mathbf{r}_{1}\right)=\psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right), \tag{8.16}
\end{equation*}
$$

the spin factor has to obey relation

$$
\begin{equation*}
\left|s_{21}\right\rangle=-\left|s_{12}\right\rangle . \tag{8.17}
\end{equation*}
$$

Let us use the ordinary $z$-basis (where $z$, in the absence of external magnetic field, is an arbitrary spatial axis) for each of the spins. In this basis, any ket-vector $\left|m_{s}\right\rangle$ of spin orientation of two particles may be represented as a linear combination of four single-spin basis vectors:

$$
\begin{equation*}
|\uparrow \uparrow\rangle, \quad|\downarrow \downarrow\rangle, \quad|\uparrow \downarrow\rangle, \quad \text { and } \quad|\downarrow \uparrow\rangle . \tag{8.18}
\end{equation*}
$$

The first two kets evidently do not satisfy Eq. (17), and cannot participate in the state. Applying to the remaining kets the same argumentation as has resulted in Eq. (11), we get

Singlet state

$$
\begin{equation*}
\left|s_{12}\right\rangle=\frac{1}{\sqrt{2}}(|\uparrow \downarrow\rangle-|\downarrow \uparrow\rangle) . \tag{8.19}
\end{equation*}
$$

Such orbital-symmetric and spin-asymmetric state is called the singlet. The origin of this name becomes clear from the analysis of the opposite (orbital-asymmetric and spin-symmetric) case:

$$
\begin{equation*}
\psi\left(\mathbf{r}_{2}, \mathbf{r}_{1}\right)=-\psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right), \quad\left|s_{12}\right\rangle=\left|s_{21}\right\rangle . \tag{8.20}
\end{equation*}
$$

For the composition of such symmetric spin state, the first two kets of Eq. (18) are completely acceptable (with arbitrary weights), and so is a specific symmetric combination of two last kets, similar to Eq. (10):

Triplet states

$$
\begin{equation*}
\left|s_{12}\right\rangle=c_{+}|\uparrow \uparrow\rangle+c_{-}|\downarrow \downarrow\rangle+c_{0} \frac{1}{\sqrt{2}}(|\uparrow \downarrow\rangle+|\downarrow \uparrow\rangle) . \tag{8.21}
\end{equation*}
$$

We may use this composite state with any values of coefficients $c$ (satisfying the normalization condition), because they correspond to the same orbital wavefunction and hence the same energy. However, each of these three states has a specific value of the $z$-component of the net spin (respectively, $+\hbar,-\hbar$, and 0$).{ }^{9}$ Because of this, an even small external magnetic field lifts their degeneracy, splitting the energy level in three, and giving it the natural name of triplet.

In the particular case when the particles do not interact at all, for example ${ }^{10}$

$$
\begin{equation*}
\hat{H}=\hat{h}_{1}+\hat{h}_{2}, \quad \hat{h}_{k}=\frac{\hat{p}_{k}^{2}}{2 m}+\hat{U}\left(\mathbf{r}_{k}\right), \quad k=1,2 \tag{8.22}
\end{equation*}
$$

the 2-particle Schrödinger equation for the symmetrical orbital wavefunction (16) is obviously satisfied by the simple product,

$$
\begin{equation*}
\psi\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=\psi_{n}\left(\mathbf{r}_{1}\right) \psi_{n^{\prime}}\left(\mathbf{r}_{2}\right), \tag{8.23}
\end{equation*}
$$

of single-particle eigenfunctions, with arbitrary sets $n$, $n$ ' of quantum numbers. For the particular (but very important!) case $n=n^{\prime}$, this means that the eigenenergy of the singlet state,

$$
\begin{equation*}
\frac{1}{\sqrt{2}} \psi_{n}\left(\mathbf{r}_{1}\right) \psi_{n}\left(\mathbf{r}_{2}\right)(|\uparrow \downarrow\rangle-|\downarrow \uparrow\rangle) \tag{8.24}
\end{equation*}
$$

is just $2 \varepsilon_{n}$, where $\varepsilon_{n}$ is the single-particle energy level. It may be proved that the lowest energy of the triplet state is always higher than that. Hence, for the limited (but extremely important!) goal of finding ground-state energies of multi-electron systems, we may ignore the actual singlet structure of spinor (24), and reduce the Pauli exclusion principle to the semi-qualitative picture of single-particle levels, each "occupied" with 2 independent particles.

As a very simple example, let us find the ground energy of a deep, cubic-shaped, 3D quantum well with side $a$, filled with 5 fermions, ignoring their direct interaction. From the solution of the singleparticle Schrödinger equation in Sec. 1.5, we know the single-particle energy spectrum of the system:

$$
\begin{equation*}
\varepsilon_{n_{x}, n_{y}, n_{z}}=\varepsilon_{0}\left(n_{x}^{2}+n_{y}^{2}+n_{z}^{2}\right), \quad \text { with } \quad \varepsilon_{0} \equiv \frac{\pi^{2} \hbar^{2}}{2 m a^{2}}, \quad \text { and } n_{x}, n_{y}, n_{z}=1,2, \ldots \tag{8.25}
\end{equation*}
$$

so that the lowest-energy orbital states are:

- one ground state with $\left\{n_{x}, n_{y}, n_{z}\right\}=\{1,1,1\}$, and energy $\varepsilon_{111}=\left(1^{2}+1^{2}+1^{2}\right) \varepsilon_{0}=3 \varepsilon_{0}$, and
- three excited states, with $\left\{n_{x}, n_{y}, n_{z}\right\}$ equal to $\{2,1,1\},\{1,2,1\}$, and $\{1,1,2\}$, with equal energies $\varepsilon_{211}=\varepsilon_{121}=\varepsilon_{112}=\left(2^{2}+1^{2}+1^{2}\right) \varepsilon_{0}=6 \varepsilon_{0}$.

According to the Pauli principle, each of these energy levels states can accommodate up to 2 electrons. Hence the lowest-energy (ground) state of the 5 -electron system is achieved by placing 2 of

[^712]them on the ground level $\varepsilon_{111}=3 \varepsilon_{0}$, and the remaining 3 particles, in any of the degenerate "excited" states of energy $6 \varepsilon_{0}$. Hence the ground energy of the system is
\[

$$
\begin{equation*}
E_{g}=2 \times 3 \varepsilon_{0}+3 \times 6 \varepsilon_{0}=24 \varepsilon_{0}=\frac{12 \pi^{2} \hbar^{2}}{m a^{2}} \tag{8.26}
\end{equation*}
$$

\]

In many cases of relatively weak interaction between particles, it does not blow up such a simple quantum state classification scheme, and the Pauli principle allows tracing the order of single-particle state filling with Fermi particles. This is exactly the approach that has been used at our discussion of atoms in Sec. 3.7.

Now let us describe the results of particle interaction more quantitatively, on the simplest example ${ }^{11}$ of the lowest energy states of a neutral atom ${ }^{12}$ of helium - more exactly, helium-4, usually denoted ${ }^{4} \mathrm{He}$, consisting of a nucleus with two protons and two neutrons, of the total electric charge $q=$ $+2 e$, and two electrons "rotating" about it. Neglecting the small relativistic effects that was discussed in Sec. 6.3, the Hamiltonian describing the electron motion may be represented as

$$
\begin{equation*}
\hat{H}=\hat{h}_{1}+\hat{h}_{2}+\hat{u}_{\text {int }}, \quad \hat{h}_{k}=\frac{\hat{p}_{k}^{2}}{2 m}-\frac{2 e^{2}}{4 \pi \varepsilon_{0} r_{k}}, \quad \hat{u}_{\text {int }}=\frac{e^{2}}{4 \pi \varepsilon_{0}\left|\mathbf{r}_{1}-\mathbf{r}_{2}\right|} . \tag{8.27}
\end{equation*}
$$

As most problems of multiparticle quantum mechanics, the eigenvalue/eigenstate problem for this Hamiltonian does not have an exact analytical solution, so let us start an approximate analysis considering the electron-electron interaction as a perturbation. As was discussed in Chapter 6, we have to start with the " $0^{\text {th }}$-order" approximation in which the perturbation is ignored, so that the Hamiltonian is reduced to sum (22). In this approximation, the ground state $g$ of the atom is the singlet (24), with the orbital factor

$$
\begin{equation*}
\psi_{g}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=\psi_{100}\left(\mathbf{r}_{1}\right) \psi_{100}\left(\mathbf{r}_{2}\right), \tag{8.28}
\end{equation*}
$$

and energy $2 \varepsilon_{\mathrm{g}}$. Here each operand $\psi_{100}(\mathbf{r})$ is the single-particle wavefunction of the ground ( $1 s$ ) state of the hydrogen-like atom with $Z=2$, with quantum numbers $n=1, l=0, m=0$. According to Eqs. (3.174) and (3.198),

$$
\begin{equation*}
\psi_{100}(\mathbf{r})=Y_{0}^{0}(\theta, \varphi) R_{1,0}(r)=\frac{1}{\sqrt{4 \pi}} \frac{2}{r_{0}^{3 / 2}} e^{-r / r_{0}}, \quad \text { with } r_{0}=\frac{r_{\mathrm{B}}}{Z}=\frac{r_{\mathrm{B}}}{2}, \tag{8.29}
\end{equation*}
$$

so that according to Eq. (3.191), in this approximation the total ground state energy is

$$
\begin{equation*}
E_{g}^{(0)}=2 \varepsilon_{g}^{(0)}=2\left(-\frac{\varepsilon_{0}}{2 n^{2}}\right)_{n=1, Z=2}=2\left(-\frac{Z^{2} E_{\mathrm{H}}}{2}\right)_{Z=2}=-4 E_{\mathrm{H}} \approx-109 \mathrm{eV} . \tag{8.30}
\end{equation*}
$$

This is still somewhat far (though not terribly far!) from the experimental value $E_{g} \approx-78.8 \mathrm{eV}$ - see the bottom level in Fig. 1a.

[^713]Making a small detour from our main topic, electron indistinguishability effects, let us note that we can get a much better agreement with experiment by calculating the electron interaction energy in the $1^{\text {st }}$ order of the perturbation theory. Indeed, in application to our system, Eq. (6.13) reads

$$
\begin{equation*}
E_{g}^{(1)}=\langle g| \hat{u}_{\mathrm{int}}|g\rangle=\int d^{3} r_{1} \int d^{3} r_{2} \psi_{g}^{*}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) u_{\mathrm{int}}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) \psi_{g}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) . \tag{8.31}
\end{equation*}
$$

Plugging in Eqs. (27)-(29), we get

$$
\begin{equation*}
E_{g}^{(1)}=\left(\frac{1}{4 \pi} \frac{4}{r_{0}^{3}}\right)^{2} \int d^{3} r_{1} \int d^{3} r_{2} \frac{e^{2}}{4 \pi \varepsilon_{0}\left|\mathbf{r}_{1}-\mathbf{r}_{2}\right|} \exp \left\{-\frac{2\left(r_{1}+r_{2}\right)}{r_{0}}\right\} . \tag{8.32}
\end{equation*}
$$

As may be readily evaluated analytically (this exercise is left for the reader), this expression equals $(5 / 4) E_{\mathrm{H}}$, so that the corrected ground state energy,

$$
\begin{equation*}
E_{g} \approx E_{g}^{(0)}+E_{g}^{(1)}=\left(-4+\frac{5}{4}\right) E_{\mathrm{H}}=-74.8 \mathrm{eV} \tag{8.33}
\end{equation*}
$$

is much closer to experiment.


Fig. 8.1. The lowest energy levels of a helium atom: (a) experimental data and (b) a schematic structure of an excited state with fixed $n$ and $l$ in the first order of the perturbation theory. On panel (a), all energies are referred to that $\left(-2 E_{\mathrm{H}} \approx-55.4 \mathrm{eV}\right)$ of the ground state of ion $\mathrm{He}^{+1}$, so that their magnitudes are the (readily measurable) energies of atom's ionization starting from the corresponding bound state.

There is still a room for improvement - that may be made, for example, using the variational method, ${ }^{13}$ based on the following, very general observation. Let $n$ be the exact, full and orthonormal set of stationary states of a quantum system, and use it as the basis for expansion of a normalized but otherwise arbitrary trial state $\alpha$ (defined in the same Hilbert space):

$$
\begin{equation*}
|\alpha\rangle=\sum_{n} \alpha_{n}|n\rangle \tag{8.34}
\end{equation*}
$$

[^714]with the energy that may be calculated using the general (4.125):
\[

$$
\begin{equation*}
E_{\alpha}=\langle\alpha| \hat{H}|\alpha\rangle=\sum_{n} W_{n} E_{n}, \text { where } W_{n}=\left|\alpha_{n}\right|^{2} \geq 0 \tag{8.35}
\end{equation*}
$$

\]

Since, by definition, the exact ground state energy $E_{g}$ is the lowest one of the set $E_{n}$, we can use Eq. (35) to compose the following inequality:

Variational
method's justification

$$
\begin{equation*}
E_{\alpha} \geq \sum_{n} W_{n} E_{g}=E_{g} \sum_{n} W_{n}=E_{g} \tag{8.36}
\end{equation*}
$$

Thus, the ground state energy is always lower then (or equal to) the energy of any trial state $\alpha$. Hence, if we make several attempts with reasonably selected trial states, we may expect the lowest of the results to approximate the genuine ground state energy reasonably well.

For our particular case of a ${ }^{4} \mathrm{He}$ atom, we may try to use, as the trial state, the wavefunction given by Eqs. (28)-(29), but with the atomic number $Z$ considered as an adjustable parameter $Z_{\text {ef }}<Z=2$ rather than a fixed number. The physics behind this idea is that each the electric charge density $\rho(\mathbf{r})=-$ $e|\psi(\mathbf{r})|^{2}$ of each electron forms a negatively charged "cloud" that reduces the effective charge of the nuclei, as seen by another electron, to $Z_{\mathrm{ef}} e^{2}$, with some $Z_{\mathrm{ef}}<2$. As a result, the single-particle wavefunction spreads further in space ( $r_{0}=r_{\mathrm{B}} / Z_{\mathrm{ef}}>r_{\mathrm{B}} / Z$ ), while keeping its functional form (29) nearly intact. Since the kinetic energies $T$ in system's Hamiltonian are proportional to $r_{0}{ }^{-2}$, while the potential energies scale as $r_{0}{ }^{-1}$, we can write

$$
\begin{equation*}
E_{g}\left(Z_{\mathrm{ef}}\right)=\left(\frac{Z_{\mathrm{ef}}}{2}\right)^{2}\left\langle T_{g}\right\rangle_{Z=2}+\frac{Z_{\mathrm{ef}}}{2}\left\langle U_{g}\right\rangle_{Z=2} \tag{8.37}
\end{equation*}
$$

Now we can use the fact that according to Eq. (3.202), for any stationary state of a hydrogen-like atom (just as for the classical circular motion in the Coulomb potential), $\langle U\rangle=2 E$, and hence $\langle T\rangle=E-\langle U\rangle=-$ $E$. Using Eq. (8.30), and adding the correction $U_{g}^{(1)}=-(5 / 4) E_{\mathrm{H}}$ calculated above, to the potential energy, we get

$$
\begin{equation*}
E_{g}\left(Z_{\mathrm{ef}}\right)=\left[4\left(\frac{Z_{\mathrm{ef}}}{2}\right)^{2}+\left(-8+\frac{5}{4}\right) \frac{Z_{\mathrm{ef}}}{2}\right] E_{\mathrm{H}} \tag{8.38}
\end{equation*}
$$

The minimum of function $E_{g}\left(Z_{\mathrm{ef}}\right)$ and the corresponding "optimal" value of $Z_{\mathrm{ef}}$ are as follows:

$$
\begin{equation*}
\left(Z_{\mathrm{eff}}\right)_{\mathrm{opt}}=2\left(1-\frac{5}{32}\right)=1.6875, \quad\left(E_{g}\right)_{\min } \approx-2.85 E_{\mathrm{H}} \approx-77.5 \mathrm{eV} \tag{8.39}
\end{equation*}
$$

Given the trial function crudeness, this number is in a surprisingly good agreement with experimental value cited above, with a difference of the order of $1 \% .{ }^{14}$

Now let us return of our basic topic - the effects of electron indistinguishability. As we have just seen, the ground level energy of the helium atom is not affected directly by this fact, but the situation is

[^715]different for its excited states - even the lowest ones. The reasonably good convergence of the perturbation theory, that we have seen for the ground state, tells us that we can base our analysis of wavefunctions $\left(\psi_{e}\right)$ of the lowest excited state orbitals, on products like $\psi_{100}\left(\mathbf{r}_{k}\right) \psi_{n l m}\left(\mathbf{r}_{k}\right)$, with $n>1$. However, in order to satisfy the fermion permutation rule, $\mathcal{P}_{j}=-1$, we have to take the orbital part of the state in an either symmetric or asymmetric form:
\[

$$
\begin{equation*}
\psi_{e}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=\frac{1}{\sqrt{2}}\left[\psi_{100}\left(\mathbf{r}_{1}\right) \psi_{n m l}\left(\mathbf{r}_{2}\right) \pm \psi_{n m l}\left(\mathbf{r}_{1}\right) \psi_{100}\left(\mathbf{r}_{2}\right)\right] \tag{8.40}
\end{equation*}
$$

\]

with the proper total permutation asymmetry provided by the corresponding spin part given by, respectively, Eq. (19) or Eq. (21), so that the upper/lower signs in Eq. (40) correspond to the singlet/triplet spin state. Let us calculate the expectation values of the total energy of the system in the first order of the perturbation theory. Plugging Eq. (40) into the $0^{\text {th }}$ order expression

$$
\begin{equation*}
\left\langle E_{e}\right\rangle^{(0)}=\int d^{3} r_{1} \int d^{3} r_{2} \psi_{e}^{*}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)\left(\hat{h}_{1}+\hat{h}_{2}\right) \psi_{e}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right), \tag{8.41}
\end{equation*}
$$

we get two groups of similar terms that differ only by the particle index. We can merge the terms of each pair by changing the notation as $\left(\mathbf{r}_{1} \rightarrow \mathbf{r}, \mathbf{r}_{2} \rightarrow \mathbf{r}^{\prime}\right)$ in one of them, and $\left(\mathbf{r}_{1} \rightarrow \mathbf{r}^{\prime}, \mathbf{r}_{2} \rightarrow \mathbf{r}\right)$ in the other term. Using Eq. (27), and the mutual orthogonality of wavefunctions $\psi_{100}(\mathbf{r})$ and $\psi_{n l m}(\mathbf{r})$, we get the following result,

$$
\begin{align*}
\left\langle E_{e}\right\rangle^{(0)} & =\int \psi_{100}^{*}(\mathbf{r})\left(-\frac{\hbar^{2} \hat{\nabla}_{\mathbf{r}}^{2}}{2 m}-\frac{2 e^{2}}{4 \pi \varepsilon_{0} r}\right) \psi_{100}(\mathbf{r}) d^{3} r+\int \psi_{n l m}^{*}\left(\mathbf{r}^{\prime}\right)\left(-\frac{\hbar^{2} \hat{\nabla}_{\mathbf{r}^{\prime}}^{2}}{2 m}-\frac{2 e^{2}}{4 \pi \varepsilon_{0} r^{\prime}}\right) \psi_{n m l}\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime}  \tag{8.42}\\
& =\varepsilon_{100}+\varepsilon_{n m l}
\end{align*}
$$

which may be interpreted as the sum of eigenenergies of two separate single particles, one in the ground state 100 , and another in the excited state $n l m$ - despite that actually the electron states are entangled. Thus, in the $0^{\text {th }}$ order of the perturbation theory, the electron entanglement does not affect their energy.

However, the potential energy of the system also includes the interaction term $u_{\text {int }}$ (27) that does not allow such separation. As a result, in the first approximation of the perturbation theory, the total energy of the system may be represented as

$$
\begin{gather*}
E_{e}=\varepsilon_{100}+\varepsilon_{n l m}+E_{\text {int }}^{(1)}  \tag{8.43a}\\
E_{\text {int }}^{(1)}=\left\langle U_{\text {int }}\right\rangle=\int d^{3} r_{1} \int d^{3} r_{2} \psi_{e}^{*}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) U_{\text {int }}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) \psi_{e}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) \tag{8.43b}
\end{gather*}
$$

Plugging Eq. (40) into this result, using the symmetry of $u_{\text {int }}$ with respect to the particle number permutation, and the same particle coordinate re-numbering as above, we get

$$
\begin{equation*}
E_{\mathrm{int}}^{(1)}=E_{\mathrm{dir}} \pm E_{\mathrm{ex}} \tag{8.44}
\end{equation*}
$$

with deceivingly similar expressions for the operands:

$$
\begin{align*}
& E_{\mathrm{dir}} \equiv \int d^{3} r \int d^{3} r^{\prime} \psi_{100}^{*}(\mathbf{r}) \psi_{n l m}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{100}(\mathbf{r}) \psi_{n l m}\left(\mathbf{r}^{\prime}\right),  \tag{8.45a}\\
& E_{\mathrm{ex}} \equiv \int d^{3} r \int d^{3} r^{\prime} \psi_{100}^{*}(\mathbf{r}) \psi_{n l m}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{n l m}(\mathbf{r}) \psi_{100}\left(\mathbf{r}^{\prime}\right) \tag{8.45b}
\end{align*}
$$

Since the single-particle orbitals can be always made real, both components are positive (or at least non-negative). However, their physics is completely different. Integral (45a), called the direct electron-electron interaction, allows a simple semi-classical interpretation as the Coulomb energy of interacting electrons, each distributed in space with the electric charge density $\rho_{n m l}(\mathbf{r})=$ $e \psi_{n m l} *(\mathbf{r}) \psi_{n m l}(\mathbf{r}):{ }^{15}$

$$
\begin{equation*}
E_{\mathrm{dir}}=\int d^{3} r \int d^{3} r^{\prime} \frac{\rho_{100}(\mathbf{r}) \rho_{n l m}\left(\mathbf{r}^{\prime}\right)}{4 \pi \varepsilon_{0}\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}=\int \rho_{100}(\mathbf{r}) \phi(\mathbf{r}) d^{3} r \tag{8.46}
\end{equation*}
$$

where $\phi(\mathbf{r})$ is the electrostatic potential created, at point $\mathbf{r}$, by the counterpart electron's "electric charge cloud": ${ }^{16}$

$$
\begin{equation*}
\phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int d^{3} r^{\prime} \frac{\rho_{n l m}\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|} \tag{8.47}
\end{equation*}
$$

However, integral (45b), called the exchange interaction, evades a classical interpretation, and (as it is clear from its derivation) is the direct corollary of the electron indistinguishability. The magnitude of $E_{\text {ex }}$ is also very much different from $E_{\text {dir }}$, because the function under integral (45b) disappears in those regions where single-particle wavefunctions do not overlap. This is in a full agreement with the discussion in Sec. 1: if two particles are identical but well separated, i.e. their wavefunctions do not overlap, the exchange interaction disappears, because all effects of particle indistinguishability vanish.

Historically, the fact of having two different hydrogen-like spectra (48) and (49) was taken as an evidence for two different species of ${ }^{4} \mathrm{He}$, called, respectively, the parahelium and orthohelium. Figure 1 b shows the structure of an excited energy level, with certain quantum numbers $n>1, l$, and $m$, given by Eqs. (44)-(45). The upper level, with energy

$$
\begin{equation*}
E_{\text {para }}=\left(\varepsilon_{100}+\varepsilon_{n l m}\right)+E_{\mathrm{dir}}+E_{\mathrm{ex}}>\varepsilon_{100}+\varepsilon_{n l m}, \tag{8.48}
\end{equation*}
$$

corresponds to the "parahelium", i.e. the symmetric orbital state and hence to the singlet spin state (19), with zero net spin, $s=0$. The lower level, with

$$
\begin{equation*}
E_{\text {ortho }}=\left(\varepsilon_{100}+\varepsilon_{n l m}\right)+E_{\text {dir }}-E_{\text {ex }}<E_{\text {para }}, \tag{8.49}
\end{equation*}
$$

corresponds to "orthohelium", i.e. the antisymmetric orbital, and hence to the triplet spin state(s) with $s$ = 1 - see Eq. (21). Its degeneracy may be lifted by magnetic field, so that the splitting is identical to that of an elementary particle with spin $s=1$. Calculations of the direct and exchange interaction integrals (45) for various values of $n$ and $l$ show that the perturbation theory explains the experimental spectrum of the orthohelium and parahelium (Fig. 1) pretty well.

Encouraged by this success, and motivation by the very important task of description of atoms, molecules, and metals, we may try to apply the same approach to systems with $N>2$ electrons. In this case the mathematical expression of the Pauli principle for fermions is

[^716]\[

$$
\begin{equation*}
\hat{P}_{k k^{\prime}}=-1, \quad \text { for all } k, k^{\prime}=1,2, \ldots, N ., \tag{8.50}
\end{equation*}
$$

\]

where operator $\hat{\mathcal{P}}_{k k^{\prime}}$ permutes particle with numbers $k$ and $k^{\prime}$. In order to understand how common eigenstates of all such operators may be formed, let us return for a minute to two non-interacting electrons, and rewrite Eq. (11) in the following compact form:

$$
\left|\alpha_{-}\right\rangle=\frac{1}{\sqrt{2}}\left(|\beta\rangle \otimes\left|\beta^{\prime}\right\rangle-\left|\beta^{\prime}\right\rangle \otimes|\beta\rangle\right)=\frac{1}{\sqrt{2}} \begin{array}{cc}
\text { state } 1 & \text { state 2 }  \tag{8.51}\\
\downarrow & \downarrow \\
\| \beta\rangle \otimes & \left|\beta^{\prime}\right\rangle \\
|\beta\rangle \otimes & \left.\left|\beta^{\prime}\right\rangle\right\rangle \leftarrow \text { particle number 1, } \\
\left|\beta^{\prime}\right\rangle & \text { particle number 2. }
\end{array}
$$

In this way, the Pauli principle is mapped on the well-known property of matrix determinants: if any of two columns of a matrix coincide, its determinant vanishes. This Slater determinant approach may be readily generalized to $N$ fermions in $N$ (not necessarily lowest) single-particle states $\beta$, $\beta$, etc:


Even though the Slater determinant form is extremely nice and compact (in comparison with direct writing of a sum of $N$ ! products, each of $N$ ket factors), there are two major problems with using it for practical calculations:
(i) For the calculation of any bra-ket product (say, within the perturbation theory) we need to spell out each bra- and ket-vector as a sum of component terms. Even for a limited number of electrons (say $N \sim 10^{2}$ in a typical atom), the number $N!\sim 10^{160}$ of terms in such a sum is impracticably large for any analytical calculation.
(ii) In the case of interacting fermions, Slater determinants do not describe the eigenvectors of the system; rather the stationary state is a superposition of such determinants - each for a specific selection of $N$ states from the general set of single-particle states - that is generally different from $N$.

These challenges make the development of a more general theory that would not use particle numbers (which are superficial for indistinguishable particles to start with) a must for getting any final results for multiparticle systems.

### 8.3. Second quantization

The most useful formalism for this purpose, that avoids particle numbering at all, is called the second quantization. ${ }^{17}$ Actually, we have already discussed a particular version of this formalism, for

[^717]the a case of 1D harmonic oscillator's excitations, in Sec. 5.4. As a reminder, we have used Eqs. (5.98) to define the "creation" and "annihilation" operators via the usual operators of coordinate and momentum, and then proved their key property (5.122),
\[

$$
\begin{equation*}
\hat{a}^{\dagger}|n\rangle=(n+1)^{1 / 2}|n+1\rangle, \quad \hat{a}|n\rangle=n^{1 / 2}|n-1\rangle, \tag{8.53}
\end{equation*}
$$

\]

where $n$ are the stationary (Fock) states of the oscillator. This property allows an interpretation of operators' actions as the creation/annihilation of a single excitations of energy $\hbar \omega_{0}$ - thus justifying the operator names. In the next chapter, we will show that such an excitation of an electromagnetic field mode may be considered as a massless boson with $s=1$, called the photon.

In order to generalize this approach to arbitrary bosons, not appealing to a specific system such as the harmonic oscillator, we may use relations similar to Eq. (53) to define the creation and annihilation operators. The definition looks simple in the language of the so-called Dirac states, with ket-vectors

Dirac state

$$
\begin{equation*}
\left|N_{1}, N_{2}, \ldots N_{j}, \ldots\right\rangle \tag{8.54}
\end{equation*}
$$

where $N_{j}$ are the state occupancies, i.e. the numbers of bosons in each single-particle state $j$. Let me emphasize that here indices $1,2, \ldots j, \ldots$, are the positions of each number in the Dirac ket vector, i.e. are the numbers of single-particle states (including their spin parts) rather than particles. Thus the very notion of individual particle numbers is completely (and for indistinguishable particles, very relevantly) absent from this formalism. Generally, the set of single-particle states participating in the Dirac state may be selected in an arbitrary way (provided that it is full and orthonormal),

$$
\begin{equation*}
\left\langle N_{1}^{\prime}, N_{2}^{\prime} \ldots, N_{j^{\prime}}^{\prime}, \ldots \mid N_{1}, N_{2} \ldots, N_{j}, \ldots\right\rangle=\delta_{N_{1} N_{1}^{\prime}} \delta_{N_{2} N_{2}^{\prime}} \ldots \delta_{N_{j} N_{j}^{\prime}} \ldots \tag{8.55}
\end{equation*}
$$

though for system of non- (or weakly) interacting bosons, using the stationary states of individual particles in the system under analysis are almost always the best choice.

Now we can define the particle annihilation operator as follows:

Boson
annihilation operator

$$
\begin{equation*}
\hat{a}_{j}\left|N_{1}, N_{2}, \ldots N_{j}, \ldots\right\rangle \equiv N_{j}^{1 / 2}\left|N_{1}, N_{2}, \ldots N_{j}-1, \ldots\right\rangle . \tag{8.56}
\end{equation*}
$$

Note that the pre-ket coefficient, similar to that in Eq. (53), guarantees that an attempt to annihilate a particle in an unpopulated state gives the non-existing (null) state:

$$
\begin{equation*}
\hat{a}_{j}\left|N_{1}, N_{2}, \ldots 0_{j}, \ldots\right\rangle=0 \tag{8.57}
\end{equation*}
$$

where symbol $0_{j}$ means zero occupancy of $j$-th state. An alternative way to write Eq. (56) is

$$
\begin{equation*}
\left\langle N_{1}^{\prime}, N_{2}^{\prime}, \ldots, N_{j}^{\prime}, \ldots\right| \hat{a}_{j}\left|\cdot N_{1}, N_{2}, \ldots, N_{j}, \ldots\right\rangle=N_{j}^{1 / 2} \delta_{N_{1} N_{1}^{\prime}} \delta_{N_{2} N_{2}^{\prime}} \ldots \delta_{N_{j}^{\prime}, N_{j}-1} \ldots \tag{8.58}
\end{equation*}
$$

According to Eq. (4.65), the matrix element of the Hermitian conjugate operator $\hat{a}_{j}^{\dagger}$ is

$$
\begin{align*}
& \left\langle N_{1}^{\prime}, N_{2}^{\prime}, \ldots, N_{j}^{\prime}, \ldots\right| \hat{a}_{j}^{\dagger}\left|N_{1}, N_{2}, \ldots N_{j}, \ldots\right\rangle=\left\langle N_{1}, N_{2}, \ldots, N_{j}, \ldots\right| \hat{a}_{j}\left|N_{1}^{\prime}, N_{2}^{\prime}, \ldots, N_{j}^{\prime}, \ldots\right\rangle^{*} \\
& =\left\langle N_{1}, N_{2}, \ldots, N_{j}, \ldots\right|\left(N_{j}^{\prime}\right)^{1 / 2}\left|N_{1}^{\prime}, N_{2}^{\prime}, \ldots, N_{j}^{\prime}-1, \ldots\right\rangle=\left(N_{j}^{\prime}\right)^{1 / 2} \delta_{N_{1} N_{1}^{\prime}} \delta_{N_{2} N_{2}^{\prime}} \ldots \delta_{N_{j}, N_{j}^{\prime}-1} \ldots  \tag{8.59}\\
& =\left(N_{j}+1\right)^{1 / 2} \delta_{N_{1} N_{1}^{\prime}} \delta_{N_{2} N_{2}^{\prime}} \ldots \delta_{N_{j}+1, N_{j}^{\prime}} \ldots,
\end{align*}
$$

meaning that

$$
\begin{equation*}
\hat{a}_{j}^{\dagger}\left|N_{1}, N_{2}, \ldots, N_{j}, \ldots\right\rangle=\left(N_{j}+1\right)^{1 / 2}\left|N_{1}, N_{2}, \ldots, N_{j}+1, \ldots\right\rangle, \tag{8.60}
\end{equation*}
$$

Boson creation operator
in the total compliance with the first of Eqs. (53). In particular, this particle creation operator $\hat{a}_{j}^{\dagger}$ allows the description of the generation of a single particle from the vacuum (not null!) state $|0,0, \ldots\rangle$ :

$$
\begin{equation*}
\hat{a}_{j}^{\dagger}\left|0,0, \ldots, 0_{j}, \ldots, 0\right\rangle=\left|0,0, \ldots, 1_{j}, \ldots 0\right\rangle \tag{8.61}
\end{equation*}
$$

and hence a product of such operators may create, from the vacuum, a multiparticle state with an arbitrary set of occupancies: ${ }^{18}$

Next, combining Eqs. (56) and (60), we get

$$
\begin{equation*}
\hat{a}_{j}^{\dagger} \hat{a}_{j}\left|N_{1}, N_{2}, \ldots N_{j}, \ldots\right\rangle=N_{j}\left|N_{1}, N_{2}, \ldots, N_{j}, \ldots\right\rangle \tag{8.63}
\end{equation*}
$$

so that, just as for the particular case of harmonic oscillator excitations, operator

$$
\begin{equation*}
\hat{N}_{j} \equiv \hat{a}_{j}^{\dagger} \hat{a}_{j} \tag{8.64}
\end{equation*}
$$

Numbercounting operator
conserves the numbers of particles in all single-particle states, and simultaneously "counts" their number in the $j$-th state. Acting by the creation-annihilation operators in the reverse order, we get

$$
\begin{equation*}
\hat{a}_{j} \hat{a}_{j}^{\dagger}\left|N_{1}, N_{2}, \ldots, N_{j}, \ldots\right\rangle=\left(N_{j}+1\right)\left|N_{1}, N_{2}, \ldots, N_{j}, \ldots\right\rangle . \tag{8.65}
\end{equation*}
$$

This result shows that for any state of a multiparticle system (which always may be represented as a linear superposition of Dirac states with different sets of $N_{j}$ ), we can write

$$
\begin{equation*}
\hat{a}_{j} \hat{a}_{j}^{\dagger}-\hat{a}_{j}^{\dagger} \hat{a}_{j} \equiv\left[\hat{a}_{j}, \hat{a}_{j}^{\dagger}\right]=\hat{I}, \tag{8.66}
\end{equation*}
$$

again in agreement with what we had for the 1D oscillator - cf. Eq. (5.101). According to Eq. (55), the creation and annihilation operators corresponding to different single-particle states do commute, so that Eq. (66) may be generalized as

[^718]Commutation relations for bosonic operators

$$
\begin{equation*}
\left[\hat{a}_{j}, \hat{a}_{j^{\prime}}^{\dagger}\right]=\hat{I} \delta_{j j^{\prime}}, \tag{8.67}
\end{equation*}
$$

and that similar bosonic creation and annihilation operators commute, regardless of which states do they act upon:

$$
\begin{equation*}
\left[\hat{a}_{j}^{\dagger}, \hat{a}_{j^{\prime}}^{\dagger}\right]=\left[\hat{a}_{j}, \hat{a}_{j^{\prime}}\right]=0 \tag{8.68}
\end{equation*}
$$

Relations (66)-(68) are the mathematical expression of the independence of occupancies of different boson states.

As was mentioned earlier, a major challenge in the Dirac approach is to rewrite the Hamiltonian of a multiparticle system, that naturally carries particle numbers $k$ (see, e.g., Eq. (22) for $k=1,2$ ), in the second quantization language, in which there are no these numbers. Let us start with single-particle components of such Hamiltonians, i.e. operators of the type

$$
\begin{equation*}
\hat{F}=\sum_{k=1}^{N} \hat{f}_{k} \tag{8.69}
\end{equation*}
$$

where all $N$ operators $\hat{f}_{k}$ are similar, besides that each of them acts on one specific ( $k$-th) particle, and $N$ is the total number of particles in the system, that is naturally equal to the sum of single-particle state occupancies:

$$
\begin{equation*}
N=\sum_{j} N_{j} . \tag{8.70}
\end{equation*}
$$

The most important examples of such operators are the kinetic energy of $N$ similar single particles, and their potential energy in an external field:

$$
\begin{equation*}
\hat{T}=\sum_{k=1}^{N} \frac{\hat{p}_{k}^{2}}{2 m}, \quad \hat{U}=\sum_{k=1}^{N} \hat{u}\left(\mathbf{r}_{k}\right) . \tag{8.71}
\end{equation*}
$$

In order to express a particle-separable operator of the type (69) in terms of the Dirac formalism, we need to return for a minute to the particle-number representations used in the beginning of this chapter. Instead of the Slater determinant (52), for bosons we have to write a similar expression, but without the sign changes (sometimes called the permanent):

$$
\begin{equation*}
\left|N_{1}, \ldots N_{j}, \ldots\right\rangle=\left(\frac{N_{1}!\ldots N_{j}!\ldots}{N!}\right)^{1 / 2} \sum_{P}|\underbrace{\ldots \beta \beta^{\prime} \beta^{\prime \prime} \ldots}_{N_{\text {operands }}}\rangle . \tag{8.72}
\end{equation*}
$$

Note again that the left-hand part of this relation is written in the Dirac notation (that does not use particle numbering), while in its right-hand part, just in relations of Secs. 1-2, particle numbers are coded with the positions of the single-particle states inside the ket-vectors, and the sum is over all different permutations of the states in the ket - cf. Eq. (10). (According to the elementary combinatorics, ${ }^{19}$ there are $N!/\left(N_{1}!\ldots N_{j}!\ldots\right)$ such permutations, so that the coefficient before the sum ensures the proper normalization of the single-particle states.) Let us use Eq. (72) to spell out the following bra-ket of a system with $(N-1)$ particles:

[^719]\[

$$
\begin{align*}
& \left\langle\ldots N_{j}, \ldots N_{j^{\prime}}-1, \ldots\right| \hat{F}\left|\ldots N_{j}-1, \ldots N_{j^{\prime}}, \ldots\right\rangle \\
& =\frac{N_{1}!\ldots . .\left(N_{j}-1\right)!\ldots\left(N_{j^{\prime}}-1\right)!\ldots}{(N-1)!}\left(N_{j^{\prime}} N_{j^{\prime}}\right)^{1 / 2} \sum_{P\langle N-1|} \sum_{P|N-1\rangle}\left\langle\left.\ldots \beta \beta^{\prime} \beta^{\prime \prime} \ldots\right|_{k=1} ^{N-1} \hat{f}_{k} \mid \ldots \beta \beta^{\prime} \beta^{\prime \prime} \ldots\right\rangle, \tag{8.73}
\end{align*}
$$
\]

where all non-specified occupation numbers in the corresponding positions of the bra- and ket-vectors are equal to each other. Each single-particle operator $\hat{f}_{k}$, participating in the operator sum, acts on the bra- and ket-vectors of states $j$ and $j^{\prime}$, respectively, in a certain (say, $k^{\text {th }}$ ) position, giving the result that does not depend on the position number:

$$
\begin{equation*}
\left\langle\left.\beta_{j}\right|_{\text {in } k^{\text {th }} \text { position }} \hat{f}_{k} \mid \beta_{j^{\prime}}\right\rangle_{\text {in } k^{\text {th }} \text { position }}=\left\langle\beta_{j}\right| \hat{f}\left|\beta_{j^{\prime}}\right\rangle \equiv f_{i j^{\prime}} . \tag{8.74}
\end{equation*}
$$

Since in both permutation sets participating in Eq. (73), with ( $N-1$ ) vectors each, all positions are equivalent, we can fix the position (say, take the first one) and replace the sum over $k$ by the multiplication by factor $(N-1)$. The fraction of permutations with the necessary bra-vector (with number $j$ ) in that position is $N_{j} /(N-1)$, while that with the necessary ket-vector (with number $j^{\prime}$ ) in the same position in $N_{j} / /(N-1)$. As the result, the permutation sum in Eq. (73) reduces to

$$
\begin{equation*}
(N-1) \frac{N_{j}}{N-1} \frac{N_{j^{\prime}}}{N-1} f_{i j^{\prime}} \sum_{P\langle N-2| P|N-2\rangle} \sum\left\langle\ldots \beta \beta^{\prime} \beta^{\prime \prime} \ldots \mid \ldots \beta \beta^{\prime} \beta^{\prime \prime} \ldots\right\rangle, \tag{8.75}
\end{equation*}
$$

where our specific position $k$ is now excluded from both the bra- and ket-vector permutations. Each of these permutations now includes only $\left(N_{j}-1\right)$ states $j$ and $\left(N_{j^{\prime}}-1\right)$ states $j^{\prime}$, so that, using the state orthonormality, we finally arrive at a very simple result:

$$
\begin{align*}
& \left\langle\ldots N_{j}, \ldots N_{j^{\prime}}-1, \ldots\right| \hat{F}\left|\ldots N_{j}-1, \ldots N_{j^{\prime}}, \ldots\right\rangle \\
& =\frac{N_{1}!\ldots\left(N_{j}-1\right)!\ldots\left(N_{j^{\prime}}-1\right)!\ldots}{(N-1)!}\left(N_{j^{\prime}} N_{j^{\prime}}\right)^{1 / 2}(N-1) \frac{N_{j}}{N-1} \frac{N_{j^{\prime}}}{N-1} f_{i j^{\prime}} \frac{(N-2)!}{N_{1}!\ldots\left(N_{j}-1\right)!\ldots\left(N_{j^{\prime}}-1\right)!\ldots}  \tag{8.76}\\
& =\left(N_{j^{\prime}} N_{j^{\prime}}\right)^{1 / 2} f_{j j^{\prime}} .
\end{align*}
$$

Now let us calculate matrix elements of the following operator:

$$
\begin{equation*}
\sum_{j, j^{\prime}} f_{i j^{\prime}} \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}} \tag{8.77}
\end{equation*}
$$

A direct application of Eqs. (56) and (60) shows that the only nonvanishing of them are

$$
\begin{equation*}
\left\langle\ldots N_{j}, \ldots N_{j^{\prime}}-1, \ldots\right| f_{j j^{\prime}} \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}\left|\ldots N_{j}-1, \ldots, N_{j^{\prime}}, \ldots\right\rangle=\left(N_{j} N_{j^{\prime}}\right)^{1 / 2} f_{i j^{\prime}} . \tag{8.78}
\end{equation*}
$$

But this is exactly the last form of Eq. (76), so that in the basis of Dirac states, operator (69) may be represented as

$$
\begin{equation*}
\hat{F}=\sum_{j, j^{\prime}} f_{i j^{\prime}} \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}} \tag{8.79}
\end{equation*}
$$

This beautifully simple equation is the most important formula of the second quantization theory, and is essentially the Dirac-language analog of Eq. (4.59) of the single-particle quantum mechanics. Each term of the sum may be described by a very simple mnemonic rule: if an operator "connects" two
single-particle states $j$ and $j$ ', move the particle from state $j$ ' into state $j$, and weigh the result with the corresponding single-particle matrix element. (One of the corollaries of Eq. (79) is that the expectation value of an operator whose eigenstates coincide with the Dirac states, is

$$
\begin{equation*}
\langle F\rangle \equiv\left\langle\ldots N_{j}, \ldots\right| \hat{F}\left|\ldots N_{j}, \ldots\right\rangle=\sum_{j} f_{i j} N_{j} \tag{8.80}
\end{equation*}
$$

with an evident physical interpretation as the sum of single-particle expectation values over all states, weighed by state occupancies.)

Proceeding to fermions, which have to obey the Pauli principle, we immediately notice that any occupation number $N_{j}$ may only take two values, 0 or 1 . In order to account for that, and also make the key equation (76) valid for fermions as well, the creation-annihilation operators are now defined by relations

Fermion creationannihilation operators

$$
\begin{align*}
& \hat{a}_{j}\left|N_{1}, N_{2}, \ldots, 0_{j}, \ldots\right\rangle=0, \quad \hat{a}_{j}\left|N_{1}, N_{2}, \ldots, 1_{j}, \ldots\right\rangle=(-1)^{\Sigma(1, j-1)}\left|N_{1}, N_{2}, \ldots, 0_{j}, \ldots\right\rangle,  \tag{8.81}\\
& \hat{a}_{j}^{\dagger}\left|N_{1}, N_{2}, \ldots, 0_{j}, \ldots\right\rangle=(-1)^{\Sigma(1, j-1)}\left|N_{1}, N_{2}, \ldots, 1_{j}, \ldots\right\rangle, \quad \hat{a}_{j}^{\dagger}\left|N_{1}, N_{2}, \ldots, 1_{j}, \ldots\right\rangle=0 . \tag{8.82}
\end{align*}
$$

In these relations, symbol $\Sigma\left(J, J^{\prime}\right)$ means the sum of all occupancy numbers in state positions from $J$ to $J^{\prime}$, including the border points:

$$
\begin{equation*}
\Sigma\left(J, J^{\prime}\right) \equiv \sum_{j=J}^{J^{\prime}} N_{j} \tag{8.83}
\end{equation*}
$$

so that the sum participating in Eqs. (81) and (82) is the total occupancy of all states with the numbers below $j$. (The states have to be numbered in a fixed albeit arbitrary order.) As a result, Eqs. (81)-(82) may be readily summarized in the verbal form: if an operator replaces the $j^{\text {th }}$ state occupancy with the opposite one ( 1 with 0 , or vice versa), it also changes sign before the result if (and only if) the total number of particles in states with $j^{\prime}<j$ is odd.

One of corollaries of this (somewhat counter-intuitive) rule of sign alternation is that the sign of the ket-vector of a completely filled two-state system depends on how exactly it has been formed from the vacuum state. Indeed, if we start from creating the fermion in state 1 , we get

$$
\begin{equation*}
\hat{a}_{1}^{\dagger}|0,0\rangle=(-1)^{0}|1,0\rangle=|1,0\rangle, \quad \hat{a}_{2}^{\dagger} \hat{a}_{1}^{\dagger}|0,0\rangle=\hat{a}_{2}^{\dagger}|1,0\rangle=(-1)^{1}|1,1\rangle=-|1,1\rangle, \tag{8.84}
\end{equation*}
$$

while if the operator order is different, the result's sign is opposite:

$$
\begin{equation*}
\hat{a}_{2}^{\dagger}|0,0\rangle=(-1)^{0}|0,1\rangle=|0,1\rangle, \quad \hat{a}_{1}^{\dagger} \hat{a}_{2}^{\dagger}|0,0\rangle=\hat{a}_{1}^{\dagger}|0,1\rangle=(-1)^{0}|1,1\rangle=+|1,1\rangle . \tag{8.85}
\end{equation*}
$$

Since the action of any of these operator products on any initial state rather than vacuum gives the null ket, we can write the following operator equality:

$$
\begin{equation*}
\hat{a}_{1}^{\dagger} \hat{a}_{2}^{\dagger}+\hat{a}_{2}^{\dagger} \hat{a}_{1}^{\dagger} \equiv\left\{\hat{a}_{1}^{\dagger}, \hat{a}_{2}^{\dagger}\right\}=0 \tag{8.86}
\end{equation*}
$$

It is straightforward to check that this result is valid for the Dirac vector of an arbitrary length, and does not depend on the occupancy of other states, so that we can always write

$$
\begin{equation*}
\left\{\hat{a}_{j}^{\dagger}, \hat{a}_{j^{\prime}}^{\dagger}\right\}=\left\{\hat{a}_{j}, \hat{a}_{j^{\prime}}\right\}=0 \tag{8.87}
\end{equation*}
$$

these equalities hold for $j=j$ ' as well. On the other hand, the absolutely similar calculation shows that the mixed creation-annihilation operator products do depend on whether the states are different or not: ${ }^{20}$

$$
\begin{equation*}
\left\{\hat{a}_{j}, \hat{a}_{j^{\prime}}^{\dagger}\right\}=\hat{I} \delta_{i j^{\prime}} \tag{8.88}
\end{equation*}
$$

Commutation relations for fermionic operators

These equations look very much like Eqs. (67)-(68) for bosons, "only" with the replacement of commutators with anticommutators. Since the core laws of quantum mechanics, including the operator compatibility (Sec. 4.5) and the Heisenberg equation (4.199) of operator evolution in time, involve commutators rather than anticommutators, so that one might think that all the behavior of bosonic and fermionic multiparticle systems should be dramatically different. However, the difference is not as huge as one could expect, for one, a straightforward check shows that the sign factors in Eqs. (81)-(82) compensate those in the Slater determinant, and make the key relation (79) valid for the fermions as well. (Indeed, this is the very goal of the introduction of these factors.)

As the simplest example, let us examine what does the second quantization formalism say about dynamics of non-interacting particles in the system whose single-particle properties we know well, namely two nearly-similar, coupled quantum wells - see Fig. 2.23. If the coupling (tunneling) between the wells is so small that the states localized in the wells are only weakly perturbed, in the basis of these states, the single-particle Hamiltonian of the system may be represented by $2 \times 2$ matrix (6.27). Selecting the origin of energy at the middle between energies of unperturbed states, so that coefficient $a_{0}$ in Eq. (6.27) vanishes, we can reduce the matrix to

$$
\mathrm{h}=\mathbf{a} \cdot \boldsymbol{\sigma}=\left(\begin{array}{cc}
a_{z} & a_{-}  \tag{8.89}\\
a_{+} & -a_{z}
\end{array}\right), \quad a_{ \pm} \equiv a_{x} \pm i a_{y}
$$

with eigenvalues

$$
\begin{equation*}
\varepsilon_{ \pm}= \pm a, \quad a=|\mathbf{a}|=\left(a_{x}^{2}+a_{y}^{2}+a_{z}^{2}\right)^{1 / 2} \tag{8.90}
\end{equation*}
$$

Now following recipe (79), we can represent the Hamiltonian of the whole system of particles in terms of the creation-annihilation operators:

$$
\begin{equation*}
\hat{H}=a_{z} \hat{a}_{1}^{\dagger} \hat{a}_{1}+a_{-} \hat{a}_{1}^{\dagger} \hat{a}_{2}+a_{+} \hat{a}_{2}^{\dagger} \hat{a}_{1}-a_{z} \hat{a}_{2}^{\dagger} \hat{a}_{2}, \tag{8.91}
\end{equation*}
$$

where $\hat{a}_{1,2}^{\dagger}$ and $\hat{a}_{1,2}$ are the operators of creation and annihilation of a particle localized in the corresponding quantum well. According to Eq. (64), the first and the last terms of the right-hand part of Eq. (91) describe particle energies in uncoupled wells,

$$
\begin{equation*}
a_{z} \hat{a}_{1}^{\dagger} \hat{a}_{1}=\varepsilon_{1} \hat{N}_{1}, \quad-a_{z} \hat{a}_{2}^{\dagger} \hat{a}_{2}=\varepsilon_{2} \hat{N}_{2} \tag{8.92}
\end{equation*}
$$

[^720]while the sum of middle two terms is the second-quantization description of tunneling between the wells.

Now we can use the general Eq. (4.199) of the Heisenberg picture to find the equations of motion for the creation-annihilation operators. For example,

$$
\begin{equation*}
i \hbar \dot{\hat{a}}_{1}=\left[\hat{a}_{1}, \hat{H}\right]=a_{z}\left[\hat{a}_{1}, \hat{a}_{1}^{\dagger} \hat{a}_{1}\right]+a_{-}\left[\hat{a}_{1}, \hat{a}_{1}^{\dagger} \hat{a}_{2}\right]+a_{+}\left[\hat{a}_{1}, \hat{a}_{2}^{\dagger} \hat{a}_{1}\right]-a_{z}\left[\hat{a}_{1}, \hat{a}_{2}^{\dagger} \hat{a}_{2}\right] . \tag{8.93}
\end{equation*}
$$

Since the Bose and Fermi operators satisfy different commutation relations, one could expect the right hand part of this equation would be different for bosons and fermions. However, it is not so. Indeed, all commutators in the right-hand part of Eq. (93) have the following form:

$$
\begin{equation*}
\left[\hat{a}_{j}, \hat{a}_{j^{\prime}}^{\dagger}, \hat{a}_{j^{\prime \prime}}\right] \equiv \hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime \prime}}-\hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime \prime}} \hat{a}_{j} . \tag{8.94}
\end{equation*}
$$

According to Eqs. (67) and (88), the first pair product of the operators may be recast as

$$
\begin{equation*}
\hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger}=\hat{I} \delta_{i j^{\prime}} \pm \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j}, \tag{8.95}
\end{equation*}
$$

where the upper sign pertains to bosons and the lower to fermions, while according to Eqs. (68) and (87), the very last pair product is

$$
\begin{equation*}
\hat{a}_{j^{\prime \prime}} \hat{a}_{j}= \pm \hat{a}_{j} \hat{a}_{j^{\prime \prime}}, \tag{8.96}
\end{equation*}
$$

with the same sign convention. Plugging these expressions into Eq. (94), we see that regardless of the particle statistics, two last terms cancel, and we arrive at a universal (and generally very useful) commutation rule

$$
\begin{equation*}
\left[\hat{a}_{j}, \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime \prime}}\right]=\hat{a}_{j^{\prime \prime}} \delta_{j j^{\prime}}, \tag{8.97}
\end{equation*}
$$

valid for particles of both kinds. As a result, the Heisenberg equation of motion for operator $\hat{a}_{1}$, and the equation for $\hat{a}_{2}$ (that may be obtained absolutely similarly), are also statistics-independent: ${ }^{21}$

$$
\begin{align*}
& i \hbar \dot{\hat{a}}_{1}=a_{z} \hat{a}_{1}+a_{-} \hat{a}_{2},  \tag{8.98}\\
& i \hbar \dot{\hat{a}}_{2}=a_{+} \hat{a}_{1}-a_{z} \hat{a}_{2} .
\end{align*}
$$

Thus we have got a system of coupled, linear differential equations that are identical to equations for the $c$-number probability amplitudes of single-particle wavefunctions of a two-level system - see Eq. (2.201) and Problem 4.10. Their general solution is a linear superposition of exponents:

$$
\begin{equation*}
\hat{a}_{1,2}(t)=\sum_{ \pm} \hat{c}_{1,2}^{( \pm)} \exp \left\{\lambda_{ \pm} t\right\} . \tag{8.99}
\end{equation*}
$$

[^721]As usual, in order to find exponents $\lambda_{ \pm}$, it is sufficient to plug in a particular solution $\hat{a}_{1,2}(t)=\hat{c}_{1,2} \exp \{\lambda t\}$ into Eq. (98) and require that the determinant of the resulting homogeneous, linear system for "coefficients" (actually, time-independent operators) $\hat{c}_{1,2}$ equals zero. This gives us the following characteristic equation

$$
\left|\begin{array}{cc}
a_{z}-i \hbar \lambda & a_{-}  \tag{8.100}\\
a_{+} & -a_{z}-i \hbar \lambda
\end{array}\right|=0,
$$

with two roots $\lambda_{ \pm}= \pm i \Omega / 2$, where $\Omega \equiv 2 a / \hbar$. Now plugging each of the roots, one by one, into the system of equations for $\hat{c}_{1,2}$, we can find these operators, and hence the general solution of system (98) for arbitrary initial conditions.

Let us consider the simple case $a_{y}=a_{z}=0$ (meaning in particular that the well eigenenergies are exactly aligned), so that $\hbar \Omega / 2 \equiv a=a_{x}$; then the solution of Eq. (98) is

$$
\begin{equation*}
\hat{a}_{1}(t)=\hat{a}_{1}(0) \cos \frac{\Omega t}{2}-i \hat{a}_{2}(0) \sin \frac{\Omega t}{2}, \quad \hat{a}_{2}(t)=-i \hat{a}_{1}(0) \sin \frac{\Omega t}{2}+\hat{a}_{2}(0) \cos \frac{\Omega t}{2} . \tag{8.101}
\end{equation*}
$$

Multiplying the first of Eqs. (101) by its Hermitian conjugate, and ensemble-averaging the result, we get

$$
\begin{align*}
\left\langle N_{1}\right\rangle= & \left\langle\hat{a}_{1}^{\dagger}(t) \hat{a}_{1}(t)\right\rangle=\left\langle\hat{a}_{1}^{\dagger}(0) \hat{a}_{1}(0)\right\rangle \cos ^{2} \frac{\Omega t}{2}+\left\langle\hat{a}_{2}^{\dagger}(0) \hat{a}_{2}(0)\right\rangle \sin ^{2} \frac{\Omega t}{2}  \tag{8.102}\\
& -i\left\langle\hat{a}_{1}^{\dagger}(0) \hat{a}_{2}(0)+\hat{a}_{2}^{\dagger}(0) \hat{a}_{1}(0)\right\rangle \sin \frac{\Omega t}{2} \cos \frac{\Omega t}{2} .
\end{align*}
$$

Let us consider the particular case when the initial state of the system is a Dirac state, i.e. has a definite number of particles in each well; in this case only two first terms in the right hand part are different from zero: ${ }^{22}$

$$
\begin{equation*}
\left\langle N_{1}\right\rangle=N_{1}(0) \cos ^{2} \frac{\Omega t}{2}+N_{2}(0) \sin ^{2} \frac{\Omega t}{2} . \tag{8.103}
\end{equation*}
$$

For one particle, initially placed in either well, this gives us our old result (2.185) describing quantum oscillations of the particle between two wells with frequency $\Omega$. However, Eq. (103) is valid for any set of initial occupancies; let us use it. For example, starting from two particles, with initially one particle in each well, we get $\left\langle N_{1}\right\rangle=1$, regardless of time. So, the occupancies do not oscillate, and no experiment may detect the quantum oscillations, though their frequency $\Omega$ is still formally present in the time evolution equations. This fact may be interpreted as the simultaneous quantum oscillations of two particles exactly in anti-phase. For bosons, we can go to even larger occupancies by preparing the system, for example, in the state with $N_{1}(0)=N, N_{2}(0)=0$. Equation (103) says that in this case we see that the quantum oscillation amplitude increases $N$-fold; this is a particular manifestation of the general fact that bosons can be (and evolve in time) in the same quantum state. On the other hand, for fermions we cannot increase initial occupancies beyond 1 , so that the largest oscillation amplitude we can get is if we initially fill just one well.

[^722]The Dirac approach may be readily generalized to more complex systems. For example, an arbitrary system of quantum wells with weak tunneling coupling between the adjacent wells may be described by Hamiltonian

$$
\begin{equation*}
\hat{H}=\sum_{j} \varepsilon_{j} a_{j}^{\dagger} \hat{a}_{j}+\sum_{\left\langle j, j^{\prime}\right\rangle} \delta_{i j^{\prime}} a_{j}^{\dagger} \hat{a}_{j^{\prime}}+\text { h.c. } \tag{8.104}
\end{equation*}
$$

where symbol $\langle j, j\rangle\rangle$ means that the second sum is restricted to pairs of next-neighbor wells - see, e.g., Eq. (2.203) and its discussion. Note that this Hamiltonian is still a quadratic form of the creationannihilation operators, so the Heisenberg-picture equations of motion of these operators are linear, and its exact solutions, though possibly cumbersome, may be studied in detail. Due to this fact, Hamiltonian (104) is widely used for the study of some phenomena, for example the very interesting Anderson localization effect, in which a random distribution of eigenenergies $\varepsilon_{j}$ prevents particles within certain energy range from spreading to unlimited distances. ${ }^{23,24}$

### 8.4. Perturbative approaches

The situation becomes much more difficult if the problem requires an account of direct interactions between the particles. Let us assume that the interaction may be reduced to that between pairs - as it is the case at their Coulomb interaction ${ }^{25}$ and most other interactions, so that it may be described with the following "pair-interaction" Hamiltonian

$$
\begin{equation*}
\hat{U}_{\mathrm{int}}=\frac{1}{2} \sum_{\substack{k, k k^{\prime}=1 \\ k \neq k^{\prime}}}^{N} \hat{\mathrm{int}}\left(\mathbf{r}_{k}, \mathbf{r}_{k^{\prime}}\right) \tag{8.105}
\end{equation*}
$$

interaction Hamiltonian in two alternative forms
with the front factor of $1 / 2$ compensating the double-counting of each particle pair. The translation of this operator to the second-quantization form may be done absolutely similarly to the derivation of Eq. (77), and gives a similar (though naturally more bulky) result ${ }^{26}$

$$
\begin{equation*}
\hat{U}_{\mathrm{int}}=\frac{1}{2} \sum_{j, j^{\prime}, l, l^{\prime}} u_{i j^{\prime} l l^{\prime}} \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger}, \hat{a}_{l^{\prime}} \hat{a}_{l} \tag{8.106}
\end{equation*}
$$

where the two-particle matrix elements are defined similarly to Eq. (74):

$$
\begin{equation*}
u_{i j I^{\prime}} \equiv\left\langle\beta_{j} \beta_{j^{\prime}}\right| \hat{u}_{\mathrm{int}}\left|\beta_{l} \beta_{l^{\prime}}\right\rangle . \tag{8.107}
\end{equation*}
$$

Even in this case, the resulting Heisenberg equations of motion are nonlinear, so that solving them and calculating observables from the results is usually impossible, at least analytically. The only

[^723]case when some general results may be obtained is the weak interaction limit. In this case the unperturbed Hamiltonian contains only single-particle terms such as in Eqs. (71), so we can always (at least conceptually :-) find such a basis of orthonormal single-particle states $\beta_{j}$ in which that Hamiltonian is diagonal in the Dirac representation:
\[

$$
\begin{equation*}
\hat{H}^{(0)}=\sum_{j} \varepsilon_{j}^{(0)} \hat{a}_{j}^{\dagger} \hat{a}_{j} . \tag{8.108}
\end{equation*}
$$

\]

Now we can use Eq. (6.13) in this basis to calculate the interaction energy as a first-order perturbation:

$$
\begin{align*}
E_{\text {int }}^{(1)} & =\left\langle N_{1}, N_{2}, \ldots\right| \hat{U}_{\mathrm{int}}\left|N_{1}, N_{2}, \ldots\right\rangle=\frac{1}{2}\left\langle N_{1}, N_{2}, \ldots\right| \sum_{j, j^{\prime} l, l l^{\prime}} u_{j j^{\prime \prime l}} \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{l^{\prime}} \hat{a}_{l}\left|N_{1}, N_{2}, \ldots\right\rangle  \tag{8.109}\\
& =\frac{1}{2} \sum_{j, j^{\prime}, l, l^{\prime}} u_{\text {jjlll}}\left\langle N_{1}, N_{2}, \ldots\right| \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{l^{\prime}} \hat{a}_{l}\left|N_{1}, N_{2}, \ldots\right\rangle .
\end{align*}
$$

Since, according to Eqs. (81)-(82), the Dirac states with different occupancies are orthogonal, the last average yields nonvanishing results only for three particular subsets of the indices:
(i) $j \neq j^{\prime}, l=j$, and $l^{\prime}=j^{\prime}$. In this case the 4-operator product in Eq. (109) equals $\hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime}} \hat{a}_{j}$, and applying the commutation rules twice, we can bring it to the so-called normal ordering, with each creation operator standing to the right of the corresponding annihilation operator, thus forming the particle number operator (64):

$$
\begin{equation*}
\hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime}} \hat{a}_{j}= \pm \hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j} \hat{a}_{j^{\prime}}= \pm \hat{a}_{j}^{\dagger}\left( \pm \hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger}\right) \hat{a}_{j^{\prime}}=\hat{a}_{j}^{\dagger} \hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime}}=\hat{N}_{j} \hat{N}_{j^{\prime}} \tag{8.110}
\end{equation*}
$$

with the similar sign of the final result for bosons and fermions.
(ii) $j \neq j^{\prime}, l=j^{\prime}$, and $l^{\prime}=j$. In this case the 4-operator product equals $\hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j} \hat{a}_{j^{\prime}}$, and bringing it to the form $\hat{N}_{j} \hat{N}_{j^{\prime}}$ requires only one commutation:

$$
\begin{equation*}
\hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j} \hat{a}_{j^{\prime}}=\hat{a}_{j}^{\dagger}\left( \pm \hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger}\right) \hat{a}_{j^{\prime}}= \pm \hat{a}_{j}^{\dagger} \hat{a}_{j} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{j^{\prime}}= \pm \hat{N}_{j} \hat{N}_{j^{\prime}} \tag{8.111}
\end{equation*}
$$

with the upper sign for bosons and lower sign for fermions.
(iii) All indices equal to each other, giving $\hat{a}_{j}^{\dagger} \hat{a}_{j^{\prime}}^{\dagger} \hat{a}_{l} \hat{a}_{l}=\hat{a}_{j}^{\dagger} \hat{a}_{j}^{\dagger} \hat{a}_{j} \hat{a}_{j}$. For fermions, such operator (that "tries" to create or kill two particles in a row, in the same state) immediately gives the null vector. In the case of bosons, we may use Eq. (66) to commute the internal pair of operators, getting

$$
\begin{equation*}
\hat{a}_{j}^{\dagger} \hat{a}_{j}^{\dagger} \hat{a}_{j} \hat{a}_{j}=\hat{a}_{j}^{\dagger}\left(\hat{a}_{j} \hat{a}_{j}^{\dagger}-\hat{I}\right) \hat{a}_{j}=\hat{N}_{j}\left(\hat{N}_{j}-\hat{I}\right) \tag{8.112}
\end{equation*}
$$

Note, however, that this formula formally covers the fermion case as well (always giving zero). As a result, Eq. (109) may be rewritten in the following universal form:

$$
\begin{equation*}
E_{\mathrm{int}}^{(1)}=\frac{1}{2} \sum_{\substack{j, j^{\prime} \\ j \neq j^{\prime}}} N_{j} N_{j^{\prime}}\left(u_{j j j j^{\prime}} \pm u_{j j j^{\prime} j}\right)+\frac{1}{2} \sum_{j} N_{j}\left(N_{j}-1\right) u_{j j j j} \tag{8.113}
\end{equation*}
$$

Particle interaction: $1^{\text {st }}$-order energy perturbation

The consequences of this result are very different for bosons and fermions. In the former case, the last term usually dominates, because the matrix elements (107) are typically the largest when all basis functions coincide. Note that this term allows a very simple interpretation: the number of the diagonal matrix elements it sums up for each state $(j)$ is just the number of interacting particle pairs residing in that state.

In contrast, for fermions the last term is zero, and the interaction energy is the difference of two terms inside the first parentheses. In order to spell them out, let us consider the case when there is no direct spin-orbit interaction. Then vectors $|\beta\rangle_{j}$ of the single-particle state basis may be represented as products $|o\rangle_{j} \otimes|m\rangle_{j}$ of their orbital and spin orientation parts. (Here, for brevity, I am using $m$ instead of $m_{s}$.) For spin- $1 / 2$ particles (say, electrons), these orientations $m$ may equal only $+1 / 2$ and $-1 / 2$; in this case the spin part of the matrix element $u_{j j}{ }^{\prime j j}$, equals

$$
\begin{equation*}
\langle m| \otimes\left\langle m^{\prime} \| m\right\rangle \otimes\left|m^{\prime}\right\rangle \tag{8.114}
\end{equation*}
$$

where, as in the general Eq. (107), the position of a particular vector in a product codes the particle number. Now since spins of different electrons are defined in different Hilbert spaces, we may move their vectors around to get

$$
\begin{equation*}
\langle m| \otimes\left\langle m^{\prime} \| m\right\rangle \otimes\left|m^{\prime}\right\rangle=(\langle m \mid m\rangle)_{1} \times\left(\left\langle m^{\prime} \mid m^{\prime}\right\rangle\right)_{2}=1 \tag{8.115}
\end{equation*}
$$

for any pair of $j$ and $j^{\prime}$. On the other hand, $u_{j j^{\prime} j^{\prime} j}$ is proportional to

$$
\begin{equation*}
\langle m| \otimes\left\langle m^{\prime} \| m^{\prime}\right\rangle \otimes|m\rangle=\left(\left\langle m \mid m^{\prime}\right\rangle\right)_{1} \times\left(\left\langle m^{\prime} \mid m\right\rangle\right)_{2}=\delta_{m m^{\prime}} \tag{8.116}
\end{equation*}
$$

In this case, it is convenient to rewrite Eq. (113) in the coordinate representation, using singleparticle wavefunctions called spin-orbitals

functions

$$
\begin{equation*}
\psi_{j}(\mathbf{r}) \equiv\left\langle\mathbf{r} \mid \beta_{j}\right\rangle=\left\langle\mathbf{r} \mid o_{j}\right\rangle \otimes|m\rangle_{j} . \tag{8.117}
\end{equation*}
$$

They differ from the "usual" orbital wavefunctions of the type (5.19) only by that their index $j$ should be understood as the set of the orbital state index and the spin orientation index $m .{ }^{27}$ Also, due to the Pauliprinciple restriction of numbers $N_{j}$ to either 0 or 1, Eq. (113) may be also rewritten without the occupancy numbers, with the understanding that the summation is extended only over the pairs of occupied states. As a result, Eq. (113) becomes

[^724]\[
E_{\mathrm{int}}^{(1)}=\frac{1}{2} \sum_{\substack{j, j^{\prime}  \tag{8.118}<br>

j \neq j^{\prime}}} \int d^{3} r \int d^{3} r^{\prime}\left[$$
\begin{array}{l}
\psi_{j}^{*}(\mathbf{r}) \psi_{j^{\prime}}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{j}(\mathbf{r}) \psi_{j^{\prime}}\left(\mathbf{r}^{\prime}\right) \\
-\psi_{j}^{*}(\mathbf{r}) \psi_{j^{\prime}}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{j^{\prime}}(\mathbf{r}) \psi_{j}\left(\mathbf{r}^{\prime}\right)
\end{array}
$$\right]
\]

If, for a system of 2 electrons, we limit the summation to 2 states $\left(j, j^{\prime}=1,2\right)$, we get the result absolutely similar to Eqs. (44)-(45), with the minus sign in Eq. (44). Hence, Eq. (118) may be considered as the generalization of the direct and exchange interaction balance picture to an arbitrary number of orbitals and an arbitrary total number $N$ of electrons. Note, however, that this equation cannot

[^725]correctly describe the energy of the excited singlet state, corresponding to the plus sign in Eq. (44). ${ }^{28}$ The reason is that the description of entangled spin states, given by Eq. (19) and the last term of Eq. (21), require linear superpositions of different Dirac states, and hence not covered by our assumption (108).

Now comes a very important fact: the approximate result (118), added to the sum of unperturbed energies $\varepsilon_{j}^{(0)}$, equals the sum of exact eigenenergies of the so-called Hartree-Fock equation: ${ }^{29}$

$$
\begin{align*}
& \left(-\frac{\hbar^{2}}{2 m} \nabla^{2}+u(\mathbf{r})\right) \psi_{j}(\mathbf{r})  \tag{8.119}\\
& +\sum_{j^{\prime} \neq j} \int\left[\psi_{j^{\prime}}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{j}(\mathbf{r}) \psi_{j^{\prime}}\left(\mathbf{r}^{\prime}\right)-\psi_{j^{\prime}}^{*}\left(\mathbf{r}^{\prime}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{j^{\prime}}(\mathbf{r}) \psi_{j}(\mathbf{r})\right] d^{3} r^{\prime}=\varepsilon_{j} \psi_{j}(\mathbf{r}),
\end{align*}
$$

where $u(\mathbf{r})$ is the external-field potential acting on each particle separately - see Eq. (71). An advantage of this equation in comparison with Eq. (118) is that it allows the (approximate) calculation of not only the energy of the system, but also the corresponding spin-orbitals, taking into account the electronelectron interaction.

In the limit when the single-particle wavefunction overlaps are small and hence the exchange interaction is negligible, the last term in square brackets may be ignored, term $\psi_{j}(\mathbf{r})$ may be taken out of the integral, and becomes similar to the single-particle Schrödinger equation with the following effective potential

$$
\begin{equation*}
\left.u_{\mathrm{ef}}(\mathbf{r})=u(\mathbf{r})+u_{\mathrm{dir}}(\mathbf{r}), \quad u_{\mathrm{dir}}(\mathbf{r})=\sum_{j^{\prime} \neq j} \int_{j^{\prime}}^{*} \psi_{\mathbf{r}^{\prime}}^{*}\right) u_{\mathrm{int}}\left(\mathbf{r}, \mathbf{r}^{\prime}\right) \psi_{j^{\prime}}\left(\mathbf{r}^{\prime}\right) d^{3} r^{\prime} \tag{8.120}
\end{equation*}
$$

This is the so-called Hartree approximation - that gives reasonable results for some systems. ${ }^{30}$ However, in dense electrons systems (such as typical atoms, molecules, and condensed matter) the exchange interaction, described by the second term in the square brackets of Eq. (119), is typically of the order of $30 \%$ of the direct interaction, and frequently this effect cannot be ignored. In this case, Eq. (119) is an integro-differential rather than just differential equation.

There are efficient methods of numerical solution of such equations, typically based on iterative methods, though they require large memory and CPU-cycle resources even for systems of $\sim 10^{2}$ electrons. ${ }^{31}$ This is why the Hartree-Fock approximation is the de-facto baseline of all so-called ab-initio
${ }^{28}$ Note that due to condition $j^{\prime} \neq j$, and Eq. (116), the exchange interaction is limited to electron state pairs with the same spin direction - again in a good correspondence with the triplet states (like $\uparrow \uparrow$ or $\downarrow \downarrow$ ) of a two-electron system, in which the contribution of $E_{\text {ex }}(8.45 \mathrm{~b})$ to the total energy is also negative.
${ }^{29}$ This equation was suggested in 1929 by D. Hartree for the direct interaction, and extended to the exchange interaction by V. Fock in 1930. In order to verify its equivalence to Eq. (118), it is sufficient to multiply all terms of Eq. (119) by $\psi^{*}(\mathbf{r})$, integrate them over all $\mathbf{r}$ space (so that the right-hand part would give $\varepsilon_{j}$ ), and then sum these single-particle energies over all occupied states $j$.
${ }^{30}$ An extreme expression of the Hartree approximation is the very simple Thomas-Fermi model of heavy atoms (with the atomic number $Z \gg 1$ ), in which the gradient of the electrostatic potential is also neglected, i.e. the atomic electrons are treated essentially as an ideal Fermi gas - see SM Chapter 3.
${ }^{31}$ Surprisingly, this is sufficient to describe, with reasonable accuracy, many properties of condensed matter, by breaking it to similar elementary spatial cells (say, Bravais cells of crystals), with cyclic boundary conditions and a limited number of electrons in each cell.
("first-principle") calculations in condensed matter physics and quantum chemistry. ${ }^{32}$ In departures from this baseline, there are two opposite trends. For larger accuracy (and typically smaller systems), several "post-Hartree-Fock methods", notably including the configuration interaction method, ${ }^{33}$ that are more complex but may provide higher accuracy, have been developed.

There is also a strong opposite trend of extending ab-initio methods to larger systems, while sacrificing the result accuracy and reliability. This trend is currently dominated by the Density Functional Theory, ${ }^{34}$ universally known by its acronym DFT. In this approach, the equation solved for each eigenfunction $\psi_{j}(\mathbf{r})$ is a differential, Schrödinger-like Kohn-Sham equation

Kohn-
Sham
equation and its components
where

$$
\begin{equation*}
u_{\mathrm{dir}}^{\mathrm{KS}}(\mathbf{r})=-e \phi(\mathbf{r}), \quad \phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}} \int d^{3} r^{\prime} \frac{\rho\left(\mathbf{r}^{\prime}\right)}{\left|\mathbf{r}-\mathbf{r}^{\prime}\right|}, \quad \rho(\mathbf{r})=-e n(\mathbf{r}), \tag{8.122}
\end{equation*}
$$

and $n(\mathbf{r})$ is the total electron density in a particular point, calculated as

$$
\begin{equation*}
n(\mathbf{r}) \equiv \sum_{j} \psi_{j}^{*}(\mathbf{r}) \psi_{j}(\mathbf{r}) \tag{8.123}
\end{equation*}
$$

The effective exchange-correlation potential $u_{\mathrm{XC}}(\mathbf{r})$ (that differs from the genuine exchange potential, participating in Eq. (121), by the inclusion of the term with $j=j^{\prime}$ ) is calculated in various approximations, most valid only asymptotically in the limit when the electron number is high. The simplest of them is the Local Density Approximation (LDA) in which the effective exchange potential at each point is a function only of the electron density (123) at the same point, taken from the theory of a uniform gas of free electrons. ${ }^{35}$ Another simplification, that dramatically cuts the computing resources necessary for systems of relatively heavy atoms, is the exclusion of the filled internal electron shells (see Sec. 3.7) from the explicit calculations, because the shell states are virtually unperturbed by the valence electron effects involved in typical atomic phenomena and chemical reactions. In this approach, the Coulomb field of the shells, described by fixed, pre-calculated and tabulated pseudo-potentials, added to that of the nuclei. Unfortunately, because of lack of time, for details I have to refer the reader to specialized literature. ${ }^{36}$

[^726]Let me, however, emphasize that despite the wide use of the DFT, ${ }^{37}$ and its undisputable successes in describing some experimental data, it has problems. For me personally, its largest conceptual deficiency is the incorporation of the absolutely unphysical Coulomb interaction of an electron with itself (by dropping condition $j^{\prime} \neq j$ ). As a result, existing DFT packages require substantial artificial tinkering to use them for description of such processes as single-electron transfer. ${ }^{38} \mathrm{~A}$ little bit light-heartedly (but still correctly), one may say that an advanced DFT software package, run on a huge supercomputer, cannot be used to calculate the correct energy spectrum of a hydrogen atom - a century after this had been done by Niels Bohr on a slip of paper!

### 8.5. Quantum computation and cryptography

Now I have to review the emerging fields of quantum computation and encryption. ${ }^{39}$ These fields are currently the subject of a very intensive research effort, which has brought (besides much hype :-) a few results of genuine importance for quantum mechanics. My coverage, by necessity short, will emphasize these fundamental results, referring the reader interested in details to special literature. ${ }^{40}$ Because of the active stage of the fields, I will also provide quite a few references to recent publications, making the style of this section closer to a brief research review than to a part of a textbook.

Presently, the work on quantum computation and encryption is focused on systems of spatiallyseparated (and hence distinguishable) two-level systems - in this context, commonly called qubits. ${ }^{41}$ Due to this distinguishability, the issues that were the focus of the past few sections (including the benefits of the second quantization) are irrelevant here. On the other hand, systems of distinguishable qubits have some interesting properties that had not been yet discussed in this course.

First of all, a system of $N \gg 1$ qubits may contain much more information than the $N$ classical bits - which is the maximum information capacity of $N$ classical bistable systems. Indeed, according to the discussions in Chapter 4, an arbitrary pure state of a single qubit may be represented by its ket vector (4.37) - see also Eq. (5.1):

$$
\begin{equation*}
|\alpha\rangle_{N=1}=\alpha_{1}\left|u_{1}\right\rangle+\alpha_{2}\left|u_{2}\right\rangle, \tag{8.124}
\end{equation*}
$$

where $\{u\}$ is any orthonormal two-state basis. In the quantum information theory, it is natural and common to employ, as $u_{j}$, the eigenstates $a_{j}$ of the observable $A$ that is eventually measured in the particular physical implementation of the qubit - say, a certain spatial component of spin- $1 / 2$ particle, etc. It is also common to write the kets of these base states as $|0\rangle$ and $|1\rangle$, so that Eq. (124) takes the form ${ }^{42}$

[^727]Single qubit
state's representation

$$
\begin{equation*}
|\alpha\rangle_{N=1}=a_{0}|0\rangle+a_{1}|1\rangle=\sum_{j=0,1} a_{j}|j\rangle, \tag{8.125}
\end{equation*}
$$

where in the rest of this chapter, letter $j$ will be used to denote an integer equal to either 0 or 1 . Hence any pure state $\alpha$ of a qubit is completely defined by two complex $c$-numbers $a_{j}$, i.e. by 4 real numbers. Moreover, due to the normalization condition $\left|a_{1}\right|^{2}+\left|a_{2}\right|^{2}=1$, we need just 3 independent real numbers say, the Bloch sphere coordinates $\theta$ and $\varphi$ (see Fig. 5.1), plus the common phase $\gamma$, which becomes important when we consider coherent states of several qubits - see Eq. (5.3).

Now, if we have a system of 2 qubits, its arbitrary pure state (4.37) may be represented as a sum of $2^{2}=4$ terms, ${ }^{43}$

$$
\begin{equation*}
|\alpha\rangle_{N=2}=a_{00}|00\rangle+a_{01}|01\rangle+a_{10}|10\rangle+a_{11}|11\rangle \equiv \sum_{j_{1}, j_{2}=0,1} a_{j_{1} j_{2}}\left|j_{1} j_{2}\right\rangle, \tag{8.126}
\end{equation*}
$$

with 4 complex coefficients, i.e. $4 \times 2=8$ real numbers, subject to just one normalization condition ${ }^{44}$

$$
\begin{equation*}
\sum_{j_{1,2}=0,1}\left|a_{j_{1} j_{2}}\right|^{2}=1 \tag{8.127}
\end{equation*}
$$

An evident generalization of Eqs. (125)-(126) to an arbitrary pure state of an $N$-qubit system is given by a sum of $2^{N}$ terms:

$$
\begin{equation*}
|\alpha\rangle_{N}=\sum_{j_{1}, j_{2}, \ldots j_{N}=0,1} a_{j_{1} j_{2} \ldots j_{N}}\left|j_{1} j_{2} \ldots j_{N}\right\rangle, \tag{8.128}
\end{equation*}
$$

including all possible combinations of 0 s and 1 s inside the ket, so that the state is fully described by $2^{N}$ complex numbers, i.e. $2 \cdot 2^{N}=2^{N+1}$ real numbers, with only one constraint, similar to Eq. (127), imposed by the normalization condition. Let me emphasize that this exponential growth of the information contents would not be possible without the qubit state entanglement. Indeed, in the particular case when qubit states are unentangled (separable),

$$
\begin{equation*}
\left.|\alpha\rangle_{N}=\left|\alpha_{1}\right\rangle\left|\alpha_{2}\right\rangle \ldots \alpha_{N}\right\rangle \tag{8.129}
\end{equation*}
$$

where each $\left|\alpha_{n}\right\rangle$ is described by an equality similar to Eq. (125) with its individual expansion coefficients, the system state description requires only $3 N$ real numbers - e.g., $N$ sets $\{\theta, \varphi, \gamma\}$.

However, it is wrong (as it is sometimes done in popular reviews) to project this exponential growth of information contents directly on the capabilities of quantum computation, because this process has to include the output information readout, i.e. qubit state measurements. Due to the fundamental intrinsic uncertainty of quantum systems, the measurement of a single qubit even in a pure state (125) generally gives uncertain results, with probabilities $W_{0}=\left|a_{0}\right|^{2}$ and $W_{1}=\left|a_{1}\right|^{2}$. In order to comply with the general notion of digital computation, a quantum computer has to provide certain (or

[^728]virtually certain) results, and hence probabilities $W_{j}$ have to be very close to either 0 or 1 , so that before the measurement, each qubit has to be in a basis state - either 0 or 1 . This means that the computational system of $N$ qubits, just before the final readout, has to be one of the basis states
\[

$$
\begin{equation*}
\left.|\alpha\rangle_{N}=\left|j_{1}\right\rangle\left|j_{2}\right\rangle \ldots j_{N}\right\rangle \equiv\left|j_{1} j_{2} \ldots j_{N}\right\rangle, \tag{8.130}
\end{equation*}
$$

\]

which is a very small subset even of the set (129) of all unentangled states, and whose maximum information contents in just $N$ classical bits.

Now the reader may start thinking that this constraint strips quantum computations of any advantages over their classical counterparts, but this view is also superficial. In order to show that, let us consider the scheme of the most frequently explored type of quantum computation, shown in Fig. 2.45


Fig. 8.2. The baseline scheme of quantum computation.

Here each horizontal line (sometimes called a "wire"46) corresponds to a single qubit, tracing its time evolution in the same direction as at the usual time function plots: from left to right. This means that the left column $|\alpha\rangle_{\text {in }}$ of ket-vectors describes the initial state of qubits, ${ }^{47}$ while the right column $|\alpha\rangle_{\text {out }}$ describes their final (pre-detector) state. The box labeled $U$ represents the qubit evolution in time due to

[^729]their specially arranged interactions between each other and/or external drive "forces". Besides these forces, during this evolution the system is supposed to be isolated from the dephasing and energydissipating environment, so that it may be described by a unitary operator defined in the $2^{N}$-dimensional Hilbert space of $N$ qubits:
\[

$$
\begin{equation*}
|\alpha\rangle_{\text {out }}=\hat{U}|\alpha\rangle_{\text {in }} \tag{8.131}
\end{equation*}
$$

\]

With the condition that the input and output states have the simple form (130), this equality reads

$$
\begin{equation*}
\left|\left(j_{1}\right)_{\text {out }}\left(j_{2}\right)_{\text {out }} \ldots\left(j_{N}\right)_{\text {out }}\right\rangle=\hat{U}\left|\left(j_{1}\right)_{\text {in }}\left(j_{2}\right)_{\text {in }} \ldots\left(j_{N}\right)_{\text {in }}\right\rangle \tag{8.132}
\end{equation*}
$$

The art of quantum computer design is selecting such unitary operators $\hat{U}$ that would:

- satisfy Eq. (132),
- be physically implementable,
- enable substantial performance advantages of the quantum computation over its classical counterpart of similar functionality, at least for some digital functions (algorithms).

I will have time to demonstrate the possibility of such advantages on just one, perhaps the simplest example - the so-called Deutsch problem. ${ }^{48}$ Let us consider the family of single-bit classical Boolean functions $j_{\text {out }}=f\left(j_{\text {in }}\right)$. Since both $j$ are Boolean variables, i.e. may take only values 0 and 1 , there are evidently only 4 such functions:

| $f$ | $f(0)$ | $f(1)$ | class | $F$ | $f(1)-f(0)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $f_{1}$ | 0 | 0 | constant | 0 | 0 |
| $f_{2}$ | 0 | 1 | balanced | 1 | 1 |
| $f_{3}$ | 1 | 0 | balanced | 1 | -1 |
| $f_{4}$ | 1 | 1 | constant | 0 | 0 |

Of them, functions $f_{1}$ and $f_{4}$, whose values are independent of their arguments, are called constants, while functions $f_{2}$ (called "YES" or "IDENTITY") and $f_{3}$ ("NOT" or "INVERSION") are called balanced. The Deutsch problem is to determine the class of a single-bit function, implemented as a "black box", as being either constant or balanced, using just one experiment.

Classically, this is clearly impossible, and the simplest way to perform the function classification involves two similar black boxes $f$ - see Fig. 3a.


Fig. 8.3. The simplest (a) classical and (b) quantum ways to classify a single-bit Boolean function $f$.

[^730]This solution uses the so-called exclusive-OR (for short, XOR) gate whose output is described by the following function $F$ of its two Boolean arguments $j_{1}$ and $j_{2}$ :

$$
F\left(j_{1}, j_{2}\right) \equiv j_{1} \oplus j_{2} \equiv\left\{\begin{array}{lll}
0, & \text { if } j_{1}=j_{2}  \tag{8.134}\\
1, & \text { if } & j_{1} \neq j_{2}
\end{array}\right.
$$

In the circuit shown in Fig. 3a, the gate produces output

$$
\begin{equation*}
F=f(0) \oplus f(1), \tag{8.135}
\end{equation*}
$$

equal to 1 if $f(0) \neq f(1)$, i.e. if function $f$ is balanced, and 0 in the opposite case - see the $4^{\text {th }}$ column in Eq. (133). ${ }^{49}$

On the other hand, let us assume that all four functions $f$ may be implemented quantummechanically, for example as a unitary transform acting on two qubits (Fig. 4a), and acting as follows each of basis components $\left.\left|j_{j_{2}}\right\rangle \equiv\left|j_{1}\right\rangle j_{2}\right\rangle$ of the general input state (126):

$$
\begin{equation*}
\hat{f}\left|j_{1}\right\rangle\left|j_{2}\right\rangle=\left|j_{1}\right\rangle\left|j_{2} \oplus f\left(j_{1}\right)\right\rangle, \tag{8.136}
\end{equation*}
$$

where $f$ is any of the classical Boolean functions defined by Eq. (133).
(a)


Fig. 8.4. Two-qubit quantum gates: (a) two-qubit function $f$ and (b) its particular case $C$ (CNOT), and their actions on the basis states.

In the particular case when $f$ is the YES function: $f(j)=f_{2}(j)=j$, gate $f$ is reduced to the socalled CNOT gate - a key ingredient of other quantum computation schemes, performing transform

$$
\begin{equation*}
\hat{C}\left|j_{1} j_{2}\right\rangle=\left|j_{1}\right\rangle\left|j_{2} \oplus j_{1}\right\rangle \tag{8.137a}
\end{equation*}
$$

Let us spell out this rule for all four possible input qubit combinations:

$$
\begin{equation*}
\hat{C}|00\rangle=|00\rangle, \quad \hat{C}|01\rangle=|01\rangle, \quad \hat{C}|10\rangle=|11\rangle, \quad \hat{C}|11\rangle=|10\rangle . \tag{8.137b}
\end{equation*}
$$

In plain English, this means that acting on basis states $\left\langle j_{j} j_{2}\right\rangle$, the CNOT gate leaves the state of first, source qubit (shown by the upper lines in Fig. 4) intact, but flips the state of the second, target qubit if the first one is in the basis state $|1\rangle$. In even simpler words, the state $j_{1}$ of the source qubit controls the NOT function acting on the target qubit - hence the gate's name CNOT (the semi-acronym of "Controlled NOT").

[^731]For the quantum function (136), the Deutsch problem may be solved within the general scheme shown in Fig. 2, with the particular structure of the unitary-transform box $U$ spelled out in Fig. 3b, which involves just one implementation of the function. Here the singe-qubit quantum gate it symbolizes the so-called Hadamard (or "Walsh-Hadamard") transform" ${ }^{50}$ whose linear operator is defined by the following actions on qubit's basis states:

Hadamard transform

$$
\begin{equation*}
\hat{\forall}|0\rangle=\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle), \quad \hat{\lambda}|1\rangle=\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle), \tag{8.138}
\end{equation*}
$$

- see also the 4 left state labels in Fig. $3 b .{ }^{51}$ On the Bloch sphere (Fig. 5.1), and in the usual spin- $1 / 2$ notation, Eqs. (138) correspond to the transfer of the representing point from the North Pole's state $\uparrow$, i.e. one of the eigenstates of matrix $\sigma_{z}$, to one of equatorial states, $\rightarrow$, i.e. one of the eigenstates of matrix $\sigma_{x}$, and from the South Pole state $\downarrow$ to the another equatorial state, $\leftarrow$, see Eq. (4.122). However, a $\pi / 2$-rotation in the $[x, z]$ plane would be a poor interpretation of this function. Indeed, since its operator has to be linear (to be physically realistic), it needs to perform action (138) on the basis states even when they are parts of an arbitrary linear superposition - as they are, e.g., for the two right Hadamard gates in Fig. 3b. For example, as immediately follows from Eq. (137) and operator's linearity,

$$
\begin{equation*}
\hat{\mathcal{H}}(\hat{\nexists H}|0\rangle)=\hat{\mathcal{H}^{\prime}}\left(\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)\right)=\frac{1}{\sqrt{2}} \hat{\mathcal{H}}\left(|0\rangle+\hat{\mathcal{H}^{\prime}}|1\rangle\right)=\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)+\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\right)=|0\rangle, \tag{8.139a}
\end{equation*}
$$

Absolutely similarly, we may get ${ }^{52}$

$$
\begin{equation*}
\hat{\mathcal{H}}(\hat{\forall X}|1\rangle)=|1\rangle . \tag{8.139b}
\end{equation*}
$$

Due to this reason, a better interpretation of the Hadamard transform is a $\pi$-rotation about the axis that bisects the angle between axes $x$ and $z$.

Now let us carry out an analysis of the "circuit" shown in Fig. 3b, minding all the time the operator linearity, and the fact that the transformation rules (136)-(138) are only applicable to basis kets of the initial ("input") state vector. In particular, taking into account that according to Fig. 3b, the input states of gate $f$ in this particular circuit are described by Eqs. (138), its output state's ket is

$$
\begin{equation*}
\hat{f}(\hat{z}|0\rangle \hat{\vec{f}}|1\rangle)=\hat{f}\left(\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle) \frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)\right)=\frac{1}{2}(\hat{f}|00\rangle-\hat{f}|01\rangle+\hat{f}|10\rangle-\hat{f}|11\rangle) . \tag{8.140}
\end{equation*}
$$

Now we may apply Eq. (136) to each of the basis kets to get:

$$
\begin{align*}
\hat{f}|00\rangle-\hat{f}|01\rangle+\hat{f}|10\rangle-\hat{f}|11\rangle & \equiv \hat{f}|0\rangle|0\rangle-\hat{f}|0\rangle|1\rangle+\hat{f}|1\rangle|0\rangle-\hat{f}|1\rangle|1\rangle \\
& =|0\rangle|0 \oplus f(0)\rangle-|0\rangle|1 \oplus f(0)\rangle+|1\rangle|0 \oplus f(1)\rangle-|1\rangle|1 \oplus f(1)\rangle  \tag{8.141}\\
& =|0\rangle(|0 \oplus f(0)\rangle-|1 \oplus f(0)\rangle)+|1\rangle(|0 \oplus f(1)\rangle-|1 \oplus f(1)\rangle) .
\end{align*}
$$

[^732]Note that the expression in the first parentheses, characterizing the state of the target qubit, is equal to $(|0\rangle-|1\rangle) \equiv(-1)^{0}(|0\rangle-|1\rangle)$ if $f(0)=0($ and hence $0 \oplus f(0)=0$ and $1 \oplus f(0)=1)$, and to $(|1\rangle-|0\rangle) \equiv(-1)^{1}(|0\rangle-$ $|1\rangle$ ) in the opposite case $f(0)=1$, so that both cases may be described in one shot by rewriting the parentheses as $(-1)^{f(0)}(|0\rangle-|1\rangle)$. The second parentheses is absolutely similarly controlled by the value of $f(1)$, so that the state of the system at the output of gate $f$ is unentangled again:

$$
\begin{equation*}
\hat{f}\left(\hat{y}|0\rangle \hat{X_{X}}|1\rangle\right)=\frac{1}{2}\left((-1)^{f(0)}|0\rangle+(-1)^{f(1)}|1\rangle\right)(|0\rangle-|1\rangle)= \pm \frac{1}{\sqrt{2}}\left(|0\rangle+(-1)^{F}|1\rangle\right) \frac{1}{\sqrt{2}}(|0\rangle-|1\rangle), \tag{8.142}
\end{equation*}
$$

where the last transition has used the fact that the Boolean function $F$, defined by Eq. (135), equals to $\pm[f(1)-f(0)]$ - compare the last two columns in Eq. (133). Since the common sign (i.e. the common phase shift by $\pi$ ) is inconsequential, it may be prescribed to any of the component ket-vectors - for example to that of the target qubit, as shown by the third pair of state labels in Fig. 3b.

This intermediate result is already rather remarkable. Indeed, it shows that, despite the impression one could get from Fig. 4, gates $f$ and even $C$, being "controlled" by the source qubit, may change that qubit's state as well! This fact (partly reflected by the vertical direction of the control lines in Figs. 3, 4, symbolizing the same stage of system's evolution in time) shows how careful one should be interpreting quantum-computational "circuits".

At the second stage of the circuit shown in Fig. 3b, the qubit components of state (142) are fed into one more pair of Hadamard gates, whose outputs therefore are

Now using Eqs. (138) again, we see that the output state ket-vectors of the source and target qubits are, respectively,

$$
\begin{equation*}
\frac{1+(-1)^{F}}{2}|0\rangle+\frac{1-(-1)^{F}}{2}|1\rangle, \quad \text { and } \pm|1\rangle \tag{8.144}
\end{equation*}
$$

Since, according to Eq. (135), the Boolean function $F$ may take only values 0 or 1, the final state of the source qubit is always one of its basis states $j$, namely the one with $j=F$. Its measurement (see Fig. 2) immediately tells us whether function $f$, participating in Eq. (136), is constant or balanced. ${ }^{53}$

Thus, the quantum circuit shown in Fig. 3b indeed solves the Deutsch problem in one shot. Reviewing our analysis, we may see that this is possible because the unitary transform performed by gate $f$ is applied to quantum superpositions (138) rather than to the basis states. Due to this trick, the quantum state components depending on $f(0)$ and $f(1)$ are processed simultaneously, in parallel. This quantum parallelism may be extended to circuits with many ( $N \gg 1$ ) qubits and, for some tasks, provide a dramatic performance increase - for example, reducing the necessary circuit component number from $O(\exp \{N\})$ to $O\left(N^{p}\right)$, where $p$ is a finite (and not very big) number.

[^733]However, this efficiency comes at a high price. Indeed, let us discuss the physical implementation of quantum gates, starting from the Hadamard gate, which performs a single-qubit transform - see Eq. (138). With the linearity requirement, its action on the arbitrary state (125) should be

$$
\begin{equation*}
\hat{\mathcal{H}}|\alpha\rangle=a_{0} \hat{\forall}|0\rangle+a_{1} \hat{\mathcal{H}}|1\rangle=a_{0} \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)+a_{1} \frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)=\frac{1}{\sqrt{2}}\left(a_{0}+a_{1}\right)|0\rangle+\frac{1}{\sqrt{2}}\left(a_{0}-a_{1}\right)|1\rangle, \tag{8.145}
\end{equation*}
$$

meaning that the state expansion coefficients in the end $(t=T)$ and beginning $(t=0)$ of the qubit evolution in time have to be related as

$$
\begin{equation*}
a_{0}(T)=\frac{a_{0}(0)+a_{1}(0)}{\sqrt{2}}, \quad a_{1}(T)=\frac{a_{0}(0)-a_{1}(0)}{\sqrt{2}} \tag{8.146}
\end{equation*}
$$

This task may be again performed using the Rabi oscillations, which were discussed in Sec. 6.5, i.e. by applying to the qubit (a two-level system), for a limited time period $T$, a weak sinusoidal external signal of frequency $\omega$ equal to the intrinsic quantum oscillation frequency $\omega_{n n}$, defined by Eq. (6.85). A perturbative analysis of the Rabi oscillations was carried out in Sec. 6.5, even for nonvanishing (though small) detuning $\Delta=\omega-\omega_{n n}$, but only for the particular initial conditions when at $t=0$ the system was in one on the basis states (there labeled as $n$ '), i.e. another state (there labeled $n$ ) was empty. For our current purposes we need to find coefficients $a_{0,1}(t)$ of expansion (125) for arbitrary initial conditions $a_{0,1}(0)$, subject only to the time-independent normalization condition $\left|a_{0}\right|^{2}+\left|a_{1}\right|^{2}=1$. For the case of exact tuning, $\Delta=0$, the solution of Eqs. (6.94) is elementary, and gives, instead of Eq. (6.102), ${ }^{54}$ the following solutions:

$$
\begin{align*}
& a_{0}(t)=a_{0}(0) \cos \Omega t-i a_{1}(0) e^{i \varphi} \sin \Omega t \\
& a_{1}(t)=a_{1}(0) \cos \Omega t-i a_{0}(0) e^{-i \varphi} \sin \Omega t \tag{8.147}
\end{align*}
$$

where $\Omega$ is the Rabi oscillation frequency (6.101), in the exact-tuning case proportional to amplitude $|A|$ of the external rf drive $A=|A| \exp \{i \varphi\}$, while $\varphi$ is the phase of the driving signal - see Eqs. (6.86)(6.87). Comparing these expressions with Eqs. (146), we see that for $t=T=\pi / 4 \Omega$ and $\varphi=\pi / 2$ they "almost" coincide, besides the opposite sign of $a_{1}(T)$.

Conceptually the simplest way to correct this deficiency is to follow the rf " $\pi / 4$-pulse", just discussed, by a short dc " $\pi$-pulse" of duration $T$ " $=\pi / \delta$, which temporary creates an small additional energy difference $\delta$ between basis states 0 and 1. According to the basic Eq. (1.61), such difference creates an additional phase difference $T$ ' $\delta / \hbar$ between the states, equal to $\pi$ for the " $\pi$-pulse".

Another way (that may be also useful for two-qubit operations) is to use another, auxiliary energy level $E_{2}$ whose distances from the basic levels $E_{1}$ and $E_{0}$ are significantly different from the difference $\left(E_{1}-E_{0}\right)$ - see Fig. 5a. In this case, the weak external rf field tuned to any of 3 potential quantum transition frequencies $\omega_{n n^{\prime}} \equiv\left(E_{n^{-}} E_{n^{\prime}}\right) / \hbar$ initiates such transitions between the corresponding states only, with a negligible perturbation of the state not involved in this transition. Such transitions may be again described by Eqs. (147), with the appropriate index changes. For the Hadamard transform implementation, it is sufficient to apply (after the already discussed $\pi / 4$-pulse of frequency $\omega_{10}$, and with

[^734]the initially empty level $E_{2}$ ), an additional $\pi$-pulse of frequency $\omega_{20}$, with any phase $\varphi$. Indeed, according to the first of Eqs. (147), with the due replacement $a_{1}(0) \rightarrow a_{2}(0)=0$, such pulse flips the sign of coefficient $a_{0}(t)$, while coefficient $a_{1}(t)$, not involved in this additional transition, remains unchanged.

(a)
(b)

(c)


Fig. 8.5. Energy-level schemes used for unitary transformations of (a) single qubits and (b, c) two-qubit systems.

Now let me describe the conceptually simplest (though, for some qubit types, not practically most convenient) scheme for the implementation of the CNOT gate, whose action is described by a linear unitary operator satisfying Eq. (137). For that, evidently, qubits have to let interact for some time $T$. As was repeatedly discussed in two past chapters, in most cases such interaction of two subsystems is bilinear - see, e.g., Eq. (6.148). For qubits, i.e. two-level systems, each of the component operators may be represented by a $2 \times 2$ matrix in the basis of states 0 and 1 . According to Eq. (4.105), such matrix may be expressed as a linear combination $\left(c_{0} I+\mathbf{c} \cdot \sigma\right)$, where $c_{0}$ and three Cartesian components of vector $\mathbf{c}$ are $c$-numbers. Let us take such bilinear interaction Hamiltonian in the simplest form

$$
\hat{H}_{\mathrm{int}}(t)=\left\{\begin{array}{cc}
\kappa \hat{\sigma}_{z}^{(1)} \hat{\sigma}_{z}^{(2)}, & \text { for } 0<t<T  \tag{8.148}\\
0, & \text { otherwise }
\end{array}\right.
$$

where the upper index is the qubit number, and $\kappa$ is a $c$-number constant. ${ }^{55}$ According to Eq. (4.175), by the end of the interaction period, this Hamiltonian produces the following unitary transform:

$$
\begin{equation*}
\hat{U}_{\mathrm{int}}=\hat{I} \exp \left\{-\frac{i}{\hbar} \hat{H}_{\mathrm{int}} T\right\}=\hat{I} \exp \left\{-\frac{i}{\hbar} \kappa \hat{\sigma}_{z}^{(1)} \hat{\sigma}_{z}^{(2)} T\right\} \tag{8.149}
\end{equation*}
$$

Since in the basis of unperturbed two-bit states $\left|j_{1} j_{2}\right\rangle$ the product operator $\hat{\sigma}_{z}^{(1)} \hat{\sigma}_{z}^{(2)}$ is diagonal, so is the unitary operator (149), with the following action on the basis states:

$$
\begin{equation*}
\hat{U}_{\mathrm{int}}\left|j_{1} j_{2}\right\rangle=\exp \left\{i \theta \sigma_{z}^{(1)} \sigma_{z}^{(2)}\right\}\left|j_{1} j_{2}\right\rangle, \tag{8.150}
\end{equation*}
$$

[^735]where $\theta \equiv-\kappa T / \hbar$, and $\sigma_{z}$ are the eigenvalues of the Pauli matrix $\sigma_{z}$ for the basis states of the corresponding qubit: $\sigma_{z}=+1$ for $|j\rangle=|0\rangle$, and $\sigma_{z}=-1$ for $|j\rangle=|1\rangle$. Let me, for clarity, spell out Eq. (150) for the particular case $\theta=-\pi / 4$ (corresponding to the qubit coupling time $T=\pi \hbar / 4 \kappa$ ):
\[

$$
\begin{equation*}
\hat{U}_{\mathrm{int}}|00\rangle=e^{-i \pi / 4}|00\rangle, \quad \hat{U}_{\mathrm{int}}|01\rangle=e^{i \pi / 4}|01\rangle, \quad \hat{U}_{\mathrm{int}}|10\rangle=e^{i \pi / 4}|10\rangle, \quad \hat{U}_{\mathrm{int}}|11\rangle=e^{-i \pi / 4}|11\rangle . \tag{8.151}
\end{equation*}
$$

\]

In order to compensate the undesirable parts of this joint phase shift of the basis states, let us apply (either before or after it) similar individual "rotations" of each qubit by angle $\theta$ ' $=+\pi / 4$, using the following product of two independent operators, plus (just for the result clarity) a common, and hence inconsequential, phase shift $\theta^{\prime \prime}=-\pi / 4:^{56}$

$$
\begin{equation*}
\hat{U}_{\mathrm{com}}=\hat{I} \exp \left\{i \theta^{\prime}\left(\hat{\sigma}_{z}^{(1)}+\hat{\sigma}_{z}^{(2)}\right)+i \theta^{\prime \prime}\right\}=\hat{I} \exp \left\{i \frac{\pi}{4} \hat{\sigma}_{z}^{(1)}\right\} \exp \left\{i \frac{\pi}{4} \hat{\sigma}_{z}^{(2)}\right\} \exp \left\{-i \frac{\pi}{4}\right\} \tag{8.152}
\end{equation*}
$$

Since this operator is also diagonal in the $\left\langle j_{1} j_{2}\right\rangle$ basis, it is equally easy to calculate the change of the basis states by the total unitary operator $\hat{U}_{t} \equiv \hat{U}_{\text {com }} \hat{U}_{\text {int }}$ :

$$
\begin{equation*}
\hat{U}_{t}|00\rangle=|00\rangle, \quad \hat{U}_{t}|01\rangle=|01\rangle, \quad \hat{U}_{t}|10\rangle=|10\rangle, \quad \hat{U}_{t}|11\rangle=-|11\rangle . \tag{8.153}
\end{equation*}
$$

This result already shows the main "miracle action" of two-qubit gates, such as shown in Fig. 4: the source qubit is left intact (only if it is in a basis state!), while the state of the target qubit is altered. True, this is still different from the CNOT operator's action (137), but may be readily reduced to it by its sandwiching of transform $U_{t}$ between two Hadamard transforms applied to the target qubit:

$$
\begin{equation*}
\hat{C}=\frac{1}{2} \hat{\mathcal{H}}^{(2)} \hat{U}_{t} \hat{\mathcal{H}}^{(2)} . \tag{8.154}
\end{equation*}
$$

We have spend quite a bit of time on the discussion of the CNOT gate, ${ }^{57}$ and now I can reward the reader for his/her effort with a bit of good news: it has been proved that an arbitrary unitary transform that satisfies Eq. (132), i.e. may be used within the general scheme outlined in Fig. 2, may be decomposed into a set of CNOT gates mixed with simpler single-qubit gates - for example, the Hadamard gate plus the $\pi / 2$ rotation discussed above. ${ }^{58}$ Unfortunately, I have no time for a detailed discussion of more complex circuits. ${ }^{59}$ Perhaps the most famous of them is the scheme for integer

[^736]number factoring, suggested in 1994 by P. Shor. ${ }^{60}$ Due to its potential practical importance for breaking broadly used communication encryption schemes such as the RSA code, ${ }^{61}$ this opportunity has incited a huge wave of enthusiasm, and triggered experimental efforts to implement quantum gates and circuits using a broad variety of two-level quantum systems. Presently, the following options are most eagerly pursued: ${ }^{62}$
(i) Trapped ions. The first experimental demonstrations of quantum state manipulation (including the already mentioned first CNOT gate) have been carried out using deeply cooled atoms in optical traps, similar to those used in frequency and time standards. Their electron spins are natural qubits, whose states may be manipulated using the Rabi transfers excited by suitably tuned lasers. The spin interactions with environment may be very weak, resulting in large dephasing times ( $T_{2}$, see Sec. 7.3), up to a few seconds. Since the distances between atoms in the traps are relatively large (of the order of a micron), their direct spin-spin interaction is even weaker, but atoms may be made effectively interacting either via their mechanical oscillations about the potential minima of the trapping field, or via photons in electromagnetic resonators ("cavities"). ${ }^{63}$ Perhaps the main challenge of using this approach for quantum computation is poor "scalability", i.e. the enormous challenge of creating large, ordered systems of individually addressable qubits.
(ii) Nuclear spins are also typically very weakly connected to environment, with $T_{2}$ exceeding 10 seconds in some cases. Their eigenenergies $E_{0}$ and $E_{1}$ may be split by external dc magnetic fields (typically, of the order of 10 T ), while the interstate Rabi transfers may be readily achieved by application of external rf fields with frequencies $\omega=\left(E_{1}-E_{0}\right) / \hbar$ of a few hundred $\mathrm{MHz} .{ }^{64}$ The challenges of this option include the weakness of spin-spin interactions (typically mediated through molecular electrons), resulting in a very slow spin evolution, whose time scale $\hbar / \kappa$ may become comparable with $T_{2}$, and small level separations $E_{1}-E_{0}$, corresponding to a few K, ${ }^{65}$ i.e. much smaller than the room temperature, creating a problem with qubit state preparation. ${ }^{66}$

Despite these challenges, the nuclear spin option was used for the first implementation of the Shor algorithm for factoring of a small number $(15=5 \times 3)$ as early as in $2001 .{ }^{67}$ However, the extension of this success to larger systems, beyond the set of spins inside one molecule, is problematic.
(iii) Josephson-junction devices. Much better scalability may be achieved with solid state devices, especially in superconductor integrated circuits including weak contacts - Josephson junctions. As was already discussed in Sec. 2.8, if the coupling of a Josephson junction to its dissipative environment is sufficiently weak (in particular if its effective parallel resistance is much higher than the

[^737]quantum resistance unit $R_{Q} \sim 10^{4} \Omega$ ), the Josephson phase variable $\varphi$ behaves as a coordinate of a 1D quantum particle with effective mass (2.252), moving in a $2 \pi$-periodic potential - see Eq. (2.250). This fact creates several opportunities for qubit implementation using quantum behavior of this macroscopic degree of freedom.

In an insulated junction, ${ }^{68}$ the phase motion in the periodic potential $U(\varphi)=-E_{j} \cos \varphi$ creates the energy band structure $E(q)$ that was discussed in detain in Sec. 2.7. In particular, in the weak potential limit (which, for the Josephson junction case, is valid at $E_{J} \ll e^{2} / 2 C-$ see the discussion in Sec. 2.8), the lowest bandgaps are very narrow, and function $E(q)$ in their vicinity is well described by the usual level anticrossing - see Figs. 2.28 and 2.29 and their discussion. The translation of this fact to the Josephson junction language (see, in particular, Eq. (2.256) and its discussion) shows that the values of the effective electric charge $Q$ of the junction, on two anticrossing energy branches, differ by charge $2 e$ of one Cooper pair. Since, according to Eq. (2.222) and its discussion, the system dynamics in this case is reduced to the interaction of these two states with different $Q$, in application to quantum computation this system is called the charge qubit. Unfortunately, the states of such qubit are rather sensitive to random charged impurities in junction's vicinity, causing strong fluctuations, and hindering its control, so this option is not actively pursued nowadays.

Other options are based on the modification of potential $U(\varphi)$ at Josephson junction incorporation into superconducting loops, i.e. in SQUIDs. ${ }^{69}$ In the simplest case of a single loop of inductance $L$ closed by one junction with critical current $I_{C}$, the total potential energy of the system in an external magnetic field is ${ }^{70}$

$$
\begin{equation*}
U(\varphi)=E_{J}\left[\frac{\left(\varphi-\varphi_{\mathrm{ext}}\right)^{2}}{2 \beta_{L}}-\cos \varphi\right], \quad \text { with } E_{J}=\frac{\hbar I_{C}}{2 e}, \beta_{L} \equiv \frac{4 e I_{C} L}{\hbar}, \tag{8.155}
\end{equation*}
$$

where $\varphi_{\text {ext }}$ is proportional to the external magnetic flux $\Phi_{\text {ext }}$ through the loop. According to this relation, at $E_{J} \gg e^{2} / 2 C$ (corresponding to the tight-binding limit of the energy band theory), one convenient way to implement a two-level system is to take the dimensionless inductance parameter $\beta_{L}$ above but very close to $1\left(0<\beta_{L}-1 \ll 1\right)$, the "symmetrizing" magnetic field ( $\varphi_{\mathrm{ext}} \approx \pi$ ), and $E_{J} \approx\left(e^{2} / C\right) /\left(\beta_{L}-1\right)^{3}$. In this case, the potential profile has the shape of a nearly symmetrical double well, with ground states in each well coupled by tunneling through a relatively low tunnel barrier, creating a pair of eigenstates with relatively low eigenenergy splitting $\Delta=E_{1}-E_{0} \ll E_{J}$ (Fig. 6a).
(a)

(b)


Fig. 8.6. Typical potential profiles and energy levels of SQUID-based qubits: (a) "flux qubit" and (b) "phase qubit". Red dashed lines show eigenenergies of the used states 0 and 1 .

[^738]Such flux qubits have a relatively large magnitude $\left|\Phi_{10}\right|=\left|\Phi_{01}\right|$ of the matrix elements of the operator of magnetic flux $\Phi=(\hbar / 2 e) \varphi$ piercing the SQUID loop. This certainly makes the arrangement of necessary coupling between flux qubits (see, e.g., Eq. (149) and its discussion) very easy, despite the macroscopic $(\sim 10 \mu \mathrm{~m})$ sizes of SQUIDs and hence of the distances between them, decreasing the time $T$ $\sim \hbar / \kappa$ necessary for the most critical two-bit (e.g., CNOT) operations, to a just few nanoseconds. However, the large flux matrix elements also increase the undesirable coupling of such qubits to dephasing environment, and hence decrease dephasing time $T_{2}$ - typically, to just a few tens or hundreds nanoseconds, uncomfortably close to $T$.

This coupling may be decreased, leading to a substantial increase of $T_{2}$ (up to a few microseconds) by moving the bias phase $\varphi_{\text {ext }}$ away from the symmetrizing value $\pi$, i.e. using the asymmetric potential profile sketched in Fig. 6b. The working states 0 and 1 of such phase qubit, localized in a higher potential well (shown left in Fig. 6b), are actually metastable, but with a very long lifetime because of the relatively high barrier separating the wells. An additional benefit of this arrangement is that a fast lowering of the tunnel barrier causes the system in state 1 to tunnel into the lower well, with the sequential energy relaxation (see the arrows in Fig. 6b); this process be used for qubit state readout. A major problem of phase qubits is that the part of potential $U(\varphi)$, in which qubit states are localized, is almost quadratic, so that the energy levels are nearly equidistant - cf. Eqs. (2.114), (6.15), and (6.22). ${ }^{71}$ As a result, the external rf drive of frequency $\omega=\left(E_{1}-E_{0}\right) / \hbar$, used to arrange the state transforms described by Eq. (146), may induce simultaneous undesirable transitions to (and between) higher energy levels. This effect may be mitigated by the rf drive amplitude reduction (see Problem 6.6), but at a price of the proportional increase of transfer time $T$, that may again become comparable to $T_{2}$. Despite this problem, phase qubits have been used for a successful experimental demonstration of the core single-operand and two-operand gates, and recently, for the reproduction of number 15 factoring " $48 \%$ of the time"..$^{72}$
(iv) Optical systems pose a special challenge for quantum computation: due to the virtual linearity of most electromagnetic media at reasonable light power, the implementation of interaction Hamiltonians, such as (149), is problematic. However, in 2001 a very smart way around this hurdle was invented. ${ }^{73}$ In this KLM scheme, nonlinear elements are not needed, and quantum gates may be composed just of linear devices (such as optical waveguides, mirrors and beam splitters), plus singlephoton sources and detectors. Unfortunately, a quantitative discussion of this scheme would require using the basics of quantum electrodynamics that will be discussed only in the next chapter. The work in this direction has already led to an experimental demonstration of factoring number $21=3 \times 7$ (which in some aspects is easier than that of 15)..$^{74}$

Let me, however, note that due to the statistical nature of Shore's algorithm, and the so-far imperfect fidelity of qubit manipulations, all number factoring experiments carried out so far may be more fairly described merely as demonstrations of their result consistency with the (evident) mathematical facts. So, despite a very substantial research effort, the progress is rather slow, with the

[^739]main culprit being the unintentional coupling of qubits to environment, leading most importantly to their state dephasing, and eventually to errors. (Another major problem of this research field is the lack of algorithms (besides Shor's number factoring) that would give quantum computation a substantial advantage over classical counterparts, and hence a potential customer base broader that the communication encryption community, that could provide the necessary significant support.)

Of course, some error probability exists in classical digital logic gates and memory cells as well. However, in this case, there is no conceptual problem with the device state measurement, so that the error may be detected and corrected in many ways; perhaps the simplest one is the so-called majority voting. For that, the input bit is reproduced in several (say, three) copies and sent to three similar devices whose outputs are measured and compared. If the output bits differ, at least one of the devices has made at error. The error may be not only detected, but also corrected by taking the two coinciding output bits for the correct one. If the probability of a single device error is $W \ll 1$, the probability of error of any device pair is close to $W^{2}$, and that of two pairs (and hence of the whole majority voting scheme) is close to $W^{3}$. Since for the currently dominating CMOS integrated circuits, $W$ is very small, such error correction circuit creates a dramatic fidelity improvement - at the cost of higher circuit complexity (which may be traded for larger time delay) and consumed power.

For quantum computation, the general idea of using several devices (say, qubits) for coding the same information remains the same; however, there are two major complications, both due to the analog nature of qubit states. First, as we know from Chapter 7, the dephasing effect of environment may be described as a slow random drift of coefficients $a_{j}$ in expansion (128), leading to the deviation of the output state $\alpha_{\text {fin }}$ from the basis form (132), and hence to a nonvanishing probability of wrong qubit state readout (Fig. 2). Hence the quantum error correction has to protect the result not only against possible random state flips $0 \leftrightarrow 1$ as in the classical digital computer, but also against these "creeping" analog errors.

Second, the qubit state is impossible to copy exactly (clone) without disturbing it, as follows from the following simple calculation. ${ }^{75}$ Cloning state $\alpha$ of one qubit to another qubit, initially in an independent state (say the basis state 0 ), means the following transformation of the two-qubit ket: $|\alpha 0\rangle$ $\rightarrow|\alpha \alpha\rangle$. If we want such transform to be performed by a real quantum system whose evolution is described by a unitary operator $\hat{u}$, and to be correct for an arbitrary state $\alpha$, it has to work not only for both basis states of the qubit:

$$
\begin{equation*}
\hat{u}|00\rangle=|00\rangle, \quad \hat{u}|10\rangle=|11\rangle, \tag{8.156}
\end{equation*}
$$

and also for their arbitrary linear combination (125). Since operator $\hat{u}$ has to be linear, we may use Eq. (156) to calculate

$$
\begin{equation*}
\hat{u}|\alpha 0\rangle=\hat{u}\left(a_{0}|0\rangle+a_{1}|1\rangle\right)|0\rangle=a_{0} \hat{u}|00\rangle+a_{1} \hat{u}|10\rangle=a_{0}|00\rangle+a_{1}|11\rangle . \tag{8.157}
\end{equation*}
$$

On the other hand, the desired result of cloning is

$$
\begin{equation*}
|\alpha \alpha\rangle=\left(a_{0}|0\rangle+a_{1}|1\rangle\right)\left(a_{0}|0\rangle+a_{1}|1\rangle\right)=a_{0}^{2}|00\rangle+a_{0} a_{1}(|10\rangle+|01\rangle)+a_{1}^{2}|11\rangle, \tag{8.158}
\end{equation*}
$$

i.e. evidently different, so that, for an arbitrary $\alpha$,

[^740]\[

$$
\begin{equation*}
\hat{u}|\alpha 0\rangle \neq|\alpha \alpha\rangle \tag{8.159}
\end{equation*}
$$

\]

showing that the qubit state cloning is indeed impossible. ${ }^{76}$
This problem may be circumvented in the way shown in Fig. 7a. Here the CNOT gate, whose action is described by Eq. (137), entangles an arbitrary input state (125) of the source qubit with a basis initial state of an ancillary qubit - frequently called ancilla. Using Eq. (137), we may readily calculate the output two-qubit state's vector:

$$
\begin{equation*}
|\alpha\rangle_{N=2}=\hat{C}\left(a_{0}|0\rangle+a_{1}|1\rangle\right)|0\rangle=a_{0} \hat{C}|00\rangle+a_{1} \hat{C}|10\rangle=a_{0}|00\rangle+a_{1}|11\rangle \tag{8.160}
\end{equation*}
$$

We see that this circuit does perform operation (157), i.e. re-prescribes the initial source qubit's expansion coefficients $a_{0}$ and $a_{1}$ equally to two qubits, i.e. duplicates the input information, though in contrast with the "genuine" cloning, it changes the state of the source qubit. Such "quasi-cloning" is the key to virtually all quantum error correction techniques.

(b)

Quasicloning

Fig. 8.7. (a) Quasi-cloning, and (b) detection and correction of dephasing errors in a single qubit.

Consider, for example, the three-qubit circuit shown in Fig. 7b. At its input, the double application of the quasi-cloning produces an intermediate state $A$ with the ket-vector

$$
\begin{equation*}
|A\rangle=a_{0}|000\rangle+a_{1}|111\rangle, \tag{8.161}
\end{equation*}
$$

which is an evident generalization of Eq. (160). ${ }^{77}$ Subjecting the source qubit to the Hadamard transform (138), we get three-qubit state $B$ represented by vector

$$
\begin{equation*}
|B\rangle=a_{0} \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|00\rangle+a_{1} \frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)|1\rangle . \tag{8.162}
\end{equation*}
$$

Now let us assume that at this stage, the source qubit comes into a contact with a dephasing environment (in Fig. 7, symbolized by single-qubit "gate" $\varphi$ ). As we know from Sec. 7.3, its effect

[^741](besides some inconsequential shift of common phase) may be described by a random mutual phase shift of the basis states: ${ }^{78}$
\[

$$
\begin{equation*}
|0\rangle \rightarrow e^{i \varphi}|0\rangle, \quad|1\rangle \rightarrow e^{-i \varphi}|1\rangle \tag{8.163}
\end{equation*}
$$

\]

As a result, for the intermediate state $C$ (see Fig. 7b) we may write

$$
\begin{equation*}
|C\rangle=a_{0} \frac{1}{\sqrt{2}}\left(e^{i \varphi}|0\rangle+e^{-i \varphi}|1\rangle\right)|00\rangle+a_{1} \frac{1}{\sqrt{2}}\left(e^{i \varphi}|0\rangle-e^{-i \varphi}|1\rangle\right)|11\rangle . \tag{8.164}
\end{equation*}
$$

At this stage, in this simple theoretical model, the coupling with environment is completely quenched (ahh, if this could be possible in reality! we would have quantum computers by now :-), and the source qubit is fed into one more Hadamard gate. Using Eqs. (138) again, for state $D$ after this gate we get

$$
\begin{equation*}
|D\rangle=a_{0}(\cos \varphi|0\rangle+i \sin \varphi|1\rangle)|00\rangle+a_{1}(i \sin \varphi|0\rangle+\cos \varphi|1\rangle)|11\rangle . \tag{8.165}
\end{equation*}
$$

Now the qubits are passed through the second, similar pair of CNOT gates - see Fig. 7b. Using Eq. (137), for the ket-vector of the resulting state $E$ we readily get expression

$$
\begin{equation*}
|E\rangle=a_{0} \cos \varphi|000\rangle+a_{0} i \sin \varphi|111\rangle+a_{1} i \sin \varphi|011\rangle+a_{1} \cos \varphi|100\rangle \tag{8.166a}
\end{equation*}
$$

which evidently may be grouped as

$$
\begin{equation*}
|E\rangle=\left(a_{0}|0\rangle+a_{1}|1\rangle\right) \cos \varphi|00\rangle+\left(a_{1}|0\rangle+a_{0}|1\rangle\right) i \sin \varphi|11\rangle . \tag{8.166b}
\end{equation*}
$$

This is already a rather remarkable result. It shows that if we measure the ancilla qubits at stage $E$, and both results corresponded to states 0 , we may be $100 \%$ sure that the source qubit (which is not affected by the measurement!) is in its initial state even after the interaction with environment. The only result of an increase of this interaction (as quantified by the magnitude of phase $\varphi$ ) is the growth of the probability,

$$
\begin{equation*}
W=\sin ^{2} \varphi \tag{8.167}
\end{equation*}
$$

of getting the opposite result, which signals a dephasing-induced error in the source qubit. This implicit measurement, without disturbing the source qubit, is called quantum error detection.

Even more impressive result may be achieved by adding to the circuit one more component, the so-called Toffoli (or "CCNOT") gate, denoted by the rightmost symbol in Fig. 7b. This 3-qubit gate is conceptually similar to the CNOT gate discussed above, besides that it flips the basis state of its target qubit only if both basis states of its two source qubits are 1. (In the circuit shown in Fig. 7b, the former role is played by our source qubit, while the latter role, by two ancilla qubits.) According to its

[^742]definition, the Toffoli gate has no effect on the first parentheses in Eq. (166b), but flips the source qubit's state in the second parentheses. The result may be factorized as follows,
\[

$$
\begin{equation*}
|F\rangle=\left(a_{0}|0\rangle+a_{1}|1\rangle\right)(\cos \varphi|00\rangle+i \sin \varphi|11\rangle) \tag{8.168}
\end{equation*}
$$

\]

showing that now the source qubit is again fully unentangled from the ancilla qubits. Moreover, calculating the norm squared of the second operand, we get

$$
\begin{equation*}
(\cos \varphi\langle 00|-i \sin \varphi\langle 11|)(\cos \varphi|00\rangle+i \sin \varphi|11\rangle)=\cos ^{2} \varphi+\sin ^{2} \varphi=1 \tag{8.169}
\end{equation*}
$$

Quantum
so that the final state of the source qubit always, exactly coincides with its initial state. This is the famous miracle of quantum state correction, taking place "automatically" - without any qubit measurements, and for any random phase shift $\varphi$.

The circuit shown in Fig. 7b may be improved by adding the Hadamard gate pairs, similar to that used for the source qubit, to the ancilla qubits as well. If dephasing is small in the sense that the $W$ given by Eq. (167) is much less than 1, this modified circuit may provide substantial error probability reduction (to $\sim W^{2}$ ) even if the ancilla qubits are also subjected to a similar dephasing and the source qubits, at the same stage - i.e. between two Hadamard gates. The perfect automatic correction of any error (not only inner dephasing of a qubit and its relaxation/excitation, but also the mutual dephasing between qubits) of any used qubit needs even more parallelism. The first circuit of that kind, based on 9 parallel qubits, which is a natural generalization of the circuit discussed above, had been invented in 1995 by the same P. Shor. Later, 5-qubit circuits enabling similar error correction were suggested. (The further parallelism reduction has been proved impossible.)

However, all these results assume that the error correction circuits as such are perfect, i.e. completely isolated from the environment. In the real world this cannot be done. Now the key question is what maximum level $W_{\max }$ of error probability in each gate (including those in the used error correction scheme) can be automatically corrected, thus opening a way toward large quantum computers producing some useful results - first of all, the factoring of large numbers - with at least $10^{3}$ bits to be of interest for practice. To the best of my knowledge, this critical level has not yet been strictly calculated, partly because the error correction greatly inflates the number of the total gates in the system - by a factor crudely proportional to the number $N$ of used qubits. Various authors give broadly different estimates: from $W_{\max } \sim 10^{-6}$ to $W_{\max } \sim 10^{-2}$. Whatever the critical level is, it has not been reached yet.

This situation has motivated the search for the quantum computation schemes different from that shown in Fig. 2; the most prominent alternative is called adiabatic quantum computation. ${ }^{79}$ In its most actively pursued option (for which "quantum system modeling" would be a more appropriate name), the interaction between a system of qubits is organized so that the system's Hamiltonian is similar to that of some quantum system of interest. Then the qubit system, first prepared in a certain initial state with relatively high energy, e.g., in an unentangled state described by Eq. (130), is let to evolve on its own. Due to the unavoidable dissipation due to interaction with environment, the system eventually relaxes to a final unentangled state of its qubits, which is then measured. From numerous runs of such experiment, outcome statistics may be revealed for various temperatures of the environment. Thus, at this approach (which is very close to the numerical modeling technique called quantum annealing), the interaction

[^743]with environment is allowed to play a certain role in the system evolution, though every effort is made to reduce it, to allow qubit "quantumness" to make a substantial difference at least at the beginning of the relaxation process.

Generally speaking, adiabatic quantum computation may be used for performing any quantum algorithm, including number factoring. ${ }^{80}$ Unfortunately, due to technical difficulties of the organization and precise control of long-range interaction in multi-qubit systems, ${ }^{81}$ the list of modeled systems is presently limited to a few simple 1D or 2D arrays described by the so-called extended quantum Ising ("spin-glass") model ${ }^{82}$

$$
\begin{equation*}
\hat{H}=-J \sum_{\left\{j, j^{\prime}\right\}} \hat{\sigma}_{z}^{(j)} \hat{\sigma}_{z}^{\left(j^{\prime}\right)}-\sum_{j} h_{j} \hat{\sigma}_{z}^{(j)} \tag{8.170}
\end{equation*}
$$

where the curly bracket denotes the summation over pairs of close (though not necessarily closest) neighbors. Though Hamiltonian (170) is the traditional playground of phase transitions theory (see, e.g., SM Chapter 4), to the best of my knowledge there are not many practically valuable tasks that could be achieved by studying the statistics of its solutions. Moreover, even for this limited task, the speed of the best experimental adiabatic quantum "computer" with $N=108$ qubits is still lower than that of a classical, off-the-shelf semiconductor processor (with a dollar cost lower by some 6 orders of magnitude), and no dramatic change of this comparison is predicted for realistic larger values of $N .{ }^{83}$

There may be better prospects for another application of entangled qubit systems, namely for telecommunication cryptography. ${ }^{84}$ The goal here is to replace the currently dominating classical encryption, based on the public-key RSA code mentioned above, that may be broken by factoring of very large numbers, by a quantum encryption that would be fundamentally unbreakable. The basis of this opportunity are the measurement postulate and the no-cloning theorem: if a message is carried out by a qubit such as a single photon, it is impossible for an eavesdropper (in cryptography, traditionally called Eve) to either measure or copy its faithfully, without also disturbing its state. However, as we have seen from the discussion of Fig. 7a, state quasi-cloning using entangled qubits is possible, so that the issue is far from being simple, especially if we want to use a publicly distributed quantum key, in some sense similar to the classical public key used at the RSA encryption.

Unfortunately, I do not have time/space to discuss various options for quantum encryption, but cannot help demonstrating how counter-intuitive they may be, on the famous example of the so-called quantum teleportation (Fig. 8). ${ }^{85}$ Suppose that party A (in cryptography, traditionally called Alice) wants to send party $\mathrm{B}(B o b)$ the full information about the quantum state $\alpha$ of a qubit, unknown to either party. Instead of sending her qubit directly to Bob, Alice asks him to send her one qubit ( $\beta$ ) of the pair of other qubits, prepared in a certain entangled state, for example in the singlet state (11):

[^744]\[

$$
\begin{equation*}
\left|\beta \beta^{\prime}\right\rangle=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle) \tag{8.171}
\end{equation*}
$$

\]

Using Eq. (125), the initial state of the whole 3-qubit system may be represented by the ket-vector

$$
\begin{equation*}
\left|\alpha \beta \beta^{\prime}\right\rangle=\left(a_{0}|0\rangle+a_{1}|1\rangle\right)\left|\beta \beta^{\prime}\right\rangle=\frac{a_{0}}{\sqrt{2}}|001\rangle-\frac{a_{0}}{\sqrt{2}}|010\rangle+\frac{a_{1}}{\sqrt{2}}|010\rangle-\frac{a_{1}}{\sqrt{2}}|111\rangle, \tag{8.172a}
\end{equation*}
$$

which may be rewritten as a linear superposition,

$$
\begin{align*}
\left|\alpha \beta \beta^{\prime}\right\rangle & =\frac{1}{2}|\alpha \beta\rangle_{s}^{+}\left(-a_{1}|0\rangle+a_{0}|1\rangle\right)+\frac{1}{2}|\alpha \beta\rangle_{s}^{-}\left(a_{1}|0\rangle+a_{0}|1\rangle\right)  \tag{8.172b}\\
& +\frac{1}{2}|\alpha \beta\rangle_{e}^{+}\left(-a_{0}|0\rangle+a_{1}|1\rangle\right)+\frac{1}{2}|\alpha \beta\rangle_{e}^{-}\left(-a_{0}|0\rangle-a_{1}|1\rangle\right),
\end{align*}
$$

of the following 4 states of qubit pair $\alpha \beta$ :

$$
\begin{equation*}
|\alpha \beta\rangle_{s}^{ \pm} \equiv \frac{1}{\sqrt{2}}(|00\rangle \pm|11\rangle), \quad|\alpha \beta\rangle_{e}^{ \pm} \equiv \frac{1}{\sqrt{2}}(|01\rangle \pm|10\rangle) . \tag{8.173}
\end{equation*}
$$



Fig. 8.8. Sequential stages of a quantum teleportation procedure: (a) the initial state with entangled qubits $\beta$ and $\beta^{\prime}$, (b) back transfer of qubit $\beta$, (c) measurement of pair $\alpha \beta$, (d) forward transfer of 2 classical bits with the measurement result, and (e) the final state, with the state of qubit $\beta^{\prime}$ mirroring the initial state of qubit $\alpha$.

After having received qubit $\beta$ from Bob, Alice measures which of these 4 states does pair $\alpha \beta$ have. This may be achieved, for example, by measurement of one observable represented by operator $\hat{\sigma}_{z}^{(\alpha)} \hat{\sigma}_{z}^{(\beta)}$ and another one corresponding to $\hat{\sigma}_{x}^{(\alpha)} \hat{\sigma}_{x}^{(\beta)}$ - cf. Eq. (148). ${ }^{86}$ The measured eigenvalue of the former operator enables distinguishing the couples of states (173) with different values of the lower index, while the latter measurement distinguishes the states with different upper indices.

Then Alice reports the result (that may be coded by just 2 classical bits) to Bob over a classical channel. Since the measurement places pair $\alpha \beta$ definitely in the corresponding state, the remaining Bob's bit $\beta^{\prime}$ is now definitely in the unentangled single-qubit state that is represented by the corresponding parentheses in Eq. (172b). Note that each of these parentheses contains both coefficients $a_{0,1}$, i.e. the whole information about the initial state of qubit $\alpha$ had initially. If Bob likes, he may now use appropriate single-qubit operations, similar to those discussed above, to move qubit $\beta$ into the state exactly similar to the initial state of qubit $\alpha$. (This fact does not violate the no-cloning theorem (159), because the measurement has already changed the state of $\alpha$.) This is of course a "teleportation" only in

[^745]a very special sense of this rather ambiguous term, but a good example of the importance of qubit entanglement's preservation at their spatial transfer. For us, this is also a good primer for the forthcoming discussion of the EPR paradox and Bell's inequalities in Sec. 10.1.

Returning for a minute to practical quantum cryptography, since its two most common quantum key distribution protocols ${ }^{87}$ require just a few simple quantum gates, whose experimental implementation is not a large obstacle, the main focus of the current effort is on decreasing singlephoton dephasing in long optical fiber waveguides, ${ }^{88}$ and hence increasing the maximum distance of quantum channels with sufficiently high qubit transfer fidelity. The recent progress was impressive, with demonstrated two lines (using either protocol) longer than $100 \mathrm{~km},{ }^{89}$ and active plans for 560 km and 700 km landlines and several satellite-based systems. Let me hope that if not the author, then the reader of these notes will see this technology accepted for practical secure telecommunications.

### 8.6. Exercise problems

8.1. $N$ electrons are placed in a 3D, spherically-symmetric quadratic potential $U(\mathbf{r})=m \omega_{0}^{2} r^{2} / 2$. Neglecting the direct interaction of the electrons, find the ground-state energy of the system.
8.2. $N \gg 1$ indistinguishable, non-interacting quantum particles are placed in a hard-wall, rectangular box with sides $a_{x}, a_{y}$, and $a_{z}$. Calculate the ground-state energy of the system, and the average forces it exerts on each face of the box. Can we characterize the forces by certain pressure?

Hint: Consider separately the cases of bosons and fermions.
8.3. Prove that the singlet state, and each triplet state of a system of two indistinguishable spin-1/2 particles, are eigenstates of the operator of the scalar product $\mathbf{S}_{1} \cdot \mathbf{S}_{2}$ of the spin vectors, and calculate the corresponding eigenvalues. Compare the results with the scalar product of two classical vectors of magnitude $\hbar / 2$ each, being either parallel or antiparallel.
8.4. The interaction of two, indistinguishable spin- $1 / 2$ particles (that are otherwise free) has the form

$$
\hat{H}_{\mathrm{int}}=U(\mathbf{r})+f(\mathbf{r}) \hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2},
$$

where $\mathbf{r} \equiv \mathbf{r}_{1}-\mathbf{r}_{2}$ is the distance between the particles. Reduce the problem to two independent wave mechanical problems.
8.5. Two similar spin- $1 / 2$ particles, with the gyromagnetic ratio $\gamma$, localized at two points separated by distance $a$, interact via the field of their magnetic dipole moments. Calculate the eigenstates and eigenvalues of the system.

[^746]8.6. In the simple case of just two similar spin-interacting particles, distinguishable by their spatial location, the famous Heisenberg model of ferromagnetism ${ }^{90}$ is reduced to the following Hamiltonian:
$$
\hat{H}=-J \hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2}-\gamma \boldsymbol{B} \cdot\left(\hat{\mathbf{S}}_{1}+\hat{\mathbf{S}}_{2}\right)
$$
where $J$ is the spin interaction constant, $\gamma$ is the gyromagnetic ratio of each particle, and $B$ is the external magnetic field. Find the stationary states and eigenenergies of this system for spin- $1 / 2$ particles.
8.7. Two distinguishable particles, both with spin $1 / 2$, but different gyromagnetic ratios $\gamma_{1}$ and $\gamma_{2}$, are placed into external magnetic field $\mathcal{B}$. In addition, their spins interact as
$$
\hat{H}_{\mathrm{int}}=-J \hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2} .
$$

Find the eigenstates and eigenenergies of the system. ${ }^{91}$
8.8. A system of 3 similar but distinguishable spin- $1 / 2$ particles is described by the following Hamiltonian:

$$
\hat{H}=-J\left(\hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2}+\hat{\mathbf{S}}_{2} \cdot \hat{\mathbf{S}}_{3}+\hat{\mathbf{S}}_{3} \cdot \hat{\mathbf{S}}_{1}\right)
$$

where $J$ is the spin interaction constant. Find the stationary states and eigenenergies of this system.
8.9. For a system of three distinguishable spins- $1 / 2$, find the joint eigenstates (and the corresponding eigenvalues) of operators $S_{z}$ and $S^{2}$, where

$$
\hat{\mathbf{S}} \equiv \hat{\mathbf{S}}_{1}+\hat{\mathbf{S}}_{2}+\hat{\mathbf{S}}_{3}
$$

is the vector operator of the total spin of the system. Do the corresponding quantum numbers $s$ and $m_{s}$ obey Eqs. (5.197)?
8.10. Prove that Eq. (8.32) of the lecture notes indeed yields $E_{g}{ }^{(1)}=(5 / 4) E_{\mathrm{H}}$.
8.11. For a diluted gas on helium atom in their ground state, with $n$ atoms per unit volume, on density $n$, calculate its:
(i) electric susceptibility $\chi_{e}$, and
(ii) magnetic susceptibility $\chi_{m}$,
and compare the results.
8.12. Represent the operators of the total kinetic energy and the total orbital angular momentum of a system of two particles, with masses $m_{1}$ and $m_{2}$, as combinations of terms describing their center-ofmass motion and relative motion.
8.13. Two particles, with masses $m_{1}$ and $m_{2}$, interact as described by 3D potential

[^747]$$
U\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right)=\frac{\kappa}{2}\left(\mathbf{r}_{1}-\mathbf{r}_{2}\right)^{2},
$$
but otherwise are free to move. Calculate the energy spectrum and the degeneracy of each energy level of the system for the cases when the particles are:
(i) distinguishable, and
(ii) indistinguishable spin- $1 / 2$ fermions (such as electrons).
8.14. Two particles with similar masses $m$ and charges $q$ are free to move along a round, plane ring of radius $R$. In the limit of their strong Coulomb interaction, find the lowest eigenenergies of the system, and sketch the system of its energy levels.
8.15. Two similar 1D, spin- $1 / 2$ particles are attracting each other at contact:
$$
U\left(x_{1}, x_{2}\right)=-w \delta\left(x_{1}-x_{2}\right), \quad \text { with } w>0
$$
but are otherwise free to move. Find the energy and the wavefunction of the ground state of the system.
Hint: Mind the possibility of various spin states of the particles.
8.16. Two indistinguishable, 1 D , spin- $1 / 2$ particles in a triplet spin state are attracting each other at limited distance:
\[

U\left(x_{1}, x_{2}\right)=\left\{$$
\begin{array}{rc}
-U_{0}, & \text { for }\left|x_{1}-x_{2}\right|<a / 2, \\
0, & \text { otherwise },
\end{array}
$$ \quad with U_{0}>0\right.
\]

but are otherwise free to move. How large should be $a$ for the system to have at least one localized eigenstate? Relate the result to the solution of the previous problem.
8.17. ${ }^{*}$ Two indistinguishable spin- $1 / 2$ particles are confined to move around a circle of radius $R$, and interact only at a very short distance $l=R \varphi=R\left(\varphi_{1}-\varphi_{2}\right)$ between them, so that the interaction potential $U$ may be well approximated with a delta-function of $\varphi$. Calculate their lowest ground states and their energy for the following two cases:
(i) "orbital" (spin-independent) interaction: $\hat{U}=w \delta(\varphi)$,
(ii) spin-spin interaction: $\hat{U}=-w \hat{\mathbf{S}}_{1} \cdot \hat{\mathbf{S}}_{2} \delta(\varphi)$,
both with constant $w>0$. Analyze the trends of your results in the limits $w \rightarrow 0$ and $w \rightarrow \infty$.
8.18. Low-energy spectrum of many diatomic molecules may be well described modeling the molecule as a system of two spinless particles connected with a light and elastic, but very stiff spring. Calculate the spectrum in this approximation.
8.19. Two particles of mass $M$, separated by two much lighter particles, of mass $m \ll M$, are placed on a ring of radius $R$ - see Fig. on the right. The particles strongly repulse at contact, but otherwise each of them is fee to move along the ring. Calculate the lower part of the energy spectrum of the system.

8.20.* Use the perturbation theory to calculate the contribution to the hyperfine splitting of the ground energy of the hydrogen atom, due to the interaction between spins of the nuclei (proton) and of the electron.

Hint: The proton's magnetic moment operator is described by Eq. (4.116), with a positive gyromagnetic factor $\gamma_{p}=g_{p} e / 2 m_{p} \approx 2.675 \times 10^{8} \mathrm{~s}^{-1} \mathrm{~T}^{-1}$, whose magnitude is much smaller than that of the electron $\left(\left|\gamma_{e}\right| \approx 1.761 \times 10^{11} \mathrm{~s}^{-1} \mathrm{~T}^{-1}\right)$, due to a different $g$-factor, $g_{p} \approx 5.586,{ }^{92}$ and of course a much higher mass, $m_{p} \approx 1.673 \times 10^{-27} \mathrm{~kg}$.
8.21. Discuss the factors $\pm 1 / \sqrt{ } 2$ that participate in Eqs. (19) and (21), in terms of the ClebshGordan coefficients discussed in Sec. 5.7.
8.22. Compose the simplest model Hamiltonians of the following systems, in terms of the second quantization formalism:
(i) a system of two weakly coupled quantum wells, taking into account pair on-site interactions (additional energy $J$ per each pair of particles in the same quantum well), and
(ii) same for the motion in a periodic 1D potential, in the tight-binding limit.
8.23. For each of the Hamiltonians composed in the previous problem, derive the Heisenberg equations of motion for particle creation operators, for (i) bosons, and (ii) fermions.
8.24. Express the ket-vectors all possible Dirac states for the system of 3 indistinguishable
(i) bosons, and
(ii) fermions, via those of their single-particle states.
8.25. Explain why the Hartree-Fock approximation (118), applied to the ${ }^{4} \mathrm{He}$ atom, gives "correct" ${ }^{93}$ expression (31) for the ground singlet state, and correct Eqs. (44)-(45) (with the minus sign in the former relation) for the excited triplet state, but cannot describe result (44), with the plus sign, for the excited singlet state.
8.26. Find a time-independent Hamiltonian that may cause the qubit evolution described by Eq. (147). Discuss the result and its relation to the time-dependent Hamiltonian (6.86).

[^748]
## Chapter 9. Introduction to Relativistic Quantum Mechanics

This chapter gives a brief introduction to relativistic quantum mechanics. It starts with a discussion of the basic elements of the quantum theory of electromagnetic field (quantum electrodynamics, $Q E D$ ), including the quantization scheme, photon statistics, radiative atomic transitions, the spontaneous and stimulated radiation, and the so-called cavity $Q E D$. Then I will briefly review the relativistic quantum theory of particles with nonvanishing rest mass, notably Dirac' theory of spin- $1 / 2$ particles, and mark the point of entry into the most complete relativistic quantum theory - the quantum field theory, QFT which is beyond the scope of these notes. ${ }^{1}$

### 9.1. Electromagnetic field quantization

Classical mechanics tells us ${ }^{2}$ that the relativistic relation between momentum $\mathbf{p}$ and energy $E$ of a free particle with rest mass $m$ may be simplified in two limits, non-relativistic and ultra-relativistic: relativistic energy

$$
E=\left[(p c)^{2}+\left(m c^{2}\right)^{2}\right]^{1 / 2} \rightarrow \begin{cases}m c^{2}+p^{2} / 2 m, & \text { for } p \ll m c  \tag{9.1}\\ p c, & \text { for } p \gg m c\end{cases}
$$

In both limits, the transfer from classical to quantum mechanics is easier than in the arbitrary case. Since all the previous part of this course was committed to the first, non-relativistic limit, I will now jump to a brief discussion of the ultra-relativistic limit $p \gg m c$, for a particular but very important system - the electromagnetic field. Since the excitations of this field, called photons, are currently believed to have zero rest mass $m,{ }^{3}$ the ultra-relativistic limit is valid for any photon energy $E$, and the quantization scheme is rather straightforward.

As usual, the quantization has to be based on the classical theory of the system, in this case the Maxwell equations. As the simplest case, let us consider electromagnetic field in a free-space volume limited by ideal walls that reflect incident waves perfectly. ${ }^{4}$ Inside the volume, the Maxwell equations may be reduced to a simple wave equation ${ }^{5}$ for electric field

$$
\begin{equation*}
\nabla^{2} \varepsilon-\frac{1}{c^{2}} \frac{\partial^{2} \varepsilon}{\partial t^{2}}=0 \tag{9.2}
\end{equation*}
$$

and an absolutely similar equation for magnetic field $\mathcal{B}$. We may look for the general solution of Eq. (2) in the variable-separating form

[^749]\[

$$
\begin{equation*}
\varepsilon(\mathbf{r}, t)=\sum_{j} p_{j}(t) \mathbf{e}_{j}(\mathbf{r}) . \tag{9.3}
\end{equation*}
$$

\]

Physically, each term of this sum is a standing wave whose spatial distribution and polarization ("mode") is described by vector function $\mathbf{e}_{j}(\mathbf{r})$, and the temporal dynamics, by function $p_{j}(t)$. Plugging an arbitrary term of this sum into Eq. (2), and separating variables exactly as we did, e.g., for the Schrödinger equation in Sec. 1.4, we get

$$
\begin{equation*}
\frac{\nabla^{2} \mathbf{e}_{j}}{\mathbf{e}_{j}}=\frac{1}{c^{2}} \frac{\ddot{p}_{j}}{p_{j}}=\text { const } \equiv-k_{j}^{2}, \tag{9.4}
\end{equation*}
$$

so that the spatial distribution of the mode satisfies the $3 D$ Helmholtz equation:

$$
\begin{equation*}
\nabla^{2} \mathbf{e}_{j}+k_{j}^{2} \mathbf{e}_{j}=0 \tag{9.5}
\end{equation*}
$$

Equation
for spatial distribution

The set of solutions of this equation, with appropriate boundary conditions, determines the set of functions $\mathbf{e}_{j}$ and simultaneously the spectrum of wave number moduli $k_{j}$. The latter values determine mode eigenfrequencies, following from Eq. (4):

$$
\begin{equation*}
\ddot{p}_{j}+\omega_{j}^{2} p_{j}=0, \quad \text { with } \omega_{j} \equiv k_{j} c . \tag{9.6}
\end{equation*}
$$

There is a big philosophical difference between the approaches to equations (5) and (6), despite their single origin (4). The first (Helmholtz) equation may be rather difficult to solve in realistic geometries, ${ }^{6}$ but it remains intact in quantum theory, with the scalar components of vector functions $\mathbf{e}_{j}(\mathbf{r})$ still treated (at each point $\mathbf{r}$ ) as $c$-numbers. In contrast, Eq. (6) is readily solvable (giving sinusoidal oscillations with frequency $\omega_{j}$ ), but this is exactly where we can make a transfer to quantum mechanics, because we already know how to quantize a mechanical 1D harmonic oscillator that obeys, in classics, the same equation.

As usual, we need to start with the appropriate Hamiltonian corresponding to the classical Hamiltonian function $H$ of the proper set of generalized coordinates and momenta. The electromagnetic field's Hamiltonian function (that in this case coincides with field's energy) is ${ }^{7}$

$$
\begin{equation*}
H=\int d^{3} r\left(\frac{\varepsilon_{0} \varepsilon^{2}}{2}+\frac{\mathcal{B}^{2}}{2 \mu_{0}}\right) \tag{9.7}
\end{equation*}
$$

Let us represent the magnetic field in a form similar to Eq. (3),

$$
\begin{equation*}
\mathcal{B}(\mathbf{r}, t)=-\sum_{j} \omega_{j} q_{j}(t) \mathbf{b}_{j}(\mathbf{r}) . \tag{9.8}
\end{equation*}
$$

Since, according to the Maxwell equations, in our case the magnetic field satisfies the equation similar to Eq. (2), the time-dependent amplitude $q_{j}$ of each of its modes obey the equation similar to Eq. (6), i.e. also changes in time sinusoidally, with the same frequency $\omega_{j}$. Plugging Eqs. (3) and (8) into Eq. (7), we may recast it as

[^750]\[

$$
\begin{equation*}
H=\sum_{j} \frac{p_{j}^{2}}{2} \int \varepsilon_{0} e_{j}^{2}(\mathbf{r}) d^{3} r+\frac{\omega_{j}^{2} q_{j}^{2}}{2} \int \frac{1}{\mu_{0}} b_{j}^{2}(\mathbf{r}) d^{3} r \tag{9.9}
\end{equation*}
$$

\]

Since the distribution of constant factors between two multiplication operands in each term of Eq. (3) is arbitrary, we may fix it by requiring the first integral in Eq. (9) to equal 1. It is straightforward to check that according to the Maxwell equations, which give a specific relation between vectors $\varepsilon$ and $\mathcal{B}, 8$ this normalization makes the second integral in Eq. (9) equal 1 as well, and Eq. (9) becomes

$$
\begin{equation*}
H=\sum_{j} H_{j}, \quad H_{j}=\frac{p_{j}^{2}}{2}+\frac{\omega_{j}^{2} q_{j}^{2}}{2} \tag{9.10}
\end{equation*}
$$

Now we can carry out the standard quantization procedure, namely declare $H_{j}, p_{j}$, and $q_{j}$ the quantum-mechanical operators related exactly as in Eq. (10),

Electromagnetic mode's Hamiltonian

$$
\begin{equation*}
\hat{H}_{j}=\frac{\hat{p}_{j}^{2}}{2}+\frac{\omega_{j}^{2} \hat{q}_{j}^{2}}{2} \tag{9.11}
\end{equation*}
$$

we see that this Hamiltonian coincides with that of a 1 D harmonic oscillator with the mass $m_{j}$ formally equal to $1,{ }^{9}$ and the eigenfrequency equal to $\omega_{j}$. Now, in order to plug Eq. (11) into Eq. (4.199) for the time evolution of Heisenberg-picture operators $\hat{p}_{j}$ and $\hat{q}_{j}$, we need to know the commutation relation between these operators. For that, returning to the classical case, let us calculate the Poisson bracket (4.204) for "functions" $A=q_{j}$, and $B=p_{j}$ ":

$$
\begin{equation*}
\left\{q_{j^{\prime}}, p_{j^{\prime \prime}}\right\} \equiv \sum_{j}\left(\frac{\partial q_{j^{\prime}}}{\partial p_{j}} \frac{\partial p_{j^{\prime \prime}}}{\partial q_{j}}-\frac{\partial q_{j^{\prime}}}{\partial q_{j}} \frac{\partial p_{j^{\prime \prime}}}{\partial p_{j}}\right) . \tag{9.12a}
\end{equation*}
$$

Since in the classical Hamiltonian mechanics, all generalized coordinates $q_{j}$ and momenta $p_{j}$ have to be considered independent arguments of $H$, only one term (with $j=j^{\prime}=j^{\prime \prime}$ ) in only one sum (12) (with $j^{\prime}=$ $j$ '), gives a nonvanishing value ( -1 ), so that

$$
\begin{equation*}
\left\{q_{j^{\prime}}, p_{j^{\prime \prime}}\right\}=-\delta_{j j^{\prime \prime}} \tag{9.12b}
\end{equation*}
$$

Hence, according to the general quantization rule (4.205), the commutation relation of the operators corresponding to $q_{j^{\prime}}$ and $p_{j^{\prime \prime}}$ is

$$
\begin{equation*}
\left[\hat{q}_{j^{\prime}}, \hat{p}_{j^{\prime \prime}}\right]=i \hbar \delta_{j j^{\prime \prime}} \tag{9.13}
\end{equation*}
$$

i.e. is exactly the same as for the usual Cartesian components of the radius-vector and momentum of a mechanical particle.

As the reader already knows, Eqs. (11) and (13) open for us several alternative ways to proceed:

[^751](i) Use the Schrödinger-picture wave mechanics based on wavefunctions $\Psi_{j}\left(q_{j}, t\right)$. As we know from Sec. 2.10, this way is inconvenient for most tasks, because eigenfunctions of the harmonic oscillator are rather clumsy.
(ii) A substantially better way is to write the equations of time evolution of the Heisenbergpicture operators $\hat{q}_{j}(t)$ and $\hat{p}_{j}(t)$.
(iii) An even more convenient approach is to use equations similar to Eqs. (5.99) to decompose operators $\hat{q}_{j}(t)$ and $\hat{p}_{j}(t)$ into the creation-annihilation operators $\hat{a}_{j}^{\dagger}$ and $\hat{a}_{j}$, and work with these operators using either the Schrödinger or the Heisenberg picture, depending on the problem.

I will mostly use the last route. Replacing $m$ with $m_{j} \equiv 1$, and $\omega_{0}$ with $\omega_{j}$, the last forms of Eqs. (5.98) become

$$
\begin{equation*}
\hat{a}_{j}=\left(\frac{\omega_{j}}{2 \hbar}\right)^{1 / 2}\left(\hat{q}_{j}+i \frac{\hat{p}_{j}}{\omega_{j}}\right), \quad \hat{a}_{j}^{\dagger}=\left(\frac{\omega_{j}}{2 \hbar}\right)^{1 / 2}\left(\hat{q}_{j}-i \frac{\hat{p}_{j}}{\omega_{j}}\right) \tag{9.14}
\end{equation*}
$$

and due to Eq. (13), the creation-annihilation operators obey the commutation similar to Eq.(5.101),

$$
\begin{equation*}
\left[\hat{a}_{j}, \hat{a}_{j^{\prime}}^{\dagger}\right]=\hat{I} \delta_{j j^{\prime}} \tag{9.15}
\end{equation*}
$$

so that, according to Eqs. (3) and (8), the quantum-mechanical operators corresponding to the electric and magnetic fields are

$$
\begin{align*}
& \hat{\boldsymbol{\varepsilon}}(\mathbf{r}, t)=i \sum_{j}\left(\frac{\hbar \omega_{j}}{2}\right)^{1 / 2} \mathbf{e}_{j}(\mathbf{r})\left(\hat{a}_{j}^{\dagger}-\hat{a}_{j}\right),  \tag{9.16a}\\
& \hat{\mathcal{B}}(\mathbf{r}, t)=\sum_{j}\left(\frac{\hbar \omega_{j}}{2}\right)^{1 / 2} \mathbf{b}_{j}(\mathbf{r})\left(\hat{a}_{j}^{\dagger}+\hat{a}_{j}\right), \tag{9.16b}
\end{align*}
$$

and Eq. (11) for $j^{\text {th }}$ mode's Hamiltonian becomes

$$
\begin{equation*}
\hat{H}_{j}=\hbar \omega_{j}\left(\hat{a}_{j}^{\dagger} \hat{a}_{j}+\frac{1}{2} \hat{I}\right)=\hbar \omega_{j}\left(\hat{n}_{j}+\frac{1}{2} \hat{I}\right), \quad \text { with } \hat{n}_{j} \equiv \hat{a}_{j}^{\dagger} \hat{a}_{j}, \tag{9.17}
\end{equation*}
$$

absolutely similar to Eq. (5.505) for a mechanical oscillator.
Now comes a very important conceptual step. From Sec. 5.4 we know that eigenstates (Fock states $n_{j}$ ) of Hamiltonian (17) have energies

$$
\begin{equation*}
E_{j}=\hbar \omega_{j}\left(n_{j}+\frac{1}{2}\right), \quad n_{j}=0,1,2, \ldots \tag{9.18}
\end{equation*}
$$

Electromagnetic mode's energies
and, according to Eq. (5.115), operators $\hat{a}_{j}^{\dagger}$ and $\hat{a}_{j}$ act on the eigenkets of these states as

$$
\begin{equation*}
\hat{a}_{j}\left|n_{j}\right\rangle=\left(n_{j}\right)^{1 / 2}\left|n_{j}-1\right\rangle, \quad \hat{a}_{j}^{\dagger}\left|n_{j}\right\rangle=\left(n_{j}+1\right)^{1 / 2}\left|n_{j}+1\right\rangle, \tag{9.19}
\end{equation*}
$$

regardless of the quantum states of other modes (frequently called field oscillators). These rules coincide with definitions (8.56) and (8.60) of bosonic creation-annihilation operators, and hence their action may be considered as the creation/annihilation of certain bosons. Such a "particle" (actually, an excitation of an electromagnetic field oscillator) is exactly what is, strictly speaking, called a photon. Note immediately that according to Eq. (16), such an excitation does not change the spatial distribution of the $j^{\text {th }}$ mode of the field. So, such a "global" photon is an excitation created simultaneously at all points of the field confinement region.

If this picture is too contrary to the intuitive image of a particle, please recall that we had a similar situation in Chapter 2 with eigenstates of the non-relativistic Schrödinger equation: the represented a standing de Broglie wave existing simultaneously in all points of the particle confinement region. The (partial :-) reconciliation with the classical picture of a moving particle might be obtained by using the linear superposition principle to assemble a quasi-localized wave packet of sinusoidal waves, with close wave numbers. Very similarly, we may form a quasi-localized wave packet using a linear superposition of the "global" photons with close values of $k_{j}\left(\right.$ and hence $\left.\omega_{j}\right)$. An additional simplification here is that since the dispersion relation for electromagnetic waves is linear:

$$
\begin{equation*}
\frac{\partial \omega_{j}}{\partial k_{j}}=c=\text { const, i.e. } \frac{\partial^{2} \omega_{j}}{\partial k_{j}^{2}}=0 \tag{9.20}
\end{equation*}
$$

so that, according to Eq. (2.39a), the electromagnetic wave packets (localized photons) do not spread out during their propagation.

The next important conceptual issue is that of the ground-state energy. Equation (18) implies that the total ground-state (i.e., the lowest) energy of the field is

Ground-
state energy of the field

$$
\begin{equation*}
E_{g}=\sum_{j}\left(E_{g}\right)_{j}=\sum_{j} \frac{\hbar \omega_{j}}{2} \tag{9.21}
\end{equation*}
$$

This sum diverges at high frequencies for any realistic any realistic model of the field-confining volume - either infinite or not. Any attempt to dismiss this paradox by declaring the zero-point energy unobservable and hence non-existing fails due to several experimental facts.

First of all, the ground-state "fluctuations" (sometimes called "quantum noise") can be directly observed - see Sec. 7.5 and in particular the literature cited therein. Second, there is the Casimir effect. ${ }^{10}$ The simplest manifestation of the effect involves two parallel plates separated by a vacuum gap of thickness $d \ll A^{1 / 2}$, where $A$ is the plate area (Fig. 1). Rather counter-intuitively, the plates attract each other with a force proportional to area $A$, and rapidly increasing at the decrease of gap $d$.


Fig. 9.1. Generic geometry of the Casimir effect manifestation.

[^752]The effect's explanation is that the energy of each the electromagnetic field mode, including the ground-state energy, is intimately related with the average pressure,

$$
\begin{equation*}
\left\langle P_{j}\right\rangle=-\frac{\partial E_{j}}{\partial V} \tag{9.22}
\end{equation*}
$$

exerted by the field on the walls constraining it to volume $V$. While its pressure on the external surfaces on the plates is due to sum (21) over all free-space modes, with arbitrary values of $k_{z}$ (the $z$-component of the wave vector $\mathbf{k}_{j}$ ), between the plates the spectrum of $k_{z}$ is limited to multiples of $\pi / d$, so that the pressure on the internal surfaces is lower. The net pressure may be found as the sum of contributions (22) from all "missing" low-frequency modes in the gap. The calculations are rather simple if the plates are made of an ideal conductor (which provides boundary conditions $E_{n}=0$ and $B_{\tau}=0$ on the plate surfaces), and the result is ${ }^{11}$

$$
\begin{equation*}
\langle P\rangle=\sum_{j}\left\langle P_{j}\right\rangle=-\frac{\pi^{2} \hbar c}{240 d^{4}} . \tag{9.23}
\end{equation*}
$$

[^753]Note that for this summation, the high-frequency divergence of Eq. (21) at high frequencies is not important, because it participates in the forces exerted on all surfaces of each plate, and hence cancels out from the net pressure. In this way, the Casimir effect not only gives a confirmation of Eq. (21), but also teaches us an important lesson how to deal with the divergence of this sum at $\omega_{j} \rightarrow \infty$ : just get accustomed to the idea that the divergence exists and ignore the fact while you can. However, for more complex tasks of quantum electrodynamics (and quantum theory of any other field) this approach becomes impossible, and then more complex, renormalization techniques become necessary. For their study, I have to refer the reader to a quantum field theory course - see the literature cited in the end of this chapter.

### 9.2. Photon statistics

As a matter of principle, the Casimir effect may be used to measure not only the free-space electromagnetic field, but also that arriving from local sources - lasers, etc. However, usually this is done by simpler detectors in which the absorption of a photon by a single atom leads to its ionization. This ionization, i.e. emission of a free electron, triggers a chain reaction (i.e., an electric discharge in a Geiger-type counter) that may readily be registered by appropriate electronic circuitry. In order to discuss the statistics of such photon counts, it is sufficient to consider the field interaction with just one,

[^754]"trigger" atom. The atom's size $a$ is typically much smaller that the radiation wave length $\lambda_{j}=2 \pi / k_{j}$, so that their interaction is adequately described in the electric dipole approximation,
\[

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=-\hat{\boldsymbol{\varepsilon}} \cdot \hat{\mathbf{d}}, \tag{9.24}
\end{equation*}
$$

\]

where $\hat{\mathbf{d}}$ is the dipole moment's operator. ${ }^{12}$ In Sec. 6.5 we have already developed an approach suitable for the analysis of this problem, based on the Golden Rule - see Fig. 6.14 and Eq. (6.152). ${ }^{13}$ In our current case, we may associate system $b$ with the "trigger atom" (whose ionized states form a continuum spectrum), and hence operator $\hat{\mathbf{d}}$ in Eq. (24) with operand $\hat{B}$ in Eq. (6.148), while the electromagnetic field is represented by system $a$, and its electric field operator $\hat{\varepsilon}$ is associated with operand $\hat{A}$ in that relation. Let us assume, for simplicity, that our field consists of only one mode $\mathbf{e}_{j}(\mathbf{r}) .{ }^{14}$ Then we can keep only one term in Eq. (16a), and drop index $j$, so that Eq. (6.152), for the transition from certain initial state ini to a final state fin may be rewritten as

$$
\begin{align*}
\Gamma & \left.=\frac{2 \pi}{\hbar}|\langle f i n| \hat{\varepsilon}(\mathbf{r}, t)| i n i\right\rangle\left.\right|^{2} \mid\left.\langle\text { fin }| \hat{\mathbf{d}} \cdot \mathbf{n}_{e}|i n i\rangle\right|^{2} \rho_{f} \\
& \left.=\frac{2 \pi}{\hbar} \frac{\hbar \omega}{2}\left|\langle f i n|\left(\hat{a}^{\dagger}-\hat{a}\right) e(\mathbf{r})\right| i n i\right\rangle\left.\right|^{2} \mid\left.\langle\text { fin }| \mathbf{r} \cdot \mathbf{n}_{e}|i n i\rangle\right|^{2} \rho_{f}, \tag{9.25}
\end{align*}
$$

where $e(\mathbf{r})$ is the local magnitude of vector $\mathbf{e}(\mathbf{r})$, and $\mathbf{n}_{\mathrm{e}} \equiv \mathbf{e}(\mathbf{r}) / e(\mathbf{r})$ is its local direction. ${ }^{15}$ As a reminder, in the Heisenberg picture of quantum mechanics, the initial and final states are time-independent, while the creation-annihilation operators are functions of time. In this Golden Rule formula, as in any perturbation result, this time dependence has to be calculated ignoring the perturbation - in this case the field-atom interaction. For the field's creation-annihilation operators, this dependence coincides with that of the usual 1D oscillator - see Eq. (5.171), in which $\omega_{0}$ should be now replaced with $\omega$ :

$$
\begin{equation*}
\hat{a}(t)=\hat{a}(0) e^{-i \omega t}, \quad \hat{a}^{\dagger}(t)=\hat{a}^{\dagger}(0) e^{+i \omega t} \tag{9.26}
\end{equation*}
$$

Hence Eq. (9.25) becomes

$$
\begin{equation*}
\left.\left.\Gamma=\pi \omega\left|\langle f i n|\left(\hat{a}^{\dagger}(0) e^{i \omega t}-\hat{a}(0) e^{-i \omega t}\right) e(\mathbf{r})\right| i n i\right\rangle\left.\right|^{2}\left|\langle f i n| \hat{\mathbf{d}}(t) \cdot \mathbf{n}_{e}\right| i n i\right\rangle\left.\right|^{2} \rho_{f i n} . \tag{9.27a}
\end{equation*}
$$

Now let us multiply the first bra-ket by $\exp \{i \omega t\}$, and the second one by $\exp \{-i \omega t\}$ :

[^755]\[

$$
\begin{equation*}
\left.\Gamma=\pi \omega\left|\left\langle f i n\left(\hat{a}^{\dagger}(0) e^{2 i \omega t}-\hat{a}(0)\right) e(\mathbf{r}) \mid i n i\right\rangle\right|^{2}\left|\langle f i n| \hat{\mathbf{d}}(t) \cdot \mathbf{n}_{e} e^{-i \omega t}\right| i n i\right\rangle\left.\right|^{2} \rho_{f i n} . \tag{9.27b}
\end{equation*}
$$

\]

The physical sense of this, mathematically trivial, operation is that at resonant photon absorption, only the annihilation operator gives a significant time-averaged contribution to the first bra-ket matrix element. (Similarly, according to Eq. (4.199), the Heisenberg operator of the dipole moment, corresponding to the increase of atom's energy, has only the Fourier components that differ from $\omega$ only by $\sim \Gamma \ll \omega$, so that its time dependence compensates the additional factor in the second bra-ket of Eq. (27b), so that this bra-ket is also frequency-independent and has a substantial time average.) Hence, we can neglect the fast-evolving term in the first bra-ket whose average over time interval $\sim 1 / \Gamma$ is very close to zero. ${ }^{16}$

Now let us assume that we use the same detector, characterized by the same second bra-ket and the same state density $\rho_{\text {fin }}$, for measurement of various electromagnetic fields - or just the same field at different points $\mathbf{r}$. Then we are only interested in the behavior of the first, field-related factor, and may write

$$
\begin{equation*}
\left.\Gamma \propto|\langle f i n| \hat{a} e(\mathbf{r})| i n i\rangle\left.\right|^{2}=\langle f i n| \hat{a} e(\mathbf{r})|i n i\rangle\langle f i n| \hat{a} e(\mathbf{r})|i n i\rangle^{*}=\langle i n i| \hat{a}^{\dagger} e^{*}(\mathbf{r}) \mid \text { fin }\right\rangle\langle\text { fin }| \hat{a} e(\mathbf{r})|i n i\rangle, \tag{9.28}
\end{equation*}
$$

where the creation-annihilation operators are assumed to be taken in the initial moment (i.e., in the Schrödinger picture), and the initial and final states are those of the field alone. As we know, any 1D harmonic oscillator (and hence the electromagnetic field oscillator) has many equidistant levels, so even if it initially was in a certain state, it may undergo be several coherent transitions to different final Fock states. If we want to calculate the total rate, we may sum the transition rates into all final states. Then, since these states form a full and orthonormal set, we may use the closure condition (4.44) to get

$$
\begin{equation*}
\left.\left.\Gamma \propto \sum_{f i n}\langle i n i| \hat{a}^{\dagger} e^{*}(\mathbf{r})|f i n\rangle\langle\text { fin }| \hat{a} e(\mathbf{r}) \mid \text { ini }\right\rangle=\langle\text { ini }| \hat{a}^{\dagger} \hat{a} \mid \text { ini }\right\rangle e^{*}(\mathbf{r}) e(\mathbf{r})=\langle n\rangle_{\text {ini }}|e(\mathbf{r})|^{2} \tag{9.29}
\end{equation*}
$$

Let us apply this formula to several possible quantum states of the field mode.
(i) First, as a sanity check, the ground initial state $(n=0)$ gives no photon counts at all. The interpretation is easy: the ground state cannot emit a photon that would trigger an atom in the counter. Again, this does not mean that the ground-state motion is not observable (if you still think so, please review the Casimir effect discussion in the last section), just that it cannot ionize an atom in the detector - because it does not have any spare energy for doing that.
(ii) All other coherent states (Fock, Glauber, squeezed, etc.) of the field oscillator give the same counting rate, provided that their $\langle n\rangle$ is the same. This result may be less evident if we apply Eq. (29) to an interference of two light beams from the same source (say, in the double-slit or the Bragg-scattering configurations). In this case we may present the spatial distribution of the field as a sum

$$
\begin{equation*}
e(\mathbf{r})=e_{1}(\mathbf{r})+e_{2}(\mathbf{r}) . \tag{9.30}
\end{equation*}
$$

Here each term describes one possible wave path, so that the field product in Eq. (29) may be a rapidly changing function of the detector position. For this configuration, our result (29) means that the

[^756]interference pattern (and its contrast) are independent of the particular state of the electromagnetic field's mode.
(iii) Surprisingly, the last statement is also valid for a classical mixture of the different eigenstates of the same field mode, for example for its thermal-equilibrium state. Indeed, in this case we need to average Eq. (29) over the corresponding classical ensemble, but it would only result in a different meaning of averaging $n$ in that equation; the field part describing the interference pattern is not affected.

The last result may look a bit counter-intuitive, because common sense tells us that the stochasticity associated with thermal equilibrium has to suppress the interference pattern contrast. These expectations are (partly :-) justified, because a typical thermal source of radiation produces many field modes $j$, rather than one mode we have analyzed. These modes may have different wave numbers $k_{j}$ and hence different field distribution functions $\mathbf{e}_{j}(\mathbf{r})$, resulting in shifted interference patterns. Their summation would indeed smear the interference, suppressing its contrast.

So the use of a single photon detector is not a suitable way to distinguish different quantum states of an electromagnetic field modes. This task, however, may be achieved using the photon counting correlation technique shown in Fig. 2. ${ }^{17}$


Fig. 9.2. Photon count correlation measurement.

In this experiment, the counter rate correlation may be characterized by the so-called secondorder correlation function ${ }^{18}$ of the counting rates,
 function: definition

$$
\begin{equation*}
g^{(2)}(\tau) \equiv \frac{\left\langle\Gamma_{1}(t) \Gamma_{2}(t-\tau)\right\rangle}{\left\langle\Gamma_{1}(t)\right\rangle\left\langle\Gamma_{2}(t)\right\rangle} \tag{9.31}
\end{equation*}
$$

[^757]where the averaging may be carried out either over many similar experiments, or over time $t$, due to the ergodicity of the experiment (with a stationary light source). Using the normalized correlation function (31) is very convenient, because characteristics of the detectors and beam splitter drop our from this fraction.

Very unexpectedly for the mid-1950s, Hanbury Brown and Twiss discovered that the correlation function depends on time delay $\tau$ in the way shown schematically by the solid line in Fig. 3. It is evident from Eq. (31) that if the counting events are completely independent, $g^{(2)}(\tau)$ should be equal 1 - which is always the case in the limit $\tau \rightarrow \infty$. Hence, the observed behavior at $\tau \rightarrow 0$ corresponds to the positive correlation of detector counts at small time delays, i.e. to a higher probability of the nearly-simultaneous arrival of photons to both counters. This effect is called the photon bunching.


Fig. 9.3. Photon bunching (solid line) and antibunching for various $n$ (dashed lines). The lines approach level $g^{(2)}=1$ at $\tau \rightarrow \infty$ (on the time scale depending on the light source).

Let us use our simple single-mode model to analyze this experiment. Now the elementary quantum process, characterized by the numerator of Eq. (31), is the correlated triggering of two counters, at two spatial-temporal points $\left\{\mathbf{r}_{1}, t\right\}$ and $\left(\mathbf{r}_{2}, t-\tau\right\}$, by the same field mode, so that we need to make the following replacement, in the first of Eqs. (25):

$$
\begin{equation*}
\hat{\mathcal{E}}(\mathbf{r}, t) \rightarrow \text { const } \times \hat{\mathcal{E}}\left(\mathbf{r}_{1}, t\right) \hat{\mathcal{E}}\left(\mathbf{r}_{2}, t-\tau\right) . \tag{9.32}
\end{equation*}
$$

Repeating all the manipulations done in the single-counter case, we get

$$
\begin{equation*}
\left\langle\Gamma_{1}(t) \Gamma_{2}(t-\tau)\right\rangle \propto\langle i n i| \hat{a}(t)^{\dagger} \hat{a}(t-\tau)^{\dagger} \hat{a}(t-\tau) \hat{a}(t)|i n i\rangle e^{*}\left(\mathbf{r}_{1}\right) e^{*}\left(\mathbf{r}_{2}\right) e\left(\mathbf{r}_{1}\right) e\left(\mathbf{r}_{2}\right) . \tag{9.33}
\end{equation*}
$$

Plugging this expression, as well as Eq. (29) for single-counter rates, into Eq. (31), we see that the field distribution factors (as well as the detector-specific bra-kets and the density of states $\rho_{\text {fin }}$ ) cancel, giving a very simple final expression

$$
\begin{equation*}
g^{(2)}(\tau)=\frac{\left\langle\hat{a}^{\dagger}(t) \hat{a}^{\dagger}(t-\tau) \hat{a}(t-\tau) \hat{a}(t)\right\rangle}{\left\langle\hat{a}^{\dagger}(t) \hat{a}(t)\right\rangle^{2}} \tag{9.34}
\end{equation*}
$$

where the averaging should be carried out, as before, over the initial state of the field. Still, the calculation of this expression for arbitrary $\tau$ may be quite complex, because the relaxation of the correlation function to the asymptotic value $\mathrm{g}^{(2)}(\infty)$ in many cases is due to the interaction of the light source with environment, and hence requires the open-system techniques which were discussed in Chapter 7. However, the zero-delay value $g^{(2)}(0)$ may be calculated in a straightforward way, because the time arguments of all operators are equal, so that we may write

$$
\begin{equation*}
g^{(2)}(0)=\frac{\left\langle\hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \hat{a}\right\rangle}{\left\langle\hat{a}^{\dagger} \hat{a}\right\rangle^{2}} \tag{9.35}
\end{equation*}
$$

Let us evaluate this ratio for the simplest states of the field. (Remember, we are working in the Schrödinger picture now.)
(i) $n^{\text {th }}$ Fock state. In this case, it is convenient to act by the annihilation operators upon the ketvectors, and by the creation operators, upon the bra-vectors, using Eq. (19):

Photon
anti-
bunching

$$
\begin{equation*}
g^{(2)}(0)=\frac{\langle n| \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \hat{a}|n\rangle}{\langle n| \hat{a}^{\dagger} \hat{a}|n\rangle^{2}}=\frac{\langle n-2|[n(n-1)]^{1 / 2}[n(n-1)]^{1 / 2}|n-2\rangle}{\langle n-1| n^{1 / 2} n^{1 / 2}|n-1\rangle^{2}}=\frac{n(n-1)}{n^{2}}=1-\frac{1}{n} . \tag{9.36}
\end{equation*}
$$

We see that the correlation function at small delays is suppressed rather than enhanced - see the dashed line in Fig. 3. This photon antibunching effect has a very simple explanation: a single photon emitted by the wave source may be absorbed by just one of the detectors. For the initial state $n=1$, this is the only option, and it is very natural that Eq. (36) predicts no simultaneous counts at $\tau=0$. Despite this theoretical simplicity, reliable observations of the antibunching have not been carried out until 1977, ${ }^{19}$ due to the experimental difficulty of creating Fock states of electromagnetic field oscillators - see Sec. 4 below.
(ii) The Glauber state $\alpha$. A similar procedure, but now using Eq. (5.155) and its Hermitian conjugate, $\langle\alpha| \hat{a}^{\dagger}=\langle\alpha| \alpha^{*}$, yields

Glauber
field statistics

$$
\begin{equation*}
g^{(2)}(0)=\frac{\langle\alpha| \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \hat{a}|\alpha\rangle}{\langle\alpha| \hat{a}^{\dagger} \hat{a}|\alpha\rangle^{2}}=\frac{\alpha^{*} \alpha^{*} \alpha \alpha}{\left(\alpha^{*} \alpha\right)^{2}}=1, \tag{9.37}
\end{equation*}
$$

for any parameter $\alpha$. We see that the result is very different result from the Fock states, unless in the latter case $n \rightarrow \infty$. (We know that the Fock and Glauber properties should also coincide for the ground state, but at that state the correlation function's value is uncertain, because there are no photon counts at all.)
(iii) Classical mixture. From Chapter 7, we know that such ensembles cannot be described by single state vectors, and require the density matrix $w$ for their description. In particular, we can use the key Eq. (7.5) to write

$$
\begin{equation*}
g^{(2)}(0)=\frac{\operatorname{Tr}\left(\hat{w} \hat{a}^{\dagger} \hat{a}^{\dagger} \hat{a} \hat{a}\right)}{\left[\operatorname{Tr}\left(\hat{w} \hat{a}^{\dagger} \hat{a}\right)\right]^{2}} . \tag{9.38}
\end{equation*}
$$

The calculation is easy for an ensemble in thermodynamic equilibrium, because here the density matrix is diagonal in the basis of Fock states $n$-see Eqs. (7.23)-(7.25):

[^758]\[

$$
\begin{equation*}
w_{n n^{\prime}}=W_{n} \delta_{n n^{\prime}}, \quad W_{n}=\frac{1}{Z} \exp \left\{-\frac{E_{n}}{k_{\mathrm{B}} T}\right\}=\frac{\lambda^{n}}{\sum_{n=0}^{\infty} \lambda^{n}}, \quad \text { where } \lambda \equiv \exp \left\{-\frac{\hbar \omega}{k_{\mathrm{B}} T}\right\} . \tag{9.39}
\end{equation*}
$$

\]

So, for the operators in the numerator and denominator of Eq. (38) we also need just the diagonal terms of the operator products that have already been calculated - see Eq. (36). As a result, we get

$$
\begin{equation*}
g^{(2)}(0)=\frac{\sum_{n=0}^{\infty} W_{n} n(n-1)}{\left(\sum_{n=0}^{\infty} W_{n} n\right)^{2}}=\frac{\sum_{n=0}^{\infty} \lambda^{n} n(n-1) \times \sum_{n=0}^{\infty} \lambda^{n}}{\left(\sum_{n=0}^{\infty} \lambda^{n} n\right)^{2}} . \tag{9.40}
\end{equation*}
$$

One of these sums is just the geometric progression,

$$
\begin{equation*}
\sum_{n=0}^{\infty} \lambda^{n}=\frac{1}{1-\lambda}, \tag{9.41}
\end{equation*}
$$

and the remaining two sums may be readily calculated by its differentiation over parameter $\lambda$ :

$$
\begin{align*}
& \sum_{n=0}^{\infty} \lambda^{n} n=\lambda \sum_{n=0}^{\infty} \lambda^{n-1} n=\lambda \frac{d}{d \lambda} \sum_{n=0}^{\infty} \lambda^{n}=\lambda \frac{d}{d \lambda} \frac{1}{1-\lambda}=\frac{\lambda}{(1-\lambda)^{2}}, \\
& \sum_{n=0}^{\infty} \lambda^{n} n(n-1)=\lambda^{2} \sum_{n=0}^{\infty} \lambda^{n-2} n(n-1)=\lambda^{2} \frac{d^{2}}{d^{2} \lambda}\left(\sum_{n=0}^{\infty} \lambda^{n}\right)=\lambda^{2} \frac{d^{2}}{d \lambda^{2}} \frac{1}{1-\lambda}=\frac{2 \lambda^{2}}{(1-\lambda)^{3}}, \tag{9.42}
\end{align*}
$$

and for the correlation function we get an extremely simple result independent of parameter $\lambda$ and hence of temperature:

$$
\begin{equation*}
g^{(2)}(0)=\frac{\left[2 \lambda^{2} /(1-\lambda)^{3}\right][1 /(1-\lambda)]}{\left[\lambda /(1-\lambda)^{2}\right]^{2}}=2 \tag{9.43}
\end{equation*}
$$

Photon bunching

This is the exactly the photon bunching effect first observed by Hanbury Brown and Twiss (Fig. 3). We see that in contrast to antibunching, this is an essentially classical (statistical) effect. Indeed, Eq. (43) allows a purely classical proof. In the classical theory, the counting rate is proportional to the wave intensity $I$, so that Eq. (31) is reduced to

$$
\begin{equation*}
g^{(2)}(0)=\frac{\left\langle I^{2}\right\rangle}{\langle I\rangle^{2}}, \quad \text { with } I \propto \overline{E^{2}(t)} \propto E_{\omega} E_{\omega}^{*} \tag{9.44}
\end{equation*}
$$

For a sinusoidal field, the intensity is constant, and $g^{(2)}(0)=1$. (This is also evident from Eq. (37), because the classical state may be considered as the Glauber state with $\alpha \rightarrow \infty$.) On the other hand, if intensity fluctuates (either in time, or from one experiment to another), the averages should be calculated as

$$
\begin{equation*}
\left\langle I^{N}\right\rangle=\int_{0}^{\infty} w(I) I^{N} d I, \quad \text { with } \int_{0}^{\infty} w(I) d I=1 \tag{9.45}
\end{equation*}
$$

where $w(I)$ is the probability density. For the classical (Boltzmann) statistics, the probability is an exponential function of the electromagnetic field energy, and hence its intensity:

$$
\begin{equation*}
w(I)=C e^{-\beta I}, \quad \text { where } \beta \propto 1 / k_{\mathrm{B}} T \tag{9.46}
\end{equation*}
$$

so that Eqs. (48) yield:

$$
\begin{align*}
& \int_{0}^{\infty} C \exp \{-\beta I\} d I=1, \quad \text { so that } C=\beta  \tag{9.47}\\
& \left\langle I^{N}\right\rangle=\int_{0}^{\infty} w(I) I^{N} d I=C \int_{0}^{\infty} \exp \{-\beta I\} I^{N} d I=\frac{1}{\beta^{N}} \int_{0}^{\infty} \exp \{-\xi\} \xi^{N} d \xi= \begin{cases}1 / \beta, & \text { for } N=1, \\
2 / \beta^{2}, & \text { for } N=2 .\end{cases}
\end{align*}
$$

Plugging these results into Eq. (44), we get $g^{(2)}(0)=2$, in a complete agreement with Eq. (43). ${ }^{20}$

### 9.3. Spontaneous and stimulated emission

In our simple model for photon counting, considered in the last section, trigger atoms of the photon counter absorbed light. Now let us have a look at the opposite process of spontaneous emission of photons by an atom in an excited state, still using the same electric-dipole approximation for the atom-to-field interaction. We may still use the Golden Rule for the model depicted in Fig. 6.14, but now the roles have changed: we have to associate operator $\hat{A}$ with the electric dipole moment of the atom, while operator $\hat{B}$ with the electric field, and the continuous spectrum of system $b$ represents the plurality of the electromagnetic field modes into which the spontaneous radiation may happen. Since now the transition increases the energy of the electromagnetic field, after the multiplication of the field bra-ket by $\exp \{i \omega t\}$, we may keep only the photon creation operator whose time evolution compensates this fast "rotation". As a result, the Golden Rule takes the following form:

Spontaneous photon
pmission emission
rate

$$
\begin{equation*}
\Gamma_{s}=\pi \omega \mid\left.\langle\text { fin }| \hat{a}^{\dagger}|0\rangle\right|^{2} \mid\left.\langle\text { fin }| \hat{\mathbf{d}} \cdot \mathbf{e}(\mathbf{r})|i n i\rangle\right|^{2} \rho_{f i n} \tag{9.48}
\end{equation*}
$$

where all operators and states are time-independent, and $\rho_{\text {fin }}$ is now the density of final states of the electromagnetic field - which in this problem plays the role of atom's environment. Here the electromagnetic field has been assumed to be initially in the ground state - the assumption that will be altered later in this section.

Relation (48), together with Eq. (19), shows that in order for field's matrix element be different from zero, the final state of the field has to be the first excited Fock state, $n=1$. (By the way, this is exactly the most practicable way of generating an excited Fock state of a field oscillator field - whose existence was taken for granted in our discussion in Sec. 2.) With that, Eq. (48) yields

$$
\begin{equation*}
\left.\left.\Gamma_{s}=\pi \omega|\langle f i n| \hat{\mathbf{d}} \cdot \mathbf{e}(\mathbf{r})| i n i\right\rangle\left.\right|^{2} \rho_{\mathrm{fin}}=\pi \omega\left|\langle f i n| \hat{d} e_{d}(\mathbf{r})\right| i n i\right\rangle\left.\right|^{2} \rho_{f i n}, \tag{9.49}
\end{equation*}
$$

[^759]where the density $\rho_{\text {fin }}$ of excited electromagnetic field states should be calculated at energy $\hbar \omega$, and $e_{d}$ is the component of the vector $\mathbf{e}(\mathbf{r})$ along the electric dipole direction. ${ }^{21}$ For plane waves, the calculation of this density was our first step in this course - see Eq. (1.1). ${ }^{22}$ From it, we get
\[

$$
\begin{equation*}
\rho_{\mathrm{fin}} \equiv \frac{d N}{d E}=V \frac{8 \pi v^{2}}{c^{3}} \frac{d v}{d E}=V \frac{\omega^{2}}{\pi^{2} \hbar c^{3}} \tag{9.50}
\end{equation*}
$$

\]

where the bounding volume $V$ should be large enough to ensure spectrum's virtual continuity. Because of that, in the normalization condition used to simplify Eq. (9), we may consider $e^{2}(\mathbf{r})$ constant. Let us present the square of this vector as a sum of squares of its three perpendicular components (one of those, $e_{d}$, aligned with the dipole direction), due to space isotropy we may write

$$
\begin{equation*}
e^{2} \equiv e_{d}^{2}+e_{\perp 1}^{2}+e_{\perp 2}^{2}=3 e_{d}^{2} \tag{9.51}
\end{equation*}
$$

As a result, the normalization condition yields

$$
\begin{equation*}
e_{d}^{2}=\frac{1}{3 \varepsilon_{0} V} . \tag{9.52}
\end{equation*}
$$

and Eq. (49) gives the famous (and very important) formula ${ }^{23}$

$$
\begin{equation*}
\left.\Gamma_{s}=\frac{1}{4 \pi \varepsilon_{0}} \frac{4 \omega^{3}}{3 \hbar c^{3}}|\langle f i n| \hat{\mathbf{d}}| i n i\right\rangle\left.\right|^{2}=\frac{1}{4 \pi \varepsilon_{0}} \frac{4 \omega^{3}}{3 \hbar c^{3}}\langle\text { fin }| \hat{\mathbf{d}}|i n i\rangle \cdot\langle i n i| \hat{\mathbf{d}}|f i n\rangle^{*} . \tag{9.53}
\end{equation*}
$$

Leaving a comparison of this formula with the classical theory of radiation, ${ }^{24}$ and the exact evaluation of $\Gamma_{\mathrm{s}}$ for a particular transition in the hydrogen atom, for reader's exercises, let me just estimate its order of magnitude. Assuming that $d \sim e r_{\mathrm{B}} \equiv e \hbar^{2} / m_{e}\left(e^{2} / 4 \pi \varepsilon_{0}\right)$ and $\hbar \omega \sim E_{\mathrm{H}} \equiv m_{e}\left(e^{2} / 4 \pi \varepsilon_{0}\right)^{2} / \hbar^{2}$, and taking into account the definition (6.62) of the fine structure constant $\alpha \approx 1 / 137$, we get

$$
\begin{equation*}
\frac{\Gamma}{\omega} \sim\left(\frac{e^{2}}{4 \pi \varepsilon_{0} \hbar c}\right)^{3} \equiv \alpha^{3} \sim 3 \times 10^{-7} \tag{9.54}
\end{equation*}
$$

This estimate says that the emission lines at atomic transitions are typically very sharp. With the present-day availability of high-speed electronics, it also makes sense to evaluate the time scale $\tau=1 / \Gamma$ of the typical quantum transition: for a typical optical frequency $\omega \sim 3 \times 10^{15} \mathrm{~s}^{-1}$, it is close to 1 ns . This is

[^760]exactly the time constant that determines the photon counting statistics of the emitted radiation - see Fig. 3. Colloquially, this is the temporal scale of the photon spontaneously emitted by an atom. ${ }^{25}$

Note, however, that the above estimate of $\tau$ is only valid for a transition with a non-vanishing dipole matrix element. If it equals zero - say, due to the initial and final state symmetry - the dipole transitions are "forbidden". (Another commonly used term is the transition selection rules. ${ }^{26}$ ) The "forbidden" transition may still take place due to a different, smaller interaction (say, via a magnetic dipole field of the atom, or its quadrupole electric field ${ }^{27}$ ), but would take much longer. In some cases the increase of $\tau$ is rather dramatic - sometimes to hours! Such long-lasting radiation is called luminescence - or fluorescence if the initial atom's excitation was due to an external radiation of higher frequency, followed first by non-radiative transitions down the energy level ladder.

Now let us consider a more general case when the electromagnetic field is initially in an arbitrary Fock state $n$, and from it may either get energy from the atomic system (photon emission) or, vice versa, give it back to the atom (photon absorption). For the photon emission rate, an evident generalization of Eq. (48) gives

$$
\begin{equation*}
\frac{\Gamma_{e}}{\Gamma_{s}} \equiv \frac{\Gamma_{n \rightarrow \text { fin }}}{\Gamma_{0 \rightarrow 1}}=\frac{\mid\left.\langle\text { fin }| \hat{a}^{\dagger}|n\rangle\right|^{2}}{\left.\left|\langle 1| \hat{a}^{\dagger}\right| 0\right\rangle\left.\right|^{2}}, \tag{9.55}
\end{equation*}
$$

where both bra-kets may be taken in the Schrödinger picture, and $\Gamma_{\mathrm{s}}$ is the spontaneous emission rate (53) of the same atomic system. This relation, with the account of Eq. (19), shows that at photon

$$
\begin{equation*}
\Gamma_{e}=(n+1) \Gamma_{s} . \tag{9.56}
\end{equation*}
$$

Thus the initial field increases the photon emission rate; this effect is called the stimulated emission of radiation. Note that the spontaneous emission may be considered as a particular case of stimulated emission for $n=0$, and interpreted as the emission stimulated by zero-point fluctuations of the electromagnetic field.

On the other hand, in accordance with the arguments of Sec. 2, for the description of radiation absorption the photon creation operator has to be replaced with the annihilation one, to get

$$
\begin{equation*}
\frac{\Gamma_{a}}{\Gamma_{s}}=\frac{|\langle f i n| \hat{a}| n\rangle\left.\right|^{2}}{\left.\left|\langle 1| \hat{a}^{\dagger}\right| 0\right\rangle\left.\right|^{2}} . \tag{9.57}
\end{equation*}
$$

[^761]According to this equation, the final state of the field at absorption is the Fock state with $n$ ' $=n-1$, and Eq. (57) yields ${ }^{28}$

$$
\begin{equation*}
\Gamma_{a}=n \Gamma_{s} . \tag{9.58}
\end{equation*}
$$

Photon absorption rate

Results (56) and (58) are usually be formulated in terms of between the Einstein coefficients $A$ and $B$ defined in the way shown in Fig. 4, where the two energy levels are those of the atom, $\Gamma_{a}$ is the rate of energy absorption from the electromagnetic field, and $\Gamma_{e}$ is that of the energy emission into the field. In this notation, Eqs. (56) and (58) say

$$
\begin{equation*}
A_{21}=B_{21}=B_{12} \tag{9.59}
\end{equation*}
$$

Einstein coefficients' relation
because each of these coefficients equals the spontaneous emission rate $\Gamma_{\mathrm{s}}$.


Fig. 9.4. The Einstein coefficients on the atomic energy spectrum diagram.

It is curious that from this point, there is just one step to an alternative derivation of the BoseEinstein statistics for photons. Indeed, in the thermodynamic equilibrium, the average probability flows between levels 1 and 2 should be equal:

$$
\begin{equation*}
W_{2}\left\langle\Gamma_{e}\right\rangle=W_{1}\left\langle\Gamma_{a}\right\rangle, \tag{9.60}
\end{equation*}
$$

where $W_{1}$ and $W_{2}$ are the probabilities for the atomic system to be on the corresponding levels, so that Eqs. (56) and (58) yield

$$
\begin{equation*}
W_{2} \Gamma_{s}\langle 1+n\rangle=W_{1} \Gamma_{s}\langle n\rangle, \quad \text { i.e. } \quad \frac{W_{2}}{W_{1}}=\frac{\langle n\rangle}{\langle n\rangle+1} . \tag{9.61}
\end{equation*}
$$

But, on the other hand, for the atomic subsystem, only weakly coupled to its electromagnetic environment, we ought to have the Gibbs distribution of probabilities:

$$
\begin{equation*}
\frac{W_{2}}{W_{1}}=\frac{\exp \left\{-E_{2} / k_{\mathrm{B}} T\right\}}{\exp \left\{-E_{1} / k_{\mathrm{B}} T\right\}}=\exp \left\{-\frac{\Delta E}{k_{\mathrm{B}} T}\right\}=\exp \left\{-\frac{\hbar \omega}{k_{\mathrm{B}} T}\right\} . \tag{9.62}
\end{equation*}
$$

Requiring Eqs. (61) and (62) to give the same result for the probability ratio, we get the Bose-Einstein distribution for the electromagnetic field in equilibrium:

$$
\begin{equation*}
\langle n\rangle=\frac{1}{\exp \left\{\hbar \omega / k_{\mathrm{B}} T\right\}-1}, \tag{9.63}
\end{equation*}
$$

the same as obtained in Sec. 7.1 by other means - see Eqs. (7.26).

[^762]Another, very important implication of Eqs. (56) and (58) is the possibility to achieve the stimulated emission coherence by level occupancy (or "population") inversion. Indeed, if $W_{2}>W_{1}$, then the net power flow from the atomic system into the electromagnetic field,

$$
\begin{equation*}
\text { power }=\hbar \omega \times \Gamma_{s}\left[W_{2}(\langle n\rangle+1)-W_{1}\langle n\rangle\right], \tag{9.64}
\end{equation*}
$$

may be positive. The necessary inversion may be produced using several ways, notably by a intensive quantum transitions to level 2 from an even higher level (which, in turn, is populated, e.g., by absorption of an external radiation, called pumping, at a higher frequency.)

A less obvious feature of the stimulated emission is spelled out by Eq. (55): again, it shows that the final state of the field after the absorption of energy $\hbar \omega$ from the atom is a pure (coherent) Fock state $(n+1)$. Colloquially, one may say that the new, $(n+1)^{\text {st }}$ photon emitted from the atom is automatically in phase with the $n$ photons that had been in the field mode initially. ${ }^{29}$ The idea of stimulated emission of coherent radiation using population inversion ${ }^{30}$ was implemented in the early 1950s in the microwave range (masers) and in 1960 in the optical range (lasers). Nowadays, lasers are ubiquitous and constitute one of cornerstones of our technological civilization.

A quantitative discussion of laser operation is beyond the framework of this course, and I have to refer the reader to special literature, ${ }^{31}$ and would only like to mention only two key points:
(i) In a typical laser, each generated electromagnetic field mode is in the Glauber (rather than the Fock) state, so that Eqs. (56) and (58) are applicable only for $n$ is averaged over the Fock-state decomposition of the Glauber state - see Eq. (5.165).
(ii) Since in a typical laser $\langle n\rangle \gg 1$, its operation may be well described using quasi-classical theories that use Eq. (64) to describe the electromagnetic energy balance (with the addition of a term describing the energy loss due to field absorption in external components of the laser, including the useful load), plus the equation describing the balance of occupancies $W_{1,2}$ due to all inter-level transitions - similar to Eq. (60), but including also the contribution(s) from the particular population inversion mechanism used in the laser. At this approach, the role of quantum mechanics is essentially reduced to the calculation of parameter $\Gamma_{\mathrm{s}}$.

The role becomes more prominent if one needs to describe fluctuations of the laser field. Here two approaches are possible, following the two options discussed in Chapter 7. If the fluctuations are relatively small, one can linearize the Heisenberg equations of motion of the field oscillator operators near their stationary-lasing "values", with the Langevin "forces" (also time-dependent operators) to describe the fluctuation sources, and use these Heisenberg-Langevin equations to the radiation fluctuations, just as was described in Sec. 7.5. On the other hand, near the lasing threshold the field fluctuations are relatively strong, smearing the phase transition between the no-lasing and lasing states. Here the linearization is not an option, but one can use the density-matrix approach described in Sec. 7.6 , for the fluctuation analysis. ${ }^{32}$

[^763]
### 9.4. Cavity QED

Now I have to mention, at least in passing, the cavity quantum electrodynamics (usually called cavity $Q E D$ for short) - an art and science of creating and using entanglement between quantum states of a single atomic system (either an atom, or an ion, or a molecule, etc.) and the electromagnetic field in a macroscopic volume called the resonant cavity (or just "resonator", or just "cavity"). This field is very popular nowadays, especially in the context of the quantum computation and communication research discussed in Sec. 8.5. ${ }^{33}$

Let me start its discussion by noting that the narrative of two last sections was based on an implicit assumption that the energy spectrum of the electromagnetic field interacting with an atomic system is essentially continuous. This assumption has justified the use of Golden Rule, implying that the emitted radiation is spread among many field modes, effectively loosing their coherence with the initial quantum state of the atom. However, this assumption becomes invalid if the electromagnetic field is contained inside a relatively small volume, with a linear size comparable with the radiation wavelength. Classical electrodynamics shows ${ }^{34}$ that if the walls of such a cavity mostly reflect, rather than absorb, radiation, so that in the crude approximation the power dissipation may be disregarded, then particular solutions $\mathbf{e}_{j}(\mathbf{r})$ of the Helmholtz equation (5) correspond to discrete, well separated mode wavenumbers $k_{j}$ and hence well separated eigenfrequencies $\omega_{j}$. Due to the energy conservation, an atomic transition corresponding to energy $\Delta E=\left|E_{\text {ini }}-E_{\text {fin }}\right|$ may be effective only if the corresponding quantum oscillation frequency $\Omega \equiv \Delta E / \hbar$ is close to one of $\omega_{j}$ and hence relatively far from other eigenfrequencies. ${ }^{35}$ As a result, the quantum states of a single atomic system and the resonant electromagnetic mode may become entangled.

A very popular approximation for the qualitative description of this effect is the so-called Rabi model, ${ }^{36}$ in which the atom is treated as a two-level system ${ }^{37}$ interacting with a single electromagnetic field mode of the resonant cavity. As the reader knows well from Chapters 4-6, any two-level ("spin-1/2") system may be described by Hamiltonian $\mathbf{c} \cdot \hat{\boldsymbol{\sigma}}$, and we may always select the state basis in that the Hamiltonian is diagonal:

$$
\begin{equation*}
\hat{H}_{\mathrm{atom}}=c \hat{\sigma}_{z} \equiv \frac{\hbar \Omega}{2} \hat{\sigma}_{z}, \tag{9.65}
\end{equation*}
$$

where $\hbar \Omega \equiv 2 c$ is the energy difference between the eigenenergies in the absence of interaction with the field. Next, according to Eq. (17), ignoring the constant ground-state energy $\hbar \omega / 2$ (that may be added to
while the laser radiation fluctuations may look like a peripheral issue, pioneering research in that field has led to the development of the general theory of open quantum systems (which was discussed in Chapter 7), that has much broader applications.
${ }^{33}$ This popularity was demonstrated, for example, by the 2012 Nobel Prize in Physics award to cavity QED experimentalists S. Haroche and D. Wineland.
${ }^{34}$ See, e.g., EM Sec. 7.9.
${ }^{35}$ On the contrary, if $\Omega$ is far from any $\omega_{j}$, the interaction is much suppressed; in particular, the spontaneous emission rate may be much lower than that given by Eq. (53) - so that this result is not as fundamental as it may look.
${ }^{36}$ After the pioneering work by I. Rabi in 1936-37.
${ }^{37}$ As was shown in Sec. 6.5, this model is justified, e.g., if transitions between all other energy level pairs have considerably different frequencies.
the final energy in the very end - if necessary), the contribution of a single mode of eigenfrequency $\omega$ to the Hamiltonian is

$$
\begin{equation*}
\hat{H}_{\text {cavity }}=\hbar \omega \hat{a}^{\dagger} \hat{a} \tag{9.66}
\end{equation*}
$$

Finally, according to Eq. (16a), in quantum electrodynamics the electric field of the mode may be presented as

$$
\begin{equation*}
\hat{\mathcal{E}}(\mathbf{r}, t)=\frac{1}{i}\left(\frac{\hbar \omega}{2}\right)^{1 / 2} \mathbf{e}(\mathbf{r})\left(\hat{a}-\hat{a}^{\dagger}\right), \tag{9.67}
\end{equation*}
$$

so that in the electric-dipole approximation (24), the cavity-atom interaction may be presented as a product of the field by one of Cartesian components (say, $\sigma_{y}$ ) of the "spin" operator:38

$$
\begin{equation*}
\hat{H}_{\mathrm{int}}=\mathrm{const} \times \hat{\sigma}_{y} \times \varepsilon=\mathrm{const} \times \hat{\sigma}_{y} \times\left(\frac{\hbar \omega}{2}\right)^{1 / 2} \frac{1}{i}\left(\hat{a}-\hat{a}^{\dagger}\right)=i \hbar \kappa \hat{\sigma}_{y}\left(\hat{a}-\hat{a}^{\dagger}\right) \tag{9.68}
\end{equation*}
$$

where $\kappa$ is a coupling constant (with the dimension of frequency). The sum of these terms is called the Rabi Hamiltonian,

$$
\begin{equation*}
\hat{H} \equiv \hat{H}_{\mathrm{atom}}+\hat{H}_{\mathrm{cavity}}+\hat{H}_{\mathrm{int}}=\frac{\hbar \Omega}{2} \hat{\sigma}_{z}+\hbar \omega \hat{a}^{\dagger} \hat{a}+i \hbar \kappa \hat{\sigma}_{y}\left(\hat{a}-\hat{a}^{\dagger}\right) \tag{9.69}
\end{equation*}
$$

Despite its apparent simplicity, using this Hamiltonian for calculations is not that simple. For example, an exact quasi-analytical expression for its eigenenergies (as zeros of a Taylor series in parameter $\kappa$, with coefficients determined by a recurrence relation) was found only recently. ${ }^{39}$ Only in the case when the electromagnetic field is very intensive and hence may be treated as the classical one, the results following from Eq. (69) are reduced to the Rabi oscillations discussed in Sec. 6.3.

In the opposite case when the field oscillator is in an essentially quantum state, $\left\langle\hat{a}^{\dagger} \hat{a}\right\rangle \sim 1$, Eq. (69) may be simplified in a different way, assuming that frequencies $\Omega$ and $\omega$ are very close, and the atom-to-cavity interaction is relatively weak, so that magnitudes of the coupling constant $\kappa$ and the detuning parameter (similar to parameter $\Delta$ used in Sec. 6.5),

$$
\begin{equation*}
\xi \equiv \Omega-\omega, \tag{9.70}
\end{equation*}
$$

are both much smaller than $\Omega \approx \omega$. To discuss this limit, it is convenient to use the spin ladder operators defined absolutely similarly for those of the orbital angular momentum - see Eqs. (5.182):

$$
\begin{equation*}
\hat{\sigma}_{ \pm} \equiv \hat{\sigma}_{x} \pm i \hat{\sigma}_{y}, \text { so that } \hat{\sigma}_{y}=\frac{\hat{\sigma}_{+}-\hat{\sigma}_{-}}{2 i} . \tag{9.71}
\end{equation*}
$$

From Eq. (4.105), it is easy to find matrices of these operators (in the standard $z$-basis),

$$
\sigma_{+}=\left(\begin{array}{ll}
0 & 2  \tag{9.72}\\
0 & 0
\end{array}\right), \quad \sigma_{-}=\left(\begin{array}{ll}
0 & 0 \\
2 & 0
\end{array}\right)
$$

[^764]and their commutation rules - that are naturally similar to Eqs. (5.183):
\[

$$
\begin{equation*}
\left[\hat{\sigma}_{+}, \hat{\sigma}_{-}\right]=4 \hat{\sigma}_{z}, \quad\left[\hat{\sigma}_{z}, \hat{\sigma}_{ \pm}\right]= \pm 2 \hat{\sigma}_{ \pm} \tag{9.73}
\end{equation*}
$$

\]

In this notation, the Rabi Hamiltonian looks like

$$
\begin{equation*}
\hat{H}=\frac{\hbar \Omega}{2} \hat{\sigma}_{z}+\hbar \omega \hat{a}^{\dagger} \hat{a}+\frac{\hbar \kappa}{2}\left(\hat{\sigma}_{+}-\hat{\sigma}_{-}\right)\left(\hat{a}-\hat{a}^{\dagger}\right) \tag{9.74}
\end{equation*}
$$

and it is straightforward to use Eq. (4.199) and (73) to derive the Heisenberg-picture equations of motion for the involved operators. (Doing this, we have to remember that operators of the "spin" subsystem, on one hand, and of the field mode, on the other hand, are defined in different Hilbert spaces and hence commute - at least at coinciding time moments.) The result (so far, exact!) is

$$
\begin{gather*}
\dot{\hat{a}}=-i \omega \hat{a}+\frac{i \kappa}{2}\left(\hat{\sigma}_{+}-\hat{\sigma}_{-}\right), \quad \dot{\hat{a}}^{\dagger}=i \omega \hat{a}^{\dagger}-\frac{i \kappa}{2}\left(\hat{\sigma}_{+}-\hat{\sigma}_{-}\right), \\
\dot{\hat{\sigma}}_{ \pm}= \pm i \Omega \hat{\sigma}_{ \pm}+i 2 \kappa\left(\hat{a}-\hat{a}^{\dagger}\right) \hat{\sigma}_{z}, \quad \dot{\hat{\sigma}}_{z}=i \kappa\left(\hat{a}^{\dagger}-\hat{a}\right)\left(\hat{\sigma}_{+}+\hat{\sigma}_{-}\right) . \tag{9.75}
\end{gather*}
$$

Now note that at negligible coupling, $\kappa \rightarrow 0$, equations (75) have very simple solutions,

$$
\begin{equation*}
\hat{a}(t) \propto e^{-i \omega t}, \quad \hat{a}^{\dagger}(t) \propto e^{i \omega t}, \quad \hat{\sigma}_{ \pm}(t) \propto e^{ \pm i \Omega t}, \quad \hat{\sigma}_{z}(t) \approx \mathrm{const} \tag{9.76}
\end{equation*}
$$

and small terms proportional to $\kappa$ in the right-hand parts of Eqs. (75) cannot affect these time evolution laws dramatically even if $\kappa$ is not exactly zero (but small). Of those terms, ones with frequencies close to the "basic" frequency of each variable would act in resonance and hence may have a substantial impact on system dynamics, while non-resonant terms may be ignored. In this rotating-wave approximation (RWA), used several times before in this course, Eqs. (75) are reduced to a much simpler system of equations:

$$
\begin{gather*}
\dot{\hat{a}}=-i \omega \hat{a}-\frac{i \kappa}{2} \hat{\sigma}_{-}, \quad \dot{\hat{a}}^{\dagger}=i \omega \hat{a}^{\dagger}+\frac{i \kappa}{2} \hat{\sigma}_{+},  \tag{9.77}\\
\dot{\hat{\sigma}}_{+}=i \Omega \hat{\sigma}_{+}+i 2 \kappa \hat{a}^{\dagger} \hat{\sigma}_{z}, \quad \dot{\hat{\sigma}}_{-}=-i \Omega \hat{\sigma}_{-}-i 2 \kappa \hat{a} \hat{\sigma}_{z}, \quad \dot{\hat{\sigma}}_{z}=i \kappa\left(\hat{a}^{\dagger} \hat{\sigma}_{-}-\hat{a} \hat{\sigma}_{+}\right) .
\end{gather*}
$$

Alternatively, these equations of motion may be obtained from the Rabi Hamiltonian after it has been cleared of the terms proportional to $\hat{\sigma}_{+} \hat{a}^{\dagger}$ and $\hat{\sigma}_{-} \hat{a}$, that oscillate fast and hence self-average to virtually zero:

$$
\begin{equation*}
\hat{H}=\frac{\hbar \Omega}{2} \hat{\sigma}_{z}+\hbar \omega \hat{a}^{\dagger} \hat{a}+\frac{\hbar \kappa}{2}\left(\hat{\sigma}_{+} \hat{a}+\hat{\sigma}_{-} \hat{a}^{\dagger}\right), \quad \text { at } \kappa,|\xi| \ll \omega, \Omega . \tag{9.78}
\end{equation*}
$$

Janes-
Cummings
Hamiltonian

This is the famous Janes-Cummings Hamiltonian, ${ }^{40}$ which is central to the cavity QED and its applications. ${ }^{41}$ In order to find its eigenstates and eigenenergies, let us note that at negligible interaction

[^765]( $\kappa \rightarrow 0$ ), the spectrum of the total energy $E$ of the system, that in this limit is the sum of two independent contributions from the atomic ("spin") and resonant-cavity subsystems,
\[

$$
\begin{equation*}
\left.E\right|_{\kappa=0}= \pm \frac{\hbar \Omega}{2}+\hbar \omega n \equiv E_{n} \pm \frac{\hbar \xi}{2} \tag{9.79}
\end{equation*}
$$

\]

consists ${ }^{42}$ of close level pairs (Fig. 5) centered to values

$$
\begin{equation*}
E_{n} \equiv \hbar \omega\left(n-\frac{1}{2}\right), \quad \text { with } n=1,2, \ldots \tag{9.80}
\end{equation*}
$$

(At the exact resonance $\omega=\Omega$, i.e. at $\xi=0$, each pair merges into one double-degenerate level $E_{n}$.)


Since at $\kappa \rightarrow 0$ the two subsystems do not interact, the eigenstates corresponding to the sublevels of $n$-th pair may be represented by products of their independent ket-vectors:

As we know from Chapter 6, weak interaction leads to strong hybridization of quantum states with close energies (in this case, two states (81) with each pair with the same $n$ ) and their negligible mixing with other states. Hence, at $0<\kappa \ll \omega \approx \Omega$, a good approximation of an eigenstate with $E \approx E_{n}$ is given by a linear superposition of states (81):

$$
\begin{equation*}
|\alpha\rangle=c_{+}|\uparrow\rangle \otimes|n-1\rangle+c_{-}|\downarrow\rangle \otimes|n\rangle \tag{9.82}
\end{equation*}
$$

with certain $c$-number coefficients $c_{ \pm}$. This relation describes the entanglement of atomic eigenstates $\uparrow$ and $\downarrow$ with Fock states $n$ and $n-1$ of the field mode.

Let me leave the (straightforward) calculation of coefficients $c_{ \pm}$and eigenenergies of the two entangled state pairs for reader's exercise. This calculation shows, in particular, that at the exact resonance $(\omega=\Omega),\left|c_{+}\right|=\left|c_{-}\right|=1 / \sqrt{ } 2$ for both states of each pair. This fact may be interpreted as a (coherent!) equal sharing of an energy quantum $\hbar \omega=\hbar \Omega$ by the atom and the cavity.

A by-product of the calculation of $c_{ \pm}$, is the fact that the dynamics of state $\alpha$ described by Eq. (82) is similar to that of the generic two-level system that was repeatedly discussed in this course - first

[^766]time in Sec. 2.6 and then in Chapters 4-6. In particular, if the composite system had been initially prepared to be in one component state, for example $|\uparrow\rangle \otimes|0\rangle$ (i.e. the atom excited, while the cavity in its ground state) and allowed to evolve on its own, after some time interval it may be found in the counterpart state $|\downarrow\rangle \otimes|1\rangle$, including the first excited Fock state $n=1$ of the field mode. This is one more (resonant) version of the same method for generation of Fock states of electromagnetic field which was discussed in Sec. 3.43

Unfortunately, my time devoted to cavity QED is over, and for further reading I have to refer the reader to special literature. ${ }^{44}$

### 9.5. The Klein-Gordon and relativistic Schrödinger equations

Now let us discuss the basics of relativistic quantum mechanics of particles with a nonvanishing rest mass $m$ - i.e., in terms of Eq. (1), the intermediate range of energies: $E \sim m c^{2}$, i.e. for $p \sim m c$. Historically, the first attempt ${ }^{45}$ to extend the non-relativistic wave mechanics into the relativistic energy range was based on performing the same transitions from classical observables to their quantummechanical operators as in the non-relativistic limit:

$$
\begin{equation*}
\mathbf{p} \rightarrow \hat{\mathbf{p}}=-i \hbar \nabla, \quad E \rightarrow \hat{H}=i \hbar \frac{\partial}{\partial t} \tag{9.83}
\end{equation*}
$$

Substitution of these operators, acting on the Schrödinger-picture wavefunction $\Psi(\mathbf{r}, t)$, into the classical relation between the energy $E$ and momentum $\mathbf{p}$ (for of a free particle) leads to the following equations:

Table 9.1. Deriving the Klein-Gordon equation for a free relativistic particle. ${ }^{46}$

|  | Non-relativistic limit | Relativistic case |
| :---: | :---: | :---: |
| Classical <br> mechanics | $E=\frac{1}{2 m} p^{2}$ | $E^{2}=c^{2} p^{2}+\left(m c^{2}\right)^{2}$ |
| Wave <br> mechanics | $i \hbar \frac{\partial}{\partial t} \Psi=\frac{1}{2 m}(-i \hbar \nabla)^{2} \Psi$ | $\left(i \hbar \frac{\partial}{\partial t}\right)^{2} \Psi=c^{2}(-i \hbar \nabla)^{2} \Psi+\left(m c^{2}\right)^{2} \Psi$ |

[^767]The resulting equation for the non-relativistic limit is just the usual Schrödinger equation (1.28) for a free particle. Its relativistic generalization, usually rewritten as

Klein-
Gordon
equation

$$
\begin{equation*}
\left(\frac{1}{c^{2}} \frac{\partial^{2}}{\partial t^{2}}-\nabla^{2}\right) \Psi+\mu^{2} \Psi=0, \quad \text { with } \mu \equiv \frac{m c}{\hbar} \tag{9.84}
\end{equation*}
$$

is called the Klein-Gordon (or sometimes "Klein-Gordon-Fock") equation. The most fundamental solutions of this equation are the same plane, monochromatic waves

$$
\begin{equation*}
\Psi(\mathbf{r}, t) \propto \exp \{i(\mathbf{k} \cdot \mathbf{r}-\omega t)\} . \tag{9.85}
\end{equation*}
$$

as in the non-relativistic case. Indeed, such waves are eigenstates of operators (83), with eigenvalues

$$
\begin{equation*}
\mathbf{p}=\hbar \mathbf{k}, \quad E=\hbar \omega \tag{9.86}
\end{equation*}
$$

so that their substitution into Eq. (84) immediately returns us to Eq. (1) with replacements (86):

$$
\begin{equation*}
E_{ \pm}=\hbar \omega_{ \pm}= \pm\left[(\hbar c k)^{2}+\left(m c^{2}\right)^{2}\right]^{1 / 2} \tag{9.87}
\end{equation*}
$$

Though one may say that this dispersion relation is just a simple combination of the classical relation (1) and the same basic quantum-mechanical relations (86) as in non-relativistic limit, it attracts our attention to the fact that energy $\hbar \omega$ as a function of momentum $\hbar \mathbf{k}$ has two rather than one branches, with $E_{-}(\mathbf{p})=-E_{+}(\mathbf{p})-$ see Fig. 6a.


(b)

Fig. 9.6. (a) Free-particle dispersion relation resulting from the Klein-Gordon and Dirac equations, and (b) creation of a particle-antiparticle pair from the vacuum.

Historically, this fact has played a very important role for spurring the fundamental idea of particle-antiparticle pairs. In this idea (very similar to the concept of electrons and holes in semiconductors, which was discussed in Sec. 2.8), what we call the vacuum actually corresponds to all states of the lower branch, with energies $E(\mathbf{p})<0$, being filled, while the states on the upper branch, with energies $E_{+}(\mathbf{p})>0$, being empty. Then an externally supplied energy

$$
\begin{equation*}
\Delta E=E_{+}-E_{-}=E_{+}+\left(-E_{-}\right) \geq 2 m c^{2}>0 \tag{9.88}
\end{equation*}
$$

may bring the system from the lower branch to the upper one (Fig. 6b). The resulting excited state is interpreted as a combination of a particle (formally, of the infinite spatial extension) with energy $E_{+}$and momentum $\mathbf{p}$, and a "hole" (antiparticle) of positive energy ( $-E_{-}$) and momentum $-\mathbf{p}$. This idea ${ }^{47}$ has led

[^768]to a search for, and discovery of the positron: electron's antiparticle with charge $q=+e$, in 1932, and later of the antiproton and other antiparticles.

Free particles of a finite spatial extension may be described, in this approach, just in the nonrelativistic Schrödinger equation, by wave packets: linear superpositions of de-Broglie waves (85) with close wave vectors $\mathbf{k}$, and $\omega$ given by Eq. (87), with the positive sign for the "usual" particles, and negative sign for antiparticles - see Fig. 6a above. Note that in order to form, from a particle's wave packet, a similar wave packet for the antiparticle, with the same phase and group velocities (2.33) in each direction, we need to change the sign not only before $\omega$, but also before $\mathbf{k}$, i.e. to replace all component wavefunctions (85), and hence the full wavefunction, with their complex conjugates.

Of more formal properties of the equation, it is easy to prove that its solutions satisfy the same continuity equation (1.52) with the probability current density $\mathbf{j}$ still given by Eq. (1.47), but a different expression for the probability density $w$ - which becomes very similar to that for $\mathbf{j}$ :

$$
\begin{equation*}
w=\frac{i \hbar}{2 m c^{2}}\left(\Psi^{*} \frac{\partial \Psi}{\partial t}-\text { c.c. }\right), \quad \mathbf{j}=\frac{i \hbar}{2 m}\left(\Psi \nabla \Psi^{*}-\text { c.c. }\right) . \tag{9.89}
\end{equation*}
$$

(In the non-relativistic limit $v / c \rightarrow 0$, Eq. (84) allows a reduction of the first relation to Eq. (1.22): $w \rightarrow$ $\Psi \Psi^{*}$.)

The Klein-Gordon equation may be readily generalized to describe a single particle moving in external fields; for example, the electromagnetic field effects on a particle with charge $q$ may be described by the same replacement as in the non-relativistic limit (see Sec. 3.1):48

$$
\begin{equation*}
\hat{\mathbf{p}} \rightarrow \hat{\mathbf{P}}-q \mathbf{A}(\mathbf{r}, t), \quad \hat{H} \rightarrow \hat{H}-q \phi(\mathbf{r}, t) \tag{9.90}
\end{equation*}
$$

where $\hat{\mathbf{P}}=-i \hbar \nabla$ is the canonical momentum operator (3.25), and the vector- and scalar potentials, $\mathbf{A}$ and $\phi$, should be treated appropriately - either as $c$-number functions if the electromagnetic field quantization is unimportant, or as operators (see Secs. 1-4 above) if it is.

However, the practical value of the relativistic Schrödinger equation is rather limited, because of two main reasons. First of all, it does not give the correct description of particles with spin. For example, for the hydrogen-like atom, i.e. the motion of an electron with electric charge $-e$ in the Coulomb central field (3.182) of an immobile nucleus with charge $+Z e$, the equation may be readily solved exactly ${ }^{49}$ and yields the following spectrum of (doubly-degenerate) energy levels:

$$
\begin{equation*}
E=m c^{2}\left(1+\frac{Z^{2} \alpha^{2}}{\lambda^{2}}\right)^{-1 / 2}, \quad \text { with } \lambda \equiv n+\left[\left(l+\frac{1}{2}\right)^{2}-Z^{2} \alpha^{2}\right]^{1 / 2}-\left(l+\frac{1}{2}\right) \tag{9.91}
\end{equation*}
$$

where $n=1,2, \ldots$ and $l=0,1, \ldots, n-1$ are the same quantum numbers as in the non-relativistic theory (see Sec. 3.6), and $\alpha \equiv e^{2} / 4 \pi \varepsilon_{0} \hbar c \approx 1 / 137$ is the fine structure constant - see Eq. (6.62). The three leading terms of the Taylor expansion of this result in small parameter $Z \alpha$ are as follows:

$$
\begin{equation*}
E \approx m c^{2}\left[1-\frac{Z^{2} \alpha^{2}}{2 n^{2}}-\frac{Z^{4} \alpha^{4}}{2 n^{4}}\left(\frac{n}{l+1 / 2}-\frac{3}{4}\right)\right] . \tag{9.92}
\end{equation*}
$$

[^769]The first of these terms is just the rest energy of the particle. The second term,

$$
\begin{equation*}
E_{n}=-m c^{2} \frac{Z^{2} \alpha^{2}}{2 n^{2}}=-\frac{m Z^{2} e^{4}}{\left(4 \pi \varepsilon_{0}\right)^{2} \hbar^{2}} \frac{1}{2 n^{2}}=-\frac{E_{0}}{2 n^{2}}, \quad \text { with } E_{0}=Z^{2} E_{\mathrm{H}} \tag{9.93}
\end{equation*}
$$

reproduces the non-relativistic Bohr's formula (3.191). Finally, the third term,

$$
\begin{equation*}
-m c^{2} \frac{Z^{4} \alpha^{4}}{2 n^{4}}\left(\frac{n}{l+1 / 2}-\frac{3}{4}\right)=-\frac{2 E_{n}^{2}}{m c^{2}}\left(\frac{n}{l+1 / 2}-\frac{3}{4}\right) \tag{9.94}
\end{equation*}
$$

is just the kinetic-relativistic contribution (6.52) to the fine structure of the Bohr levels (93). However, as we already know from Sec. 6.3, for a spin $-1 / 2$ particle such as the electron, the spin-orbit interaction (6.56) gives an additional contribution of the same order to the fine structure, so that the net result, confirmed by experiment, is given by Eq. (6.60), i.e. different from Eq. (94). This is very natural, because the relativistic Schrödinger equation does not have the very notion of spin.

Second, even for massive spinless particles (such as $Z^{0}$ bosons), for which this equation is believed to be valid, the most important problems are related to particle interactions at high energies of the order of $\Delta E \sim 2 m c^{2}$ (88) and beyond. Due to possibility of creation and annihilation of particleantiparticle pairs at such energies, the number of particles participating in such interactions is typically considerable (and variable), and its adequate description of the system is given not by the relativistic Schrödinger equation (which is formulated in single-particle terms), but by the quantum field theory - to which I will devote just a few sentences in the very end of this chapter.

### 9.6. Dirac's theory

The real breakthrough toward the quantum relativistic theory of electrons (and any spin- $1 / 2$ fermions) was achieved in 1928 by P. A. M. Dirac. For that time, the structure of his theory was highly nontrivial. Namely, while formally preserving, in the coordinate representation, the same Schrödingerpicture equation of quantum dynamics as in the non-relativistic quantum mechanics, ${ }^{50}$

$$
\begin{equation*}
i \hbar \frac{\partial \Psi}{\partial t}=\hat{H} \Psi \tag{9.95}
\end{equation*}
$$

it postulates that wavefunction $\Psi$ is not a scalar complex function of time and coordinates, but a fourcomponent column-vector (sometimes called the bispinor) of such functions, its Hermitian-conjugate bispinor $\Psi^{\dagger}$ being a 4-component row-vector of their complex conjugates:

$$
\Psi=\left(\begin{array}{l}
\Psi_{1}(\mathbf{r}, t)  \tag{9.96}\\
\Psi_{2}(\mathbf{r}, t) \\
\Psi_{3}(\mathbf{r}, t) \\
\Psi_{4}(\mathbf{r}, t)
\end{array}\right), \quad \Psi^{\dagger}=\left(\begin{array}{lll}
\left.\Psi_{1}^{*}(\mathbf{r}, t) \quad \Psi_{2}^{*}(\mathbf{r}, t) \quad \Psi_{3}^{*}(\mathbf{r}, t) \quad \Psi_{4}^{*}(\mathbf{r}, t)\right), ~, ~
\end{array}\right.
$$

[^770]and that the Hamiltonian participating in Eq. (95) is a $4 \times 4$ matrix in the Hilbert space of bispinors $\Psi$. For a free particle, the postulated Hamiltonian looks amazingly simple: ${ }^{51}$
\[

$$
\begin{equation*}
\hat{H}=c \hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}}+\hat{\beta} m c^{2} \tag{9.97}
\end{equation*}
$$

\]

where $\hat{\mathbf{p}}=-i \hbar \nabla$ is the same 3D vector of momentum component operators as in the non-relativistic case, while operators $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ may be presented in the following shorthand $2 \times 2$ form:

$$
\hat{\boldsymbol{\alpha}} \equiv\left(\begin{array}{cc}
0 & \hat{\boldsymbol{\sigma}}  \tag{9.98a}\\
\hat{\boldsymbol{\sigma}} & 0
\end{array}\right), \quad \hat{\beta} \equiv\left(\begin{array}{cc}
\hat{I} & 0 \\
0 & -\hat{I}
\end{array}\right)
$$

Dirac operators

Operator $\hat{\boldsymbol{\alpha}}$, composed of the Pauli vector operators $\hat{\boldsymbol{\sigma}}$, is also a vector in the usual 3D space, so that each of its 3 Cartesian components is a $4 \times 4$ matrix. The particular form of the $2 \times 2$ matrices corresponding to operators $\hat{\boldsymbol{\sigma}}$ and $\hat{I}$ in Eq. (98a) depends on the basis selected for representation of the spin states of the particle; for example, in the standard $z$-basis, in which the Cartesian components $\hat{\sigma}_{x}$, $\hat{\sigma}_{y}$, and $\hat{\sigma}_{z}$ of $\hat{\boldsymbol{\sigma}}$ are represented by the Pauli matrices (4.105), the full matrix form of Eq. (98a) is

$$
\alpha_{x}=\left(\begin{array}{cccc}
0 & 0 & 0 & 1  \tag{9.98b}\\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{array}\right), \quad \alpha_{y}=\left(\begin{array}{cccc}
0 & 0 & 0 & -i \\
0 & 0 & i & 0 \\
0 & -i & 0 & 0 \\
i & 0 & 0 & 0
\end{array}\right), \quad \alpha_{z}=\left(\begin{array}{cccc}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0
\end{array}\right), \quad \beta=\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{array}\right) .
$$

(According to the second of Eq. (98a), $\beta$ has this form in any spin basis.) It is straightforward to use Eqs. (98) to verify that matrices $\alpha_{x}, \alpha_{y}, \alpha_{z}$ and $\beta$ satisfy the following relations:

$$
\begin{gather*}
\alpha_{x}^{2}=\alpha_{y}^{2}=\alpha_{z}^{2}=\beta^{2}=1,  \tag{9.99}\\
\alpha_{x} \alpha_{y}+\alpha_{y} \alpha_{x}=\alpha_{y} \alpha_{z}+\alpha_{z} \alpha_{y}=\alpha_{z} \alpha_{x}+\alpha_{x} \alpha_{z}=\alpha_{x} \beta+\beta \alpha_{x}=\alpha_{y} \beta+\beta \alpha_{y}=\alpha_{z} \beta+\beta \alpha_{z}=0, \tag{9.100}
\end{gather*}
$$

i.e. anticommute.

Acting essentially as in Sec. 4.1, but using commutation relations (99)-(100), it is straightforward to show that any solution to the Dirac equation obeys the probability conservation law, i.e. the continuity equation (1.52), with the probability density,
${ }^{51}$ Moreover, if the time derivative participating in Eq. (95) and the three coordinate derivatives participating (via the momentum operator) in Eq. (97), are merged into one 4 -vector operator $\partial / \partial x_{k} \equiv\{\nabla, \partial / \partial(c t)\}$, the Dirac equation (95) may be rewritten in an even simpler, manifestly Lorentz-invariant 4 -vector form (with the implicit summation over the repeated index $k=1, \ldots, 4-\mathrm{see}$, e,g., EM Sec. 9.4):

$$
\left(\hat{\gamma}_{k} \frac{\partial}{\partial x_{k}}+\mu\right) \Psi=0, \quad \text { where } \hat{\boldsymbol{\gamma}} \equiv\left\{\hat{\gamma}_{1}, \hat{\gamma}_{2}, \hat{\gamma}_{3}\right\}=\left(\begin{array}{cc}
0 & -i \hat{\boldsymbol{\sigma}} \\
i \hat{\boldsymbol{\sigma}} & 0
\end{array}\right), \quad \hat{\gamma}_{4}=\hat{\boldsymbol{\beta}},
$$

where $\mu \equiv m c / \hbar$ - just as in Eq. (84). Note also that, very counter-intuitively, the Dirac Hamiltonian (97) is linear in momentum, while the non-relativistic Hamiltonian of a particle, as well as the relativistic Schrödinger equation, are quadratic in $\mathbf{p}$. In my humble opinion, the Dirac theory (including the concept of antiparticles) may compete for the title of the most revolutionary theoretical idea in physics, despite such heavy contenders as the Newton laws, the Maxwell equations, the Einstein's relativity, the Bohr atom, and the Gibbs' statistical distributions.

$$
\begin{equation*}
w=\Psi^{\dagger} \Psi \tag{9.101}
\end{equation*}
$$

and the probability current,

$$
\begin{equation*}
\mathbf{j}=c \Psi^{\dagger} \hat{\boldsymbol{\alpha}} \Psi \tag{9.102}
\end{equation*}
$$

looking almost as in the non-relativistic theory - cf. Eqs. (1.22) and (1.47). Note, however, the Hermitian conjugation used in these formulas instead of the complex conjugation, in order to form scalars $w, j_{x}, j_{y}$, and $j_{z}$ from 4-component vectors (96).

This qualified similarity is extended to the fundamental, plane-wave solutions of the Dirac equations is free space. Indeed, plugging such solution, in the form

$$
\Psi=\mathrm{u} e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)}=\left(\begin{array}{l}
u_{1}  \tag{9.103}\\
u_{2} \\
u_{3} \\
u_{4}
\end{array}\right) e^{i(\mathbf{k} \cdot \mathbf{r}-\omega t)}
$$

into Eqs. (95) and (97), we get a system of 4 coupled, linear algebraic equations for 4 complex $c$-number amplitudes $u_{1,2,3,4}$. The condition of their consistency yields the same dispersion relation (87), i.e. the same two-branch diagram shown in Fig. 6, as follows from the Klein-Gordon equation. The difference is that plugging each value of $\omega$, given by Eq. (87), back into the system of equations for amplitudes $u$, we get two solutions for vector $u$ for each of the energy branches. In the standard spin $z$-basis they may be presented as:

$$
\begin{align*}
& \text { for } E=E_{+}>0: \quad \mathbf{u}_{+\uparrow}=c_{+\uparrow}\left(\begin{array}{c}
1 \\
0 \\
\frac{c p_{z}}{E_{+}+m c^{2}} \\
\frac{c\left(p_{x}+i p_{y}\right)}{E_{+}+m c^{2}}
\end{array}\right), \quad \mathbf{u}_{+\downarrow}=c_{+\downarrow}\left(\begin{array}{c}
0 \\
\frac{c\left(p_{x}-i p_{y}\right)}{E_{+}+m c^{2}} \\
\frac{-c p_{z}}{E_{+}+m c^{2}}
\end{array}\right),  \tag{9.104a}\\
& \text { for } E=E_{-}<0: \quad \mathrm{u}_{-\uparrow}=c_{\uparrow}\left(\begin{array}{c}
\frac{c p_{z}}{E_{-}-m c^{2}} \\
\frac{c\left(p_{x}+i p_{y}\right)}{E_{-}-m c^{2}} \\
1 \\
0
\end{array}\right), \quad \mathbf{u}_{-\downarrow}=c_{\downarrow}\left(\begin{array}{c}
\frac{c\left(p_{x}-i p_{y}\right)}{E_{-}-m c^{2}} \\
\frac{-c p_{z}}{E_{-}-m c^{2}} \\
0 \\
1
\end{array}\right), \tag{9.104b}
\end{align*}
$$

where $c$ are normalization coefficients.
The simplest interpretation of these solutions is that Eq. (103) with vectors $u_{+}$, given by Eq. (104a), represents a spin- $1 / 2$ particle (say, an electron), while that with vectors u. given by Eq. (104b) represents an antiparticle (a positron), and two solutions for each particle correspond to two opposite directions of spin, $\sigma_{z}= \pm 1, S_{z}= \pm \hbar / 2$. This interpretation is indeed solid in the non-relativistic limit, when two last components of vector (104a) and two first components of vector (104b) are negligibly small:

$$
u_{+\uparrow} \rightarrow\left(\begin{array}{l}
1  \tag{9.105}\\
0 \\
0 \\
0
\end{array}\right), \quad \mathbf{u}_{+\downarrow} \rightarrow\left(\begin{array}{l}
0 \\
1 \\
0 \\
0
\end{array}\right), \quad \mathbf{u}_{-\uparrow} \rightarrow\left(\begin{array}{l}
0 \\
0 \\
1 \\
0
\end{array}\right), \quad \mathbf{u}_{-\downarrow} \rightarrow\left(\begin{array}{l}
0 \\
0 \\
0 \\
1
\end{array}\right), \quad \text { at } \frac{p_{k}}{m c} \rightarrow 0
$$

In order to show this, let us use the Dirac equation to calculate the Heisenberg-picture law of time evolution of operators of the Cartesian components of the orbital angular momentum $\mathbf{L} \equiv \mathbf{r} \times \mathbf{p}$, for example of $L_{x}=y p_{z}-z p_{y}$, taking into account that operators (98a) commute with those of $\mathbf{r}$ and $\mathbf{p}$, and also the Heisenberg commutation relations (2.14):

$$
\begin{equation*}
i \hbar \frac{\partial \hat{L}_{x}}{\partial t}=\left[\hat{L}_{x}, \hat{H}\right]=c \hat{\boldsymbol{a}} \cdot\left[\left(\hat{y} \hat{p}_{z}-\hat{z} \hat{p}_{y}\right), \hat{\mathbf{p}}\right]=-i \hbar c\left(\hat{\alpha}_{z} \hat{p}_{y}-\hat{\alpha}_{y} \hat{p}_{z}\right) \tag{9.106}
\end{equation*}
$$

with similar relations for two other Cartesian components of the operator. Since the right-hand part of these equations is different from zero, the orbital momentum is generally not conserved - even for a free particle! Let us, however, consider the following vector operator,

$$
\hat{\mathbf{S}} \equiv \frac{\hbar}{2}\left(\begin{array}{ll}
\hat{\boldsymbol{\sigma}} & 0  \tag{9.107a}\\
0 & \hat{\boldsymbol{\sigma}}
\end{array}\right)
$$

whose Cartesian components, in the $z$-basis, are represented by $4 \times 4$ matrices

$$
\mathrm{S}_{x}=\frac{\hbar}{2}\left(\begin{array}{cccc}
0 & 1 & 0 & 0  \tag{9.107b}\\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right), \quad \mathrm{S}_{y}=\frac{\hbar}{2}\left(\begin{array}{cccc}
0 & -i & 0 & 0 \\
i & 0 & 0 & 0 \\
0 & 0 & 0 & -i \\
0 & 0 & i & 0
\end{array}\right), \quad \mathrm{S}_{z}=\frac{\hbar}{2}\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1
\end{array}\right)
$$

and calculate the Heisenberg-picture law of time evolution of these components, for example

$$
\begin{equation*}
i \hbar \frac{\partial \hat{S}_{x}}{\partial t}=\left[\hat{S}_{x}, \hat{H}\right]=c\left[\hat{S}_{x},\left(\hat{\alpha}_{x} \hat{p}_{x}+\hat{\alpha}_{y} \hat{p}_{y}+\hat{\alpha}_{z} \hat{p}_{z}\right)\right] \tag{9.108}
\end{equation*}
$$

A direct calculation of the commutators of matrices (98) and (107) yields

$$
\begin{equation*}
\left[\hat{S}_{x}, \hat{\alpha}_{x}\right]=0, \quad\left[\hat{S}_{x}, \hat{\alpha}_{y}\right]=i \hbar \hat{\alpha}_{z}, \quad\left[\hat{S}_{x}, \hat{\alpha}_{z}\right]=-i \hbar \hat{\alpha}_{y} \tag{9.109}
\end{equation*}
$$

so that we finally get

$$
\begin{equation*}
i \hbar \frac{\partial \hat{S}_{x}}{\partial t}=i \hbar c\left(\hat{\alpha}_{z} \hat{p}_{y}-\hat{\alpha}_{y} \hat{p}_{z}\right) \tag{9.110}
\end{equation*}
$$

with similar expressions for other two components of the operator. Comparing this result with Eq. (106), we see that any Cartesian component of operator (5.198),

$$
\begin{equation*}
\hat{\mathbf{J}} \equiv \hat{\mathbf{L}}+\hat{\mathbf{S}} \tag{9.111}
\end{equation*}
$$

is an integral of motion, ${ }^{52}$ so that this operator may be interpreted as the one presenting the total angular momentum. Hence, operator (104) may be interpreted as the spin operator of a spin-1/2 particle (e.g., electron). As it follows from the last of Eq. (107b), columns (105) represent the eigenkets of the $z$ component of that operator, with eigenstates $S_{z}= \pm \hbar / 2$, depending on the arrow index. So, the Dirac theory provides a justification for spin- $1 / 2$ - or, somewhat more humbly, replaces the spin hypothesis by an assumption of a simpler (and hence more plausible), Lorentz-invariant Hamiltonian (97).

Note, however, that this fact is not true for the exact solutions (103)-(104), so that generally the eigenstates of the Dirac Hamiltonian are certain linear (coherent) superpositions of component wavefunctions describing the particle and its antiparticle - each with both directions of spin. This fact leads to several interesting effects, including the so-called Klien paradox at reflection of a particle from a tunnel barrier. ${ }^{53}$ It is curious that some of these effects may be reproduced in such non-relativistic systems as electron moving in a 2D honeycomb lattice (e.g., in graphene), since they also feature a (locally) linear dispersion relation - see Eq. (3.122). ${ }^{54}$

### 9.7. Low-energy limit

The generalization of the Dirac's theory to the case of a particle with electric charge $q$, moving in a classically-described electromagnetic field may be obtained using the same Eqs. (90). As a result, Eq. (95) becomes

$$
\begin{equation*}
\left[c \hat{\boldsymbol{\alpha}} \cdot(-i \hbar \nabla-q \mathbf{A})+m c^{2} \hat{\beta}+(q \phi-\hat{H})\right] \Psi=0 \tag{9.112}
\end{equation*}
$$

where the Hamiltonian operator $\hat{H}$ is understood in the sense of Eq. (95), i.e. as the partial time derivative with multiplier $i \hbar$. Let us prepare this equation for a low-energy approximation by acting on its left-hand part by a similar square bracket (also an operator!), but with the opposite sign before the last parentheses. Using relations (99) and (100), and the fact that space- and time-independent operators $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ commute with the spin-independent functions $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$, as well as with the Hamiltonian operator $i \hbar \partial / \partial t$, the result is

$$
\begin{equation*}
\left\{c^{2}[\hat{\boldsymbol{\alpha}} \cdot(-i \hbar \nabla-q \mathbf{A})]^{2}+\left(m c^{2}\right)^{2}-c[\hat{\boldsymbol{\alpha}} \cdot(-i \hbar \nabla-q \mathbf{A}),(q \phi-\hat{H})]-(q \phi-\hat{H})^{2}\right\} \Psi=0 . \tag{9.113}
\end{equation*}
$$

A direct calculation of the first square bracket, using Eqs. (98) and (107), yields

$$
\begin{equation*}
[\hat{\boldsymbol{\alpha}} \cdot(-i \hbar \nabla-q \mathbf{A})]^{2}=(-i \hbar \nabla-q \mathbf{A})^{2}-2 q \hat{\mathbf{S}} \cdot \nabla \times \mathbf{A} . \tag{9.114}
\end{equation*}
$$

But according to the last of Eqs. (3.21), the last vector product in the right-hand part is just the magnetic field

$$
\begin{equation*}
\boldsymbol{B}=\nabla \times \mathbf{A} . \tag{9.115}
\end{equation*}
$$

Similarly, we may use the first of Eqs. (3.21), for the electric field,

$$
\begin{equation*}
\varepsilon=-\nabla \phi-\frac{\partial \mathbf{A}}{\partial t} \tag{9.116}
\end{equation*}
$$

[^771]to simplify the commutator participating in Eq. (9.113):
\[

$$
\begin{equation*}
[\hat{\boldsymbol{\alpha}} \cdot(-i \hbar \nabla-q \mathbf{A}),(q \phi-\hat{H})]=-q \hat{\boldsymbol{\alpha}} \cdot[\hat{H}, \mathbf{A}]-i \hbar q \hat{\boldsymbol{\alpha}} \cdot[\nabla, \phi]=-i \hbar q \frac{\partial \mathbf{A}}{\partial t}-i \hbar \hat{\boldsymbol{\alpha}} \cdot \nabla \phi=i \hbar q \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\varepsilon} . \tag{9.117}
\end{equation*}
$$

\]

As a result, Eq. (110) becomes

$$
\begin{equation*}
\left\{c^{2}(-i \hbar \nabla-q \mathbf{A})^{2}+(q \phi-\hat{H})^{2}-\left(m c^{2}\right)^{2}-2 q c^{2} \hat{\mathbf{S}} \cdot \boldsymbol{B}+i \hbar c q \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\varepsilon}\right\} \Psi=0 . \tag{9.118}
\end{equation*}
$$

So far, this is an exact result, equivalent to Eq. (112), but more convenient for an analysis of the low-energy limit in that not only the offset energy $E-m c^{2}$ (which is the energy used in non-relativistic quantum mechanics), but also the electrostatic energy of the particle, $|q\langle\phi\rangle|$, are much smaller than the rest energy $m c^{2}$. In this limit, the second and third terms of Eq. (118) almost cancel, and introducing the offset Hamiltonian

$$
\begin{equation*}
\hat{\tilde{H}} \equiv \hat{H}-m c^{2} \hat{I} \tag{9.119}
\end{equation*}
$$

we may approximate their difference, up to the first nonvanishing term, as

$$
\begin{equation*}
(q \phi \hat{I}-\hat{H})^{2}-\left(m c^{2}\right)^{2} \hat{I} \equiv\left(q \phi \hat{I}-m c^{2} \hat{I}-\hat{\tilde{H}}\right)^{2}-\left(m c^{2}\right)^{2} \hat{I} \approx 2 m c^{2}(\hat{\tilde{H}}-q \phi \hat{I}) . \tag{9.120}
\end{equation*}
$$

As a result, after division of all terms by $2 m c^{2}$, Eq. (118) may be approximated as

$$
\begin{equation*}
\hat{\tilde{H}} \Psi=\left[\frac{1}{2 m}(-i \hbar \nabla-q \mathbf{A})^{2}+q \phi-\frac{q}{m} \hat{\mathbf{S}} \cdot \boldsymbol{B}+\frac{i \hbar q}{2 m c} \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\varepsilon}\right] \Psi . \tag{9.121}
\end{equation*}
$$

Let us discuss this important result. The first two terms in the square brackets give the Hamiltonian (3.26) that was extensively used in Chapter 3 for the discussion of non-relativistic motion of charged particles. Note again that the contribution of the vector-potential $\mathbf{A}$ into that Hamiltonian is essentially relativistic, in the following sense: when used for the description of magnetic interaction of two charged particles, due to their orbital motion with speed $v \ll c$, the magnetic interaction is a factor of $(v / c)^{2}$ smaller than the electrostatic interaction of the particles. ${ }^{55}$ The reason why we did discuss the effects of $\mathbf{A}$ in Chapter 3 was that is was used there to describe external magnetic fields, keeping our analysis valid even for the cases when that field is strong by being produced by relativistic effects - such as aligned spins in a permanent magnet.

The next, third term in the square brackets is also familiar to the reader: it was introduced informally in Sec. 4.1, and then formally in Sec. 4.4 to describe the effect of magnetic field on particle's spin - see Eqs. (4.3), (4.5), and (4.163). When justifying this form of interaction, I referred mostly to results of Stern-Gerlach-type experiments, but it is extremely pleasing that this result ${ }^{56}$ follows from such a fundamental relativistic treatment as Dirac's theory. As we already know from the discussion of

[^772]the Zeeman effect in Sec. 6.4, the effects of magnetic field on the orbital motion of an electron (described by orbital angular momentum $\mathbf{L}$ ) and its spin $\mathbf{S}$ are of the same order, i.e. present an essentially relativistic effect.

Finally, the last term in the square brackets of Eq. (121) is also not quite new for us: in particular it describes the spin-orbit interaction. Indeed, in the case of classical, spherical-symmetric electric field $\varepsilon$ with potential $\phi(r)=U(r) / q$, the term may be reduced to Eq. (6.56b):

$$
\begin{equation*}
\hat{H}_{\mathrm{so}}=\frac{1}{2 m^{2} c^{2}} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}} \frac{1}{r} \frac{d U}{d r}=-\frac{q}{2 m^{2} c^{2}} \hat{\mathbf{S}} \cdot \hat{\mathbf{L}} \frac{1}{r} \varepsilon . \tag{9.122}
\end{equation*}
$$

The proof of this correspondence requires a bit of additional work, ${ }^{57}$ because in Eq. (121), the term responsible for the spin-orbit interaction acts on 4-component wavefunctions, while Hamiltonian (122) is supposed to act on non-relativistic wavefunctions with account of spin, whose coordinate representation is given by 2 -component columns - spinors: ${ }^{58}$

$$
\begin{equation*}
\psi=\binom{\psi_{\uparrow}}{\psi_{\downarrow}} . \tag{9.123}
\end{equation*}
$$

The simplest way to prove the identity of the two formulas is not to use Eq. (121) directly, but to return to the Dirac equation (112), for the particular case of motion in a stationary electric field with no magnetic field, when Dirac's Hamiltonian is reduced to

$$
\begin{equation*}
\hat{H}=c \hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}}+\hat{\beta} m c^{2}+U(\mathbf{r}) \tag{9.124}
\end{equation*}
$$

Since this Hamiltonian is time-independent, we may look for its 4-component eigenfunctions in the form

$$
\begin{equation*}
\Psi(\mathbf{r}, t)=\binom{\psi_{+}(\mathbf{r})}{\psi_{-}(\mathbf{r})} \exp \left(-i \frac{E}{\hbar} t\right) \tag{9.125}
\end{equation*}
$$

where each of $\psi_{ \pm}$is a 2-component column of the type (123), representing two spin states of the particle (index + ) and antiparticle (index -). Plugging Eq. (125) into Eq. (124), and using Eq. (98a), we get the following system of two linear equations:

$$
\begin{align*}
& {\left[E-m c^{2}-U(\mathbf{r})\right] \psi_{+}-c \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \psi_{-}=0}  \tag{9.126}\\
& {\left[E+m c^{2}-U(\mathbf{r})\right] \psi_{-}-c \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \psi_{+}=0}
\end{align*}
$$

[^773]Expressing $\psi$ - from the latter equation, and plugging the result into the former one, we get the following single equation for particle's spinor:

$$
\begin{equation*}
\left[E-m c^{2}-U(\mathbf{r})-c^{2} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \frac{1}{E+m c^{2}-U(\mathbf{r})} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\right] \psi_{+}=0 . \tag{9.127}
\end{equation*}
$$

So far, this is an exact equation for eigenstates and eigenvalues of Hamiltonian (124). It may be substantially simplified in the low-energy limit when both the potential energy ${ }^{59}$ and the non-relativistic eigenenergy

$$
\begin{equation*}
\widetilde{E} \equiv E-m c^{2} \tag{9.128}
\end{equation*}
$$

are much less than $m c^{2}$. Indeed, in this case the expression in denominator of the last term in the brackets of Eq. (127) is close to $2 m c^{2}$. Since $\sigma^{2}=1$, with that replacement, Eq. (127) is reduced to the non-relativistic Schrödinger equation, similar for both spin components of $\psi_{+}$, and hence giving spindegenerate energy levels. In order to recover small relativistic and spin-orbit effects, we need a slightly more accurate approximation:

$$
\begin{equation*}
\frac{1}{E+m c^{2}-U(\mathbf{r})} \equiv \frac{1}{2 m c^{2}+\widetilde{E}-U(\mathbf{r})}=\frac{1}{2 m c^{2}}\left[1+\frac{\widetilde{E}-U(\mathbf{r})}{2 m c^{2}}\right]^{-1} \approx \frac{1}{2 m c^{2}}\left[1-\frac{\widetilde{E}-U(\mathbf{r})}{2 m c^{2}}\right] \tag{9.129}
\end{equation*}
$$

in which Eq. (127) is reduced to

$$
\begin{equation*}
\left[\widetilde{E}-U(\mathbf{r})-\frac{\hat{p}^{2}}{2 m}+\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \frac{\widetilde{E}-U(\mathbf{r})}{\left(2 m c^{2}\right)^{2}} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}\right] \psi_{+}=0 . \tag{9.130}
\end{equation*}
$$

As follows from Eqs. (5.46)-(5.47), the operators of momentum and of a function of coordinates commute as

$$
\begin{equation*}
[\hat{\mathbf{p}}, U(\mathbf{r})]=-i \hbar \nabla U, \tag{9.131}
\end{equation*}
$$

so that the last term in square brackets of Eq. (130) may be rewritten as

$$
\begin{equation*}
\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}} \frac{\widetilde{E}-U(\mathbf{r})}{(2 m c)^{2}} \hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}=\frac{\widetilde{E}-U(\mathbf{r})}{(2 m c)^{2}} \hat{p}^{2}-\frac{i \hbar}{(2 m c)^{2}}(\hat{\boldsymbol{\sigma}} \cdot \nabla U)(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}) . \tag{9.132}
\end{equation*}
$$

Since in the low-energy limit both terms in the right-hand part of this relation are much smaller than the three leading terms of Eq. (130), in the first of them we may replace the numerator with its nonrelativistic value $\hat{p}^{2} / 2 m$. With this replacement, the term coincides with the first relativistic correction to the kinetic energy operator - see Eqs. (6.47) and (6.49a). The second term, proportional to the electric field $\varepsilon=-\nabla \phi=-\nabla U / q$, may be transformed further on, using a readily verifiable relation

$$
\begin{equation*}
(\hat{\boldsymbol{\sigma}} \cdot \nabla U)(\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}})=(\nabla U) \cdot \hat{\mathbf{p}}+i \hat{\boldsymbol{\sigma}} \cdot[(\nabla U) \times \hat{\mathbf{p}}] . \tag{9.133}
\end{equation*}
$$

Of the two terms in the right-hand part, only the second one depends on spin, ${ }^{60}$ giving the following spin-orbital interaction contribution to the Hamiltonian,

[^774]\[

$$
\begin{equation*}
\hat{H}_{\mathrm{so}}=\frac{\hbar}{(2 m c)^{2}} \hat{\boldsymbol{\sigma}} \cdot[(\nabla U) \times \hat{\mathbf{p}}]=\frac{q}{2 m^{2} c^{2}} \hat{\mathbf{S}} \cdot[(\nabla \phi) \times \hat{\mathbf{p}}] . \tag{9.134}
\end{equation*}
$$

\]

For a central electric field with $\phi(\mathbf{r})=\phi(r)$, the potential gradient has only one, radial component: $\nabla \phi=$ $(d \phi / d r) \mathbf{r} / \mathbf{r}=-\varepsilon \mathbf{r} / r$, and with the angular momentum definition $\hat{\mathbf{L}} \equiv \mathbf{r} \times \hat{\mathbf{p}}$, Eq. (134) is reduced to Eq. (122).

As was shown in Sec. 6.3, the perturbative treatment of Eq. (122), together with the kineticrelativistic correction (6.49), in the hydrogen-like atom problem, leads to the fine structure of each Bohr level $E_{n}$, given by Eq. (6.60):

$$
\begin{equation*}
\Delta E_{\mathrm{so}}=-\frac{2 E_{n}}{m c^{2}}\left(3-\frac{4 n}{j+1 / 2}\right) . \tag{9.135}
\end{equation*}
$$

This result gets a confirmation from the surprising fact that for the hydrogen-like atom problem, the Dirac equation may be solved exactly - without any assumptions. I do not have time/space to reproduce the solution, ${ }^{61}$ and will list just the final result for the energy spectrum:

H-like
atom's eigenenergies

$$
\begin{equation*}
\frac{E}{m c^{2}}=\left\{1+\frac{Z^{2} \alpha^{2}}{\left[n+\left\{(j+1 / 2)^{2}-Z^{2} \alpha^{2}\right\}^{1 / 2}-(j+1 / 2)\right]^{2}}\right\}^{-1 / 2} . \tag{9.136}
\end{equation*}
$$

Here $n=1,2, \ldots$ is the same main quantum number as in Bohr's theory, while $j$ is the quantum number specifying eigenvalues (5.203) of the total angular momentum's square $J^{2}$ in the units of $\hbar^{2}$, taking halfinteger values: $j=l \pm 1 / 2=1 / 2,3 / 2,5 / 2, \ldots$ - see Eq. (5.215). Such set of quantum numbers is rather natural, because due to the spin-orbit interaction, the orbital and spin angular momenta are not conserved, while their vector sum, $\mathbf{J}=\mathbf{L}+\mathbf{S}$, is - in the absence of external magnetic field. Each energy level (136) is doubly-degenerate, with two eigenstates representing two directions of spin - i.e. two values of $l=j \mp 1 / 2$ at fixed j .

Since according to Eq. (1.9), the square of the fine-structure constant $\alpha \equiv e^{2} / 4 \pi \varepsilon_{0} \hbar \mathrm{c}$ may be presented as the ratio $E_{\mathrm{H}} / m c^{2}$, the low-energy limit $\left(E-m c^{2} \sim E_{\mathrm{H}} \ll m c^{2}\right)$ may be pursued by expanding Eq. (136) into the Taylor series in $(Z \alpha)^{2} \ll 1$. The result,

$$
\begin{equation*}
E \approx m c^{2}\left[1-\frac{Z^{2} \alpha^{2}}{2 n^{2}}-\frac{Z^{4} \alpha^{4}}{2 n^{4}}\left(\frac{n}{j+1 / 2}-\frac{3}{4}\right)\right], \tag{9.137}
\end{equation*}
$$

has the same structure, and allows the same interpretation as Eq. (92), but with the last term coinciding with Eq. (6.52) - and with experimental results. Historically, this correct description of the fine structure of atomic levels provided a decisive proof of Dirac's theory.

However, even such an impressive theory does not have too many direct applications. The main reason for that was already discussed in brief in the end of Sec. 5: due to the possibility of creation and

[^775]annihilation of particle-antiparticle pairs at energies higher than $2 m c^{2}$, the number of particles participating in high-energy interactions is not fixed. An adequate general description of such situation is given by the quantum field theory, in which the particle wavefunction is treated as a field to be quantized, using so-called field operators $\hat{\Psi}(\mathbf{r}, t)$ - very much as the electromagnetic field was treated in Secs. 1-4 above. (The Dirac equation follows from the quantum field theory in the single-particle approximation.)

As was mentioned above on several occasions, the quantum field theory is beyond the scope of this course, and I have to stop here, referring the interested reader to one of several excellent available textbooks on this discipline. ${ }^{62}$ (I would strongly encourage the student going in this direction to start with playing with the field operators on this or her own, taking clues from Eqs. (16), but replacing the creation / annihilations operators $\hat{a}_{j}^{\dagger}$ and $\hat{a}_{j}$ of the harmonic oscillator with those of the general second quantization formalism outlined in Sec. 8.3.)

### 9.8. Exercise problems

9.1.* Prove the Casimir formula (23) for the attraction force $F=-P A$ between two perfectly conducting parallel plates of area $A$, separated by a narrow vacuum gap $d \ll A^{1 / 2}$.

Hint: You may like to use the Euler-Maclaurin formula. ${ }^{63}$
9.2. Radiation of some single-mode quantum sources may have such a high degree of coherence that it is possible to observe interference from two independent sources with virtually the same frequency, incident on one detector.
(i) Generalize Eq. (29) to this case.
(ii) Use the generalized expression to show that incident waves in different Fock states do not create an interference pattern.
9.3. Calculate the zero-delay value $g^{(2)}(0)$ of the second-order correlation function of a singlemode electromagnetic field in the so-called Schrödinger-cat state: a coherent superposition of two Glauber states, with equal amplitudes, equal but sign-opposite parameters $\alpha$, and a certain phase shift between them.
9.4. Calculate the zero-delay value $g^{(2)}(0)$ of the second-order correlation function of singlemode electromagnetic field in the squeezed ground state $=$ defined by Eq. (5.172).
9.5. Calculate the rate of spontaneous photon emission (into the unrestricted free space) by a hydrogen atom, initially in the $2 p$ state $(n=2, l=1)$ with $m=0$. Would the result be different for $m= \pm$

[^776]1? for the $2 s$ state $(n=2, l=0, m=0)$ ? Discuss the relation between these quantum-mechanical results and those given by the classical theory of radiation, using the simplest classical model of the atom.
9.6. An electron has been placed at the lowest excited level of a spherically-symmetric, quadratic potential well $U(\mathbf{r})=m_{e} \omega^{2} r^{2} / 2$. Calculate the rate of its relaxation to the ground state, with emission of a photon (to the free space). Compare the rate with that for a similar transition of the hydrogen atom, for the case when the radiation frequencies of these two systems are equal.
9.7. Derive an analog of Eq. (53) for the spontaneous photon emission into the free space, due to a change of its magnetic dipole moment $\mathbf{m}$ of a small-size system.
9.8. A spin- $1 / 2$ particle, with the gyromagnetic ratio $\gamma$, is in its orbital ground state in a dc magnetic field $\boldsymbol{B}_{0}$. Calculate the rate of its spontaneous transition from the higher to the lower energy level, with the emission of a photon into the free space. Evaluate the rate for in an electron in a field of 10 T , and discuss the implications of this result for experiments with electron spins.
9.9. Calculate the rate of spontaneous transitions between the two sublevels of the ground state of a hydrogen atom, formed as a result of its hyperfine splitting. Discuss the implications of the result for the width of the $21-\mathrm{cm}$ spectral line.
9.10. Find the eigenstates and eigenvalues of the Janes-Cummings Hamiltonian (78), and discuss their behavior near the resonance point $\omega=\Omega$.
9.11. Analyze the Purcell effect, mentioned in Secs. 3 and 4, qualitatively; in particular, calculate the so-called Purcell factor $F_{\mathrm{P}}$, defined as the ratio of the spontaneous emission rates $\Gamma_{s}$ of an atom in a resonant cavity (tuned exactly to the quantum transition frequency) and that in the free space.
9.12. Prove that the Klein-Gordon equation (9.84) may be rewritten in the form similar to the non-relativistic Schrödinger equation,

$$
i \hbar \frac{\partial \psi}{\partial t}=\hat{H} \psi
$$

for a two-component wavefunction $\psi,{ }^{64}$ with the Hamiltonian represented (in the usual $z$-basis) by the following $2 \times 2$-matrix:

$$
\mathrm{H}=-\left(\sigma_{z}+i \sigma_{y}\right) \frac{\hbar^{2}}{2 m} \nabla^{2}+m c^{2} \sigma_{z} .
$$

Use your solution to discuss the physical meaning of the wavefunction's components.
9.13. Calculate and discuss the energy spectrum of a relativistic, spinless, charged particle placed into an external uniform, time-independent magnetic field $\mathcal{B}$. Use the result to formulate the condition of validity of the non-relativistic theory.

[^777]Hint: Reduce the relativistic Schrödinger equation, describing the problem, to the non-relativistic one describing the same problem, with some effective parameter(s).
9.14. Prove Eq. (91) for the energy spectrum of a hydrogen-line atom, calculated from the relativistic Schrödinger equation.

Hint: Use the fact that, as a mathematical analysis of Eq. (3.184) shows, its eigenvalues are given by Eq. (3.191), $\varepsilon_{n}=-1 / 2 n^{2}$, with $n=l+1+n_{r}$, where $n_{r}=0,1,2, \ldots$, even if $l$ is not integer. ${ }^{65}$
9.15. Derive the general expression for the differential cross-section of the elastic scattering of a spinless relativistic particle by a static potential $U(\mathbf{r})$, in the Born approximation, and formulate the conditions of its validity. Use these results to calculate the differential cross-section of scattering of a particle with electric charge $-e$ by the Coulomb electrostatic potential $\phi(\mathbf{r})=Z e / 4 \pi \varepsilon_{0} r$.
9.16. Calculate the commutator of operator $\hat{L}^{2}$ and the Dirac Hamiltonian of a free particle. Compare the result with that for the non-relativistic Hamiltonian of a free particle, and interpret the difference.
9.17.* In the Heisenberg picture of quantum dynamics, derive an equation describing time evolution of free electron's velocity in the Dirac theory. Solve the equation for the simplest state, with constant energy and momentum, and discuss the solution.
9.18. ${ }^{*}$ Calculate the eigenstates and eigenenergies of a spin- $1 / 2$ particle with charge $q$, placed into a uniform, time-independent external magnetic field $B$. Compare the calculated energy spectrum with those following from the non-relativistic theory and the relativistic Schrödinger equation.
9.19. ${ }^{*}$ Following the recommendation in the end of Chapter 9 of the lecture notes, introduce the quantum field operators $\hat{\psi}$, which would be related to the usual wavefunctions $\psi$ just as the EM field operators (9.16) are related to the classical electromagnetic fields, and explore the basic properties of these operators. (For this preliminary study, consider just the fixed-time situation.)

[^778]
## Chapter 10. Making Sense of Quantum Mechanics

This (very cryptic) chapter addresses the issues of quantum mechanics interpretation that are still a subject of debate - fortunately not affecting practical applications of the quantum theory.

### 10.1. Hidden variables and local reality

Only now, with a quantitative understanding of the principles of quantum mechanics, we are ready to proceed to the discussion of its interpretation ${ }^{1}$ - the issue which is very closely related to problems of measurements, already discussed in Sec. 7.7. As was already mentioned in that section, the founding fathers of quantum mechanics have not left much guidance on these topics, because in the first years after the advent of this exciting new theory they gave understandable preference to using it for deriving new particular results, and then were much distracted by the development of nuclear physics and its applications. This is why, after a very important but inconclusive discussion between A. Einstein and N . Bohr in the mid-30s, the debates of quantum measurements and the related conceptual issues of quantum mechanics have resumed only in the 1950s. They have led to a key contribution by J. Bell in the early 1960s, and an important experimental work on verifying Bell's inequalities (see below), but besides that work, the recent progress is marginal, and opinions of even prominent physicists on certain issues are still very much different.

Perhaps the central controversial issue is question (iii) posed in Sec. 7.7: what (if any :-) is the "real" state of a quantum-mechanical system before a nearly-perfect measurement giving a certain outcome? In order to be specific, let us focus again on the simplest example of Stern-Gerlach measurements of spin $-1 / 2$ particles - because of their physical transparency and technical simplicity. ${ }^{2}$ As the reader knows very well by now, even in a pure quantum spin state (for example, $\uparrow$ ), i.e. the least uncertain state of the system, the results of the Stern-Gerlach measurements of other spin component are still uncertain. Indeed, as we know from Sec. 4.4, the ket-vector of this state may be presented as

$$
\begin{equation*}
|\uparrow\rangle=\frac{1}{\sqrt{2}}(|\rightarrow\rangle+|\leftarrow\rangle), \tag{10.1}
\end{equation*}
$$

so that the probabilities of measuring any of values $S_{x}=+\hbar / 2$ and $S_{x}=-\hbar / 2$ equal $50 \%$. So, has the spin had a certain value of $S_{x}$ a split second before the Stern-Gerlach measurement that gave a certain outcome, for example $S_{x}=+\hbar / 2$ ? For a classical system, with perfect detectors, the answer is definitely yes. In this case, the pre-measurement probability of $50 \%$ just reflects the degree of our ignorance about the real state of the system, and the detector merely reveals it.

However, the situation in quantum mechanics is different, and such interpretation is impossible, as was clearly shown in the famous EPR paper published in 1935 by A. Einstein, B. Podolsky, and N.

[^779]Rosen. Its original discussed thought experiments with a pair of 1D particles prepared in a quantum state in that both the sum of their momenta and difference of their coordinates are exactly fixed: $p_{1}+p_{2}$ $=0, x_{1}-x_{2}=a .{ }^{3}$ However, usually the discussion is recast into an equivalent Stern-Gerlach experiment shown in Fig. 1a. ${ }^{4}$ A source emits rare pairs of spin- $1 / 2$ particles, propagating in opposite directions, with exactly zero net spin, but otherwise in random spin states. After the spatial separation of the particles has become sufficiently large (see below), the spin state of each of them is measured with a SternGerlach detector, one of them (Fig. 1, detector $\mathrm{SG}_{1}$ ) somewhat closer to the particle source, so it makes the measurement first, at time $t_{1}<t_{2}$.


Fig. 10.1. (a) General scheme of two-particle Stern-Gerlach experiments, and (b) the orientation of the detectors, assumed at the devivation of Bell's inequality (14).

First, let the detectors be oriented say along the same direction, say axis z. Evidently, the probability of each detector to give any of values $S_{z}= \pm \hbar / 2$ is $50 \%$. However, if the first detector had given result $S_{z}=-\hbar / 2$, even before the second detector's measurement, we know that it will give result $S_{z}$ $=+\hbar / 2$ with $100 \%$ probability. So far, the result allows for a classical interpretation, just for the singleparticle measurements discussed in Secs. 2.5 and 7.7. Thus we may fancy that the second particle really has a definite spin before the measurement, and the first measurement has just removes our ignorance about that reality. In other words, the change of probability is due to the statistical ensemble redefinition: the $50 \%$ probability belongs to the ensemble of all experiments, while the $100 \%$ probability, to the sub-ensemble of experiments with the $S_{z}=-\hbar / 2$ outcome of the first experiment.

However, let the source generate the particle pairs in the entangled, singlet state (8.19),

$$
\begin{equation*}
\left|s_{12}\right\rangle=\frac{1}{\sqrt{2}}(|\uparrow \downarrow\rangle-|\downarrow \uparrow\rangle), \tag{10.2}
\end{equation*}
$$

that certainly satisfies the above assumptions: the probability of each $S_{z}$ value of any particle is $50 \%$, the sum of both $S_{z}$ is exactly zero, and if the first detector's result is $S_{z}=-\hbar / 2$, then the state of the remaining particle is $\uparrow$, with zero uncertainty. Now let us use Eq. (1), and its counterpart for vector $|\downarrow\rangle,{ }^{5}$ to present the same initial state (2) in the form

[^780]\[

$$
\begin{equation*}
\left|s_{12}\right\rangle=\frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}(|\rightarrow\rangle+|\leftarrow\rangle) \frac{1}{\sqrt{2}}(|\rightarrow\rangle-|\leftarrow\rangle)-\frac{1}{\sqrt{2}}(|\rightarrow\rangle-|\leftarrow\rangle) \frac{1}{\sqrt{2}}(|\rightarrow\rangle+|\leftarrow\rangle)\right] . \tag{10.3}
\end{equation*}
$$

\]

Opening the parentheses (without swapping the ket-vector order!), we get an expression similar to Eq. (2), but now for the $x$-basis:

$$
\begin{equation*}
\left|s_{12}\right\rangle=\frac{1}{\sqrt{2}}(|\rightarrow \leftarrow\rangle-|\leftarrow \rightarrow\rangle) . \tag{10.4}
\end{equation*}
$$

Hence if we use the first detector (closest to the particle source) to measure $S_{x}$ rather than $S_{z}$, then after it had given as certain result (say, $S_{x}=-\hbar / 2$ ), we know for sure, before the second particle spin's measurement, that its $S_{x}$ component equals $+\hbar / 2$.

So, depending on the experiment performed on the first particle, the second particle turns out to be in one of two states - either with a definite component $S_{z}$ or with a definite component $S_{x}$, in each case without any uncertainty. Evidently, this situation cannot be interpreted in classical terms if the particles do not interact during the measurements. A. Einstein in was deeply unhappy with such situation, because it did not satisfy the general requirement to any theory, which nowadays is called the local reality. His definition of this requirement was as follows:
"The real factual situation of system 2 is independent of what is done with system 1 that is spatially separated from the former".
(Here the term "separated" in this sentence is a bit uncertain, but from the context it is clear that Einstein meant the detector separation by a superluminal interval, i.e. by distance

$$
\begin{equation*}
\left|\mathbf{r}_{1}-\mathbf{r}_{2}\right|>c\left|t_{1}-t_{2}\right|, \tag{10.5}
\end{equation*}
$$

where the measurement time difference, participating in the right-hand part, includes the measurement duration.) In Einstein's view, since quantum mechanics does not satisfy the local reality condition, it cannot be considered a complete theory of Nature.

This situation naturally raises the question whether something (usually called hidden variables) may be added to the quantum-mechanical description in order to satisfy the local reality requirement. The first definite statement in this regards was J. von Neumann's "proof" (first famous, then infamous :-) that such variables cannot be introduced; for a while his work satisfied quantum mechanics practitioners. ${ }^{7}$ A major new contribution to the problem was made only in the 1960s by J. Bell. ${ }^{8}$ First of all, he has found an elementary (in his words, "foolish") error in von Neumann's logic, which voids his "proof". Second, he demonstrated that Einstein’s local reality condition is incompatible with conclusions of quantum mechanics - that had been, by that time, confirmed by too many experiments to be seriously questioned. Since no hidden variable introduction can change this situation, in this sense such introduction is impossible.

[^781]Let me describe a particular version of Bell's proof (suggested by E. Wigner), using the same EPR pair experiment (Fig. 1a), in that each SG detector may be oriented in any of 3 directions: $a, b$, or $c$ - see Fig. 1b. As we know from Chapter 4, if a fully-polarized beam of spin-1/2 particles is passed through a Stern-Gerlach apparatus forming angle $\phi$ with the polarization axis, the probabilities of two counterpart outcomes of the experiment are

$$
\begin{equation*}
W\left(\phi_{+}\right)=\cos ^{2} \frac{\phi}{2}, \quad W\left(\phi_{-}\right)=\sin ^{2} \frac{\phi}{2} . \tag{10.6}
\end{equation*}
$$

Let us use this formula to calculate all joint probabilities of measurement outcomes, starting from the detectors 1 and 2 oriented, respectively, in directions $a$ and $c$. Since the angle between negative direction of axis $a$ and positive direction of axis $c$ is $\phi_{a+, c-}=\pi-\varphi$ (see the dashed arrow in Fig. 1b), we get

$$
\begin{equation*}
W\left(a_{+}, c_{+}\right)=W\left(a_{+}\right) W\left(c_{+} \mid a_{+}\right)=\frac{1}{2} \cos ^{2} \frac{\phi_{a-, c+}}{2}=\frac{1}{2} \cos ^{2} \frac{\pi-\varphi}{2}=\frac{1}{2} \sin ^{2} \frac{\varphi}{2} . \tag{10.7}
\end{equation*}
$$

Absolutely similarly,

$$
\begin{gather*}
W\left(c_{+}, b_{+}\right)=W\left(c_{+}\right) W\left(b_{+} \mid c_{+}\right)=\frac{1}{2} \sin ^{2} \frac{\varphi}{2},  \tag{10.8}\\
W\left(a_{+}, b_{+}\right)=W\left(a_{+}\right) W\left(b_{+} \mid a_{+}\right)=\frac{1}{2} \cos ^{2} \frac{\pi-2 \varphi}{2}=\frac{1}{2} \sin ^{2} \varphi . \tag{10.9}
\end{gather*}
$$

Now note that for any angle $\varphi$ smaller than $\pi / 2$ (as in the case shown in Fig. 1b),

$$
\begin{equation*}
\frac{1}{2} \sin ^{2} \varphi \geq \frac{1}{2} \sin ^{2} \frac{\varphi}{2}+\frac{1}{2} \sin ^{2} \frac{\varphi}{2} \equiv \sin ^{2} \frac{\varphi}{2} . \tag{10.10}
\end{equation*}
$$

(For example, for $\varphi \rightarrow 0$ the left-hand part of this relation tends to $\varphi^{2} / 2$, while the right-hand part, to $\varphi^{2} / 4$.) Hence the quantum-mechanical result gives, in particular,

$$
\begin{equation*}
W\left(a_{+}, b_{+}\right) \geq W\left(a_{+}, c_{+}\right)+W\left(c_{+}, b_{+}\right), \quad \text { for }|\varphi| \leq \pi / 2 . \tag{10.11}
\end{equation*}
$$

On the other hand, we may compose another inequality for the same probabilities without calculating them from any particular theory, but using the local reality assumption. Let us list all possible outcomes of detector measurements, taking into account the zero net spin:

| $W\left(a_{+}, b_{+}\right) \xrightarrow{W\left(a_{+}, c_{+}\right) \longrightarrow} \xrightarrow{\bullet}$ | Detector 1 results | Detector 2 results | Probability |
| :---: | :---: | :---: | :---: |
|  | $a_{+}, b_{+}, c_{+}$ | $a_{\text {-, }}, b_{\text {-, }}, c_{\text {- }}$ | $W_{1}$ |
|  | $a_{+}, b_{+}, c_{-}$ | $a_{\text {-, }}, b_{\text {-, }} c_{+}$ | $W_{2}$ |
|  | $a_{+}, b_{-}, c_{+}$ | $a_{\text {-, }}, b_{+}, c_{-}$ | $W_{3}$ |
|  | $a_{+}, b_{-}, c_{-}$ | $a_{\text {-, }}, b_{+}, c_{+}$ | $W_{4}$ |
|  | $a_{\text {a }}, b_{+}, c_{+}$ | $a_{+}, b_{-}, c_{-}$ | $W_{5}$ |
|  | $a_{\text {. }}, b_{+}, c_{\text {- }}$ | $a_{+}, b_{-}, c_{+}$ | $W_{6}$ |
|  | $a_{\text {-, }}, b_{-}, c_{+}$ | $a_{+}, b_{+}, c_{-}$ | $W_{7}$ |
|  | $a_{\text {- , }}, b_{-}, c_{\text {- }}$ | $a_{+}, b_{+}, c_{+}$ | $W_{8}$ |

Quantummechanical result for joint probabilities

From the local reality point of view, these measurement options are independent, so we may write:

$$
\begin{equation*}
W\left(a_{+}, c_{+}\right)=W_{2}+W_{4}, \quad W\left(c_{+}, b_{+}\right)=W_{3}+W_{7}, \quad W\left(a_{+}, b_{+}\right)=W_{3}+W_{4} . \tag{10.12}
\end{equation*}
$$

On the other hand, since no probability may be negative (by its very definition), we may always write

$$
\begin{equation*}
W_{3}+W_{4} \leq\left(W_{2}+W_{4}\right)+\left(W_{3}+W_{7}\right) \tag{10.13}
\end{equation*}
$$

Plugging into this inequality the values of these two parentheses, given by Eq. (12), we get

Bell's inequality for local-reality theories

$$
\begin{equation*}
W\left(a_{+}, b_{+}\right) \leq W\left(a_{+}, c_{+}\right)+W\left(c_{+}, b_{+}\right) . \tag{10.14}
\end{equation*}
$$

This is (one of several possible forms of) the Bell's inequality that has to be satisfied by any local-reality theory; it directly contradicts the quantum-mechanical result (11).

Though experimental tests of the Bell's inequalities had been started in the late 1960s, the interpretation of first results was vulnerable to two criticisms:
(i) The detectors were not fast enough and not far enough to have relation (5) satisfied. This is why, as the matter of principle, there was a chance that information on one measurement had been transferred (by some, mostly implausible) means to particles before the second measurement - the socalled locality loophole.
(ii) Particle detection efficiencies were too low to have sufficiently small error bars for both parts of the inequality - the detection loophole.

Gradually, these loopholes have been closed. ${ }^{9}$ As expected, substantial violations of Bell inequalities equivalent to Eq. (14) have been proved, essentially rejecting any possibility to reconcile quantum mechanics with Einstein's local reality requirement.

### 10.2. Interpretations of quantum mechanics

The fact that quantum mechanics is incompatible with local reality, makes it reconciliation with our (classically-bred) "common sense" rather challenging. Here is a brief list of the major interpretations of quantum mechanics, that try to provide at least a partial reconciliation of this kind:
(i) The so-called Copenhagen interpretation, to which most physicists subscribe. This "interpretation" does not really interpret anything; it just states the internal randomness of measurement results in quantum mechanics, essentially saying: "Do not worry; this is just how it is; live with it". For me personally, this interpretation, at least in its most frequently repeated forms, has only one, rather pedagogical weakness: though it implies statistical ensembles (otherwise, how would you define the probability?), but does not put a sufficient emphasis on their role, in particular the possible ensemble

[^782]redefinition as the only key point of human involvement in the measurement process. ${ }^{10}$ Perhaps the most impressive objection to the Copenhagen interpretation was given by A. Einstein during his 1935 discussion with N. Bohr: "God does not play dice." OK, when Einstein speaks, we all should listen, but perhaps when God speaks (through the experimental results), we have to pay even more attention.
(ii) Non-local reality. After the dismissal of von Neumann's "proof" by J. Bell, to the best of my knowledge, there has been no proof that hidden parameters could not be introduced, provided that they do not imply the local reality. Of constructive approaches, perhaps the most notable contribution was made by D. Bohm ${ }^{11}$ who developed the L. de Broglie's interpretation of the wavefunction as a "pilot wave", making it quantitative. In the wave mechanics version of this concept, the wavefunction, governed by the Schrödinger equation, just guides a real, point-like classical particle whose coordinates serve as hidden variables. However, this concept does not satisfy the notion of local reality. Namely, the measurement of particle's coordinate at a certain point $\mathbf{r}_{1}$ has to instantly change the wavefunction everywhere, including points $\mathbf{r}_{2}$ in the superluminal interval range (4). So, Bohm's hidden variables would hardly make A. Einstein happy. After having recognized this problem, D. Bohm abandoned his theory - in J. Bell's view, perhaps too early. In my personal taste, however, the assumption of such (in Einstein's words) "spooky action at a distance" is too large a sacrifice to save the classical determinism.
(iii) The many-world interpretation introduced in 1957 by H . Everitt and popularized in the 1960s and 1970s by B. de Witt. In this interpretation, all possible measurement outcomes do happen, splitting the Universe into the corresponding number of "parallel" Universes, so that from one of them, other Universes and hence other outcomes cannot be observed. Let me leave to the reader an estimate of the rate at which the parallel Universes being constantly generated (say, per second), taking into account that such generation should take place not only at explicit lab experiments, but at any irreversible process such as fission of any atom nucleus or absorption of a photon, everywhere in each Universe whether its result is recorded or not. Even the main proponent of this interpretation, B. de Witt, has confessed: "The idea is not easy to reconcile with common sense". I agree.
(iv) The quantum logic. In desperation, some physicists turned philosophers have decided to dismiss the very logic we are using - in science and elsewhere, so that a statement like "the Bell inequalities are violated" would not make any definite sense. OK, if we dismiss the formal logic, I do not know how we can use any scientific theory and make any predictions - until the quantum logic experts tell us what to replace the classical logic with. To the best of my knowledge, so far they have not done that, at least for the measurement process. I personally trust J. Bell's opinion: "It is my impression that the whole vast subject of Quantum Logic has arisen [...] from the misuse of a word."

The weakness of all interpretations of quantum mechanics is that, as far as I know, neither of them has yet provided any suggestion how this particular interpretation might be tested experimentally to exclude other ones. On the positive side, there is a consensus that quantum mechanics makes correct, if sometimes probabilistic, predictions of all reliable experimental results we are aware of. Maybe, this is not that bad for a scientific theory. ${ }^{12}$

[^783]

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# Part CM: Statistical Mechanics 

Last corrections: 2019/08/01

A revised version of this material is now published by the IOP under the title "Statistical Mechanics: Lecture notes" (Essential Advanced Physics - Volume 7, ISBN 978-0-7503-1416-6), with the model solutions of the exercise problems published under the title

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## Chapter 1. Review of Thermodynamics

This chapter starts from a brief discussion of the subject of statistical physics and thermodynamics, and the relation between these two disciplines. Then I proceed to a review of the basic notions and relations of thermodynamics. Most of this material is supposed to be known to the reader from his or her undergraduate studies, ${ }^{1}$ so the discussion is rather brief.

### 1.1. Introduction: Statistical physics and thermodynamics

Statistical physics (alternatively called "statistical mechanics") and thermodynamics are two different approaches to the same goal: a description of internal dynamics of large physical systems, notably those consisting of many, $N \gg 1$, identical particles - or other components. The traditional example of such a system is a human-scale portion of a gas, with the number $N$ of molecules of the order of the Avogadro number $N_{\mathrm{A}} \sim 10^{23} .^{2}$ The "internal dynamics" is an (admittedly loose) term meaning all the physics unrelated to the motion of the system as a whole. The most important example of the internal dynamics is the thermal motion of atoms and molecules.

The motivation for the statistical approach to such systems is straightforward: even if the laws governing the dynamics of each particle and their interactions were exactly known, and we had infinite computing resources at our disposal, calculating the exact evolution of the system in time would be impossible, at least because it is completely impracticable to measure the exact initial state each component, e.g., the initial position and velocity of each particle. The situation is further exacerbated by the phenomena of chaos and turbulence, ${ }^{3}$ and the quantum-mechanical uncertainty, ${ }^{4}$ which do not allow the exact calculation of final positions and velocities of the component particles even if their initial state is known with the best possible precision. As a result, in most situations only statistical predictions about behavior of such systems may be made, with the probability theory becoming a major part of the mathematical tool arsenal.

However, the statistical approach is not as bad as it may look. Indeed, it is almost self-evident that any measurable macroscopic variable characterizing a stationary system of $N \gg 1$ particles as a whole (think, e.g., about pressure $P$ of a gas contained in a fixed volume $V$ ) is almost constant in time. Indeed, we will see below that, besides certain exotic exceptions, the relative fluctuations - either in time, or among macroscopically similar systems - of such a variable are of the order of $1 / \sqrt{ } N$, i.e. for $\mathrm{N} \sim$ $N_{\mathrm{A}}$ are extremely small. As a result, the average values of macroscopic variables may characterize the state of the system rather well. Their calculation is the main task of statistical physics. (Though the analysis of fluctuations is also an important task, but due to the fluctuation smallness, the analysis in most cases may be based on perturbative approaches - see Chapter 5.)

[^784]Let us have a look at typical macroscopic variables the statistical physics and thermodynamics should operate with. Since I have already mentioned pressure $P$ and volume $V$, let me start with this famous pair. First of all, note that volume is an extensive variable, i.e. a variable whose value for a system consisting of several non-interacting (or weakly interacting) parts is the sum of those of its parts. On the other hand, pressure is an example of intensive variables whose value is the same for different parts of a system - if they are in equilibrium. In order to understand why $P$ and $V$ form a natural pair of variables, let us consider the classical playground of thermodynamics, a portion of a gas contained in a cylinder, closed with a movable piston of area $A$ (Fig. 1). Neglecting friction between the walls and the piston, and assuming that it is being moved slowly enough (so that the pressure $P$, at any instant, is virtually the same for all parts of the volume), the elementary work of the external force $\neq P A$, compressing the gas, at a small piston displacement $d x=-d V / A$, is

$$
\begin{equation*}
d w=7 d x=(7 / A)(A d x)=-P d V \tag{1.1}
\end{equation*}
$$

It is clear that the last expression is more general than the model shown in Fig. 1, and does not depend on the particular shape of the system surface.


Fig. 1.1. Compressing a gas.

From the point of analytical mechanics, ${ }^{5} \quad V$ and $(-P)$ is just one of many possible canonical pairs of generalized coordinates $q_{j}$ and generalized forces $\mathcal{Z}_{j}$, whose products $d w_{j}=\mathcal{Z}_{j} d q_{j}$ give independent contributions to the total work of the environment on the system under analysis. For example, the reader familiar with the basics of electrostatics knows that if the spatial distribution $\mathscr{E}(\mathbf{r})$ of an external electric field does not depend on the electric polarization $\mathscr{P}(\mathbf{r})$ of the dielectric medium placed into the field, its elementary work on the medium is

$$
\begin{equation*}
d w=\int \mathscr{E}(\mathbf{r}) \cdot d \mathscr{P}(\mathbf{r}) d^{3} r \equiv \int \sum_{j=1}^{3} \mathscr{E}_{j}(\mathbf{r}) d \mathscr{T}_{j}(\mathbf{r}) d^{3} r . \tag{1.2a}
\end{equation*}
$$

The most important cases when this condition is fulfilled (and hence Eq. (2a) is valid) are, first, long cylindrical samples in a parallel external field (see, e.g., EM Fig. 3.13) and, second, the polarization of a sample (of any shape) due to that of discrete dipoles $\boldsymbol{\mu}_{\mathrm{k}}$, whose electric interaction is negligible. In the latter case, Eq. (2a) may be also rewritten as the sum over the single dipoles, located at points $\mathbf{r}_{\mathrm{k}}$ :

$$
\begin{equation*}
d w=\sum_{k} d w_{k}, \quad \text { with } d w_{k}=\mathscr{E}\left(\mathbf{r}_{k}\right) \cdot d \boldsymbol{p}_{k} . \tag{1.2b}
\end{equation*}
$$

Very similarly, and at the similar conditions upon the external magnetic field $\mathscr{H}(\mathbf{r})$, its elementary work on a magnetic medium may be also represented in either of two forms:

$$
\begin{equation*}
d w=\mu_{0} \int \mathscr{H}(\mathbf{r}) \cdot d \mathscr{M}(\mathbf{r}) d^{3} r \equiv \mu_{0} \int \sum_{j=1}^{3} \mathscr{H}_{j}(\mathbf{r}) d \mathscr{M}_{j}(\mathbf{r}) d^{3} r \tag{1.3a}
\end{equation*}
$$

[^785]\[

$$
\begin{equation*}
d w=\sum_{k} d w_{k}, \quad \text { with } d w_{k}=\mu_{0} \mathscr{H}\left(\mathbf{r}_{k}\right) \cdot d \boldsymbol{m}_{k} \tag{1.3b}
\end{equation*}
$$

\]

where $\mathscr{M}$ and $\boldsymbol{m}$ are the vectors of, respectively, the magnetization and the moment of a single magnetic dipole. These expressions show that the roles of generalized coordinates may be played by Cartesian components of the vectors $\mathscr{P}$ (or $\boldsymbol{\mu}$ ) and $\mathscr{M}$ (or $\boldsymbol{m}$ ), with the components of the electric and magnetic fields serving as the corresponding generalized forces. This list may be extended to other interactions (such as gravitation, surface tension in fluids, etc.).

Again, the specific relations between the variables of each pair listed above are typically affected by the statistics of the components (particles) of a body, but their definition is not based on statistics. The situation is very different for a very specific pair of variables, temperature $T$ and entropy $S$, although these "sister variables" participate in many formulas of thermodynamics exactly like one more canonical pair $\left\{\mathcal{Z}_{j}, q_{j}\right\}$. However, the very existence of these two variables is due to statistics. Temperature $T$ is an intensive variable that characterizes the degree of thermal "agitation" of system components. On the contrary, entropy $S$ is an extensive variable that in most cases evades immediate perception by human senses; it is a qualitative measure of disorder of the system, i.e. the degree of our ignorance about its exact microscopic state. ${ }^{6}$

The reason for the appearance of the $\{T, S\}$ pair of variables in formulas is that the statistical approach to large systems of particles brings some qualitatively new results, most notably the notion of irreversible time evolution of collective (macroscopic) variables describing the system. On one hand, such irreversibility looks absolutely natural in such phenomena as the diffusion of an ink drop in a glass of water. In the beginning, the ink molecules are located in a certain small part of system's volume, i.e. to some extent ordered, while at the late stages of diffusion, the position of each molecule is essentially random. However, as a second thought, the irreversibility is rather surprising, ${ }^{7}$ taking into account that it takes place even if the laws governing the motion of system's components are time-reversible - such as the Newton laws or the basic laws of quantum mechanics. Indeed, if, at a late stage of the diffusion process, we exactly reversed the velocities of all molecules simultaneously, the ink molecules would again gather (for a moment) into the original spot. ${ }^{8}$ The problem is that getting the information necessary for the exact velocity reversal is not practicable. This example shows a deep connection between the statistical mechanics and the information theory.

A qualitative discussion of the reversibility-irreversibility dilemma requires a strict definition of the basic notion of statistical mechanics (and indeed the probability theory), the statistical ensemble, and I would like to postpone it until the beginning of Chapter 2. In particular, in that chapter we will see that the basic law of irreversible behavior is the increase of entropy $S$ in any closed system. Thus, statistical mechanics, without defying the "microscopic" laws governing evolution of system's components,

[^786]introduces on top of them some new "macroscopic" laws, intrinsically related to the evolution of information, i.e. the degree of our knowledge of the microscopic state of the system.

To conclude this brief discussion of variables, let me mention that as in all fields of physics, a very special role in statistical mechanics is played by energy $E$. In order to emphasize the commitment to disregard the motion of the system as a whole, in thermodynamics it is frequently called the internal energy, though for brevity, I will mostly skip the adjective. Its simplest example is the kinetic energy of the thermal motion of molecules in a dilute gas, but in general $E$ also includes not only the individual energies of all system's components, but also their interactions with each other. Besides a few pathological cases of very-long-range interactions (such as the Coulomb interactions in plasma with uncompensated charge density), the interactions may be treated as local; in this case the internal energy is proportional to $N$, i.e. is an extensive variable. As will be shown below, other extensive variables with the dimension of energy are often very useful, including the (Helmholtz) free energy $F$, the Gibbs energy $G$, enthalpy $H$, and grand potential $\Omega$. (The collective name for such variables is thermodynamic potentials.)

Now, we are ready for a brief discussion of the relation between statistical physics and thermodynamics. While the task of statistical physics is to calculate the macroscopic variables discussed above, ${ }^{9}$ using this or that particular microscopic model of the system, the main role of thermodynamics is to derive some general relations between the average values of the macroscopic variables (called thermodynamic variables) that do not depend on specific models. Surprisingly, it is possible to accomplish such a feat using a few either evident or very plausible general assumptions (sometimes called the laws of thermodynamics), which find their proof in statistical physics. ${ }^{10}$ Such general relations allow us to reduce rather substantially the amount of calculations we have to do in statistical physics; in many cases it is sufficient to calculate from statistics just one or two variables, and then use thermodynamic relations to calculate all other properties of interest. Thus the thermodynamics, sometimes snubbed at as a phenomenology, deserves every respect not only as a discipline which is, in a certain sense, more general than statistical physics as such, but also as a very useful science. This is why the balance of this chapter is devoted to a brief review of thermodynamics.

### 1.2. The $2^{\text {nd }}$ law of thermodynamics, entropy, and temperature

Thermodynamics accepts a phenomenological approach to entropy $S$, postulating that there is such a unique extensive measure of disorder, and that in a closed system, ${ }^{11}$ it may only grow in time, reaching its constant (maximum) value at equilibrium: ${ }^{12}$

$$
\begin{equation*}
d S \geq 0 \tag{1.4}
\end{equation*}
$$

This postulate is called the $2^{\text {nd }}$ law of thermodynamics - arguably its only substantial new law.

[^787]Surprisingly, this law, together with the additivity of $S$ in composite systems of non-interacting parts (as an extensive variable), is sufficient for a formal definition of temperature, and a derivation of its basic properties that comply with our everyday notion of this variable. Indeed, let us consider a particular case: a closed system consisting of two fixed-volume subsystems (Fig. 2) whose internal relaxation is very fast in comparison with the rate of the thermal flow (i.e. the energy and entropy exchange) between the parts. In this case, on the latter time scale, each part is always in some quasiequilibrium state, which may be described by a unique relation $E(S)$ between its energy and entropy. ${ }^{13}$


Fig. 1.2. Composite thermodynamic system.
Neglecting the interaction energy between the parts (which is always possible at $N \gg 1$, in the absence of long-range interactions), we may use the extensive character of variables $E$ and $S$ to write

$$
\begin{equation*}
E=E_{1}\left(S_{1}\right)+E_{2}\left(S_{2}\right), \quad S=S_{1}+S_{2}, \tag{1.5}
\end{equation*}
$$

for the full energy and entropy of the system. Now let us calculate the following derivative:

$$
\begin{equation*}
\frac{d S}{d E_{1}}=\frac{d S_{1}}{d E_{1}}+\frac{d S_{2}}{d E_{1}}=\frac{d S_{1}}{d E_{1}}+\frac{d S_{2}}{d E_{2}} \frac{d E_{2}}{d E_{1}}=\frac{d S_{1}}{d E_{1}}+\frac{d S_{2}}{d E_{2}} \frac{d\left(E-E_{1}\right)}{d E_{1}} . \tag{1.6}
\end{equation*}
$$

Since the total energy $E$ of the system is fixed and hence independent of its re-distribution between the sub-systems, $d E / d E_{1}=0$, and we get

$$
\begin{equation*}
\frac{d S}{d E_{1}}=\frac{d S_{1}}{d E_{1}}-\frac{d S_{2}}{d E_{2}} \tag{1.7}
\end{equation*}
$$

According to the $2^{\text {nd }}$ law of thermodynamics, when the two parts reach the thermodynamic equilibrium, the total entropy $S$ reaches its maximum, so that $d S / d E_{1}=0$, and Eq. (7) yields

$$
\begin{equation*}
\frac{d S_{1}}{d E_{1}}=\frac{d S_{2}}{d E_{2}} \tag{1.8}
\end{equation*}
$$

Thus we see that if a thermodynamic system may be partitioned into weakly interacting macroscopic parts, their derivatives $d S / d E$ should be equal in the equilibrium. The reciprocal of such derivative is called temperature. Taking into account that our analysis pertains to the situation (Fig. 2) when both volumes $V_{1,2}$ are fixed, we may write this definition as

$$
\begin{equation*}
\left(\frac{\partial E}{\partial S}\right)_{V} \equiv T \tag{1.9}
\end{equation*}
$$

[^788]subscript $V$ meaning that volume is kept constant at differentiation. (Such notation is common and very useful in thermodynamics, with its broad range of variables.)

Note that according to Eq. (9), if temperature is measured in energy units (as I will do in this course for the brevity of notation), $S$ is dimensionless. ${ }^{14}$ The transfer to the SI or Gaussian units, i.e. to temperature $T_{\mathrm{K}}$ measured in kelvins (not "Kelvins", not "degrees Kelvin", please!), is given by relation $T=k_{\mathrm{B}} T_{\mathrm{K}}$, where the Boltzmann constant $k_{\mathrm{B}} \approx 1.38 \times 10^{-23} \mathrm{~J} / \mathrm{K}=1.38 \times 10^{-16} \mathrm{erg} / \mathrm{K} .{ }^{15}$ In these units, the entropy becomes dimensional: $S_{\mathrm{K}}=k_{\mathrm{B}} S$.

The definition of temperature, given by Eq. (9), is of course in a sharp contract with the popular notion of $T$ as a measure of the average energy per particle. However, as we will repeatedly see below, is most cases these two notions may be reconciled. In particular, let us list some properties of $T$, which are in accordance with our everyday notion of temperature:
(i) according to Eq. (9), temperature is an intensive variable (since both $E$ and $S$ are extensive), i.e., in a system of similar particles, independent of the particle number $N$;
(ii) temperatures of all parts of a system are equal at equilibrium - see Eq. (8);
(iii) in a closed system whose parts are not in equilibrium, thermal energy (heat) always flows from a warmer part (with higher $T$ ) to the colder part.

In order to prove the last property, let us come back to the closed, composite system shown in Fig. 2, and consider another derivative:

$$
\begin{equation*}
\frac{d S}{d t}=\frac{d S_{1}}{d t}+\frac{d S_{2}}{d t}=\frac{d S_{1}}{d E_{1}} \frac{d E_{1}}{d t}+\frac{d S_{2}}{d E_{2}} \frac{d E_{2}}{d t} . \tag{1.10}
\end{equation*}
$$

If the internal state of each part is very close to equilibrium (as was assumed from the very beginning) at each moment of time, we can use Eq. (9) to replace derivatives $d S_{1,2} / d E_{1,2}$ for $1 / T_{1,2}$ and get

$$
\begin{equation*}
\frac{d S}{d t}=\frac{1}{T_{1}} \frac{d E_{1}}{d t}+\frac{1}{T_{2}} \frac{d E_{2}}{d t} \tag{1.11}
\end{equation*}
$$

Since in a closed system $E=E_{1}+E_{2}=$ const, these time derivatives are related as $d E_{2} / d t=-d E_{1} / d t$, and Eq. (11) yields

$$
\begin{equation*}
\frac{d S}{d t}=\left(\frac{1}{T_{1}}-\frac{1}{T_{2}}\right) \frac{d E_{1}}{d t} \tag{1.12}
\end{equation*}
$$

But in accordance with the $2^{\text {nd }}$ law of thermodynamics, the derivative cannot be negative: $d S / d t \geq 0$. Hence,

$$
\begin{equation*}
\left(\frac{1}{T_{1}}-\frac{1}{T_{2}}\right) \frac{d E_{1}}{d t} \geq 0 \tag{1.13}
\end{equation*}
$$

[^789]For example, if $T_{1}>T_{2}$ (i.e. $1 / T_{1}<1 / T_{2}$ ), then $d E_{1} / d t \leq 0$, i.e. the warmer part gives energy to its colder counterpart.

Note also that at such a heat exchange, at fixed volumes $V_{1,2}$, and $T_{1} \neq T_{2}$, increases the total system entropy, without performing any "useful" mechanical work.

### 1.3. The $1^{\text {st }}$ and $3^{\text {rd }}$ laws of thermodynamics, and heat capacity

Now let us consider a thermally insulated system whose volume $V$ may be changed by a deterministic force - see, for example, Fig. 1. Such system is different from the fully closed one, because its energy $E$ may be changed by the external force's work - see Eq. (1):

$$
\begin{equation*}
d E=d w=-P d V . \tag{1.14}
\end{equation*}
$$

Let the volume change be so slow $(d V / d t \rightarrow 0)$ that the system is virtually at equilibrium at any instant without much error. Such a slow process is called reversible, and in this particular case of a thermally insulated system, it is also called adiabatic. If pressure $P$ (or any a generalized external force $7_{j}$ ) is deterministic, i.e. is a predetermined function of time independent on the state of the system under analysis, it may be considered as coming from a fully ordered system, i.e. the one having zero entropy, with the total system completely closed. Since according to the second of Eqs. (5), the entropy of the total closed system should stay constant, $S$ of the system under analysis should stay constant on its own. Thus we arrive at a very important conclusion: an adiabatic process, the entropy of a system cannot change. ${ }^{16}$ This means that we can use Eq. (14) to write

$$
\begin{equation*}
P=-\left(\frac{\partial E}{\partial V}\right)_{S} . \tag{1.15}
\end{equation*}
$$

Let us now consider an even more general thermodynamic system that may also exchange thermal energy ("heat") with the environment (Fig. 3).


Fig. 1.3. General thermodynamic process involving both the mechanical work and heat exchange with the environment.

For such a system, our previous conclusion about the entropy constancy is not valid, so that $S$, in equilibrium, may be a function of not only energy $E$, but also of volume $V$. Let us resolve this relation for energy: $E=E(S, V)$, and write the general mathematical expression for the full differential of $E$ as a function of these two independent arguments:

$$
\begin{equation*}
d E=\left(\frac{\partial E}{\partial S}\right)_{V} d S+\left(\frac{\partial E}{\partial V}\right)_{S} d V \tag{1.16}
\end{equation*}
$$

[^790]This formula, based on the stationary relation $E=E(S, V)$, is evidently valid not only in equilibrium, but also for very slow, reversible ${ }^{17}$ processes. Now, using Eqs. (9) and (15), we may rewrite Eq. (16) as

$$
\begin{equation*}
d E=T d S-P d V \tag{1.17}
\end{equation*}
$$

[^791]The second term in the right-hand part of this equation is just the work of the external force, so that due to the conservation of energy, ${ }^{18}$ the first term has to be equal to the heat $d Q$ transferred from the environment to the system (see Fig. 3):

$$
\begin{gather*}
d E=d Q+d w  \tag{1.18}\\
d Q=T d S \tag{1.19}
\end{gather*}
$$

[^792]The last relation, divided by $T$ and then integrated along an arbitrary (but reversible!) process,

$$
\begin{equation*}
S=\int \frac{d Q}{T}+\text { const }, \tag{1.20}
\end{equation*}
$$

is sometimes used as an alternative definition of entropy $S$ - provided that temperature is defined not by Eq. (9), but in some independent way. It is useful to recognize that entropy (like energy) may be defined to an arbitrary constant, which does not affect any other thermodynamic observables. The common convention is to take

$$
\begin{equation*}
S \rightarrow 0 \text { at } T \rightarrow 0 . \tag{1.21}
\end{equation*}
$$

This condition is sometimes called the $3^{\text {rd }}$ law of thermodynamics, but it is important to realize that this is just a convention rather than a real law. ${ }^{19}$ Indeed, the convention corresponds well to the notion of the full order at $T=0$ in some systems (e.g., perfect crystals), but creates ambiguity for other systems, e.g., amorphous solids (like the usual glasses) that may remain, for "astronomic" times, highly disordered even at $T \rightarrow 0$.

Now let us discuss the notion of heat capacity that, by definition, is the ratio $d Q / d T$, where $d Q$ is the amount of heat that should be given to a system to raise its temperature by a small amount $d T .{ }^{20}$ (This notion is very important, because it may be most readily measured experimentally.) The heat capacity depends, naturally, on whether the heat $d Q$ goes only into an increase of the internal energy $d E$

[^793]of the system (as it does if volume $V$ is constant), or also into the mechanical work ( $-d w$ ) that may be performed at expansion - as it happens, for example, if pressure $P$, rather than volume $V$, is fixed (the socalled isobaric process - see Fig. 4). ${ }^{21}$


Fig. 1.4. The simplest implementation of an isobaric process.

Hence we should discuss two different quantities, the heat capacity at fixed volume,

$$
\begin{equation*}
C_{V} \equiv\left(\frac{\partial Q}{\partial T}\right)_{V} \tag{1.22}
\end{equation*}
$$

and heat capacity at fixed pressure

$$
\begin{equation*}
C_{P} \equiv\left(\frac{\partial Q}{\partial T}\right)_{P}, \tag{1.23}
\end{equation*}
$$

and expect that for all "normal" (mechanically stable) systems, $C_{P} \geq C_{V}$. The difference between $C_{P}$ and $C_{V}$ is rather minor for most liquids and solids, but may be very substantial for gases - see Sec. 4.

### 1.4. Thermodynamic potentials

A technical disadvantage of Eqs. (22) and (23) is that $\partial Q$ is not a differential of a function of state of the system, ${ }^{22}$ and hence (in contrast with temperature and pressure) does not allow an immediate calculation of heat capacity, even if the relation between $E, S$, and $V$ is known. For $C_{V}$ the situation is immediately correctable, because at fixed volume, $d w=-P d V=0$ and hence, according to Eq. (18), $d Q$ $=d E$. Hence we may write

$$
\begin{equation*}
C_{V}=\left(\frac{\partial E}{\partial T}\right)_{V} . \tag{1.24}
\end{equation*}
$$

[^794]so that in order to calculate $C_{V}$ from a certain statistical-physics model, we only need to calculate $E$ as a function of temperature and volume.

If we want to write similarly a convenient expression for $C_{P}$, the best way is to introduce a new notion of so-called thermodynamic potentials - whose introduction and effective use is perhaps one of the most impressive formalisms of thermodynamics. For that, let us combine Eqs. (1) and (18) to write the " $1^{\text {st }}$ law of thermodynamics" in its most common form

$$
\begin{equation*}
d Q=d E+P d V \tag{1.25}
\end{equation*}
$$

At an isobaric process (Fig. 4), i.e. at $P=$ const, this expression is equivalent to

$$
\begin{equation*}
(d Q)_{P}=d E+d(P V)=d(E+P V)_{P} \tag{1.26}
\end{equation*}
$$

Thus, if we introduce a new function with the dimensionality of energy: ${ }^{23}$

$$
\begin{equation*}
H \equiv E+P V \tag{1.27}
\end{equation*}
$$

called enthalpy (or, more rarely, the "heat function" or "heat contents"), ${ }^{24}$ we may rewrite Eq. (23) as

$$
\begin{equation*}
C_{P}=\left(\frac{\partial H}{\partial T}\right)_{P} \tag{1.28}
\end{equation*}
$$

Comparing Eq. (28) with (24) we see that for the heat capacity, enthalpy $H$ plays the same role at fixed pressure as the internal energy $E$ plays at fixed volume.

Now let us explore properties of the enthalpy for an arbitrary reversible process, i.e. lifting the restriction $P=$ const, but still keeping definition (27). Differentiating it, we get

$$
\begin{equation*}
d H=d E+P d V+V d P \tag{1.29}
\end{equation*}
$$

so that plugging in Eq. (17) for $d E$, we see that two terms $P d V$ cancel, yielding a very simple expression

$$
\begin{equation*}
d H=T d S+V d P \tag{1.30}
\end{equation*}
$$

Enthalpy: definition

This equation shows that if $H$ has been found (say, experimentally measured or calculated for a certain microscopic model) as a function of entropy $S$ and pressure $P$, we can find temperature $T$ and volume $V$ by simple partial differentiation:

$$
\begin{equation*}
T=\left(\frac{\partial H}{\partial S}\right)_{P}, \quad V=\left(\frac{\partial H}{\partial P}\right)_{S} \tag{1.31}
\end{equation*}
$$

The comparison of the first of these relations with Eq. (9) shows that not only for the heat capacity, but for temperature as well, enthalpy plays the same role at fixed pressure as played by the intrinsic energy at fixed volume. Moreover, the comparison of the second of Eqs. (31) with Eq. (15) shows that the transfer between $E$ to $H$ corresponds to a simple swap of $(-P)$ and $V$ in the expressions for the differentials of these variables.

[^795]This success immediately raises the question whether we could develop it further on, by defining other useful thermodynamic potentials - variables with the dimensionality of energy that would have similar properties, first of all a potential which would enable a similar swap of $T$ and $S$ in its full differential. We already know that the adiabatic processes is the reversible process with fixed entropy, so that now we should analyze a reversible process with fixed temperature. Such isothermal process may be implemented, for example, by placing the system under consideration into a thermal contact with a much larger system (called either the heat bath, or "heat reservoir", or "thermostat") that remains in thermodynamic equilibrium at all times - see Fig. 5.


Fig. 1.5. The simplest implementation of an isothermal process.

Due to its large size, the heat bath temperature $T$ does not depend on what is being done with our system, and if the change is being done slowly enough (i.e. reversibly), that temperature is also the temperature of our system - see Eq. (8) and its discussion. Let us calculate the elementary work $d w$ for such a reversible isothermal process. According to the general Eq. (18), $d w=d E-d Q$. Plugging in $d Q$ from Eq. (19), for $T=$ const we get

$$
\begin{equation*}
(d w)_{T}=d E-T d S=d(E-T S)=d F \tag{1.32}
\end{equation*}
$$

where the following combination,

Free
energy: definition

$$
\begin{equation*}
F \equiv E-T S \tag{1.33}
\end{equation*}
$$

is called the free energy (or the "Helmholtz free energy", or just the "Helmholtz energy"25). Just as we have done for the enthalpy, let us establish properties of this new thermodynamic potential for an arbitrary (not necessarily isothermal) small reversible variation of variables, while keeping definition (33). Differentiating this relation and using Eq. (17), we get

$$
\begin{equation*}
d F=-S d T-P d V \tag{1.34}
\end{equation*}
$$

Thus, if we know function $F(T, V)$, we can calculate $S$ and $P$ by simple differentiation:

$$
\begin{equation*}
S=-\left(\frac{\partial F}{\partial T}\right)_{V}, \quad P=-\left(\frac{\partial F}{\partial V}\right)_{T} . \tag{1.35}
\end{equation*}
$$

It is easy to see that we can make the derivative system full and symmetric if we introduce one more thermodynamic potential. Indeed, we have shown that each of three already introduced thermodynamic potentials $(E, H$, and $F$ ) has especially simple full differential if it is considered a

[^796]function of two canonical arguments: one of "thermal variables" (either $S$ or $T$ ) and one of "mechanical variables" (either $P$ or $V$ ): ${ }^{26}$
\[

$$
\begin{equation*}
E=E(S, V), \quad H=H(S, P), \quad \text { and } \quad F=F(T, V) . \tag{1.36}
\end{equation*}
$$

\]

In this list of pair of 4 arguments, only one pair is missing: $(T, P)$. The thermodynamic function of this pair, which gives two other variables ( $S$ and $V$ ) by simple differentiation, is called the Gibbs energy (or sometimes the "Gibbs free energy"): $G=G(T, P)$. The way to define it in a symmetric way is evident from the so-called circular diagram shown in Fig. 6.

(b)

Fig. 1.6. (a) Circular diagram and (b) its use for variable calculation. The thermodynamic potentials are shown in boldface, each flanked by its two canonical arguments.

In this diagram, each thermodynamic potential is placed between its two canonical arguments see Eq. (36). The left two arrows in Fig. 6a show the way the potentials $H$ and $F$ have been obtained from energy $E$ - see Eqs. (27) and (33). This diagram hints that $G$ has to be defined as shown by the right two arrows on that panel, i.e. as

$$
\begin{equation*}
G \equiv E-T S+P V=H-T S=F+P V \tag{1.37}
\end{equation*}
$$

Gibbs
energy: definition
so that if we know the function $G(T, P)$, we can indeed readily calculate entropy and volume:

$$
\begin{equation*}
S=-\left(\frac{\partial G}{\partial T}\right)_{P}, \quad V=\left(\frac{\partial G}{\partial P}\right)_{T} \tag{1.39}
\end{equation*}
$$

The circular diagram completed in this way is a good mnemonic tool for describing Eqs. (9), (15), (31), (35), and (39), which express thermodynamic variables as partial derivatives of the thermodynamic potentials. Indeed, the variable in any corner of the diagram may be found as a derivative of any of two potentials that are not its immediate neighbors, over the variable in the opposite corner. For example, the red line in Fig. 6b corresponds to the second of Eqs. (39), while the blue line, to the second of Eqs. (31). At this, the derivatives giving variables of the upper row ( $S$ and $P$ ) have to be

[^797]taken with negative signs, while those giving the variables of the bottom row ( $V$ and $T$ ), with positive signs. ${ }^{27}$

Now I have to justify the collective name "thermodynamic potentials" used for $E, H, F$, and $G$. For that, let us consider an irreversible process, for example, a direct thermal contact of two bodies with different initial temperatures. As we have seen in Sec. 2, at such a process, the entropy may grow even without the external heat flow: $d S \geq 0$ at $d Q=0$ - see Eq. (12). For a more general process with $d Q \neq 0$, this means that entropy may grow faster than predicted by Eq. (19), which has been derived for a reversible process, so that

$$
\begin{equation*}
d S \geq \frac{d Q}{T} \tag{1.40}
\end{equation*}
$$

with the equality approached in the reversible limit. Plugging Eq. (40) into Eq. (18) (which, being just the energy conservation law, remains valid for irreversible processes as well), we get

$$
\begin{equation*}
d E \leq T d S-P d V \tag{1.41}
\end{equation*}
$$

Now we can use this relation to have a look at the behavior of other thermodynamic potentials in irreversible situations, still keeping their definitions given by Eqs. (27), (33), and (37). Let us start from the (very common) case when both temperature $T$ and volume $V$ are kept constant. If the process was reversible, according to Eq. (34), the full time derivative of free energy $F$ would equal zero. Equation (41) says that at the irreversible process it is not necessarily so: if $d T=d V=0$, then

$$
\begin{equation*}
\frac{d F}{d t}=\frac{d}{d t}(E-T S)=\frac{d E}{d t}-T \frac{d S}{d t} \leq T \frac{d S}{d t}-T \frac{d S}{d t}=0 . \tag{1.42}
\end{equation*}
$$

Hence, in the general (irreversible) situation, function $F$ can only decrease, but not increase in time. This means that $F$ eventually approaches its minimum value $F(T, S)$, which is given by the equations of reversible thermodynamics.

Thus in the case $T=$ const, $V=$ const, the free energy $F$, i.e. the difference $E-T S$, plays the role of the potential energy in the classical mechanics of dissipative processes: its minimum corresponds to the (in the case of $F$, thermodynamic) equilibrium of the system. This is one of the key results of thermodynamics, and I invite the reader to give it some thought. One of its possible handwaving interpretations is that the heat bath with fixed $T>0$, i.e. with a substantial thermal agitation of its components, "wants" to impose thermal disorder in the system immersed in it by "rewarding" it (by lowering its $F$ ) for any increase of disorder.

Repeating the calculation for the case $T=$ const, $P=$ const, it is easy to see that in this case the same role is played by the Gibbs energy:

$$
\begin{equation*}
\frac{d G}{d t}=\frac{d}{d t}(E-T S+P V)=\frac{d E}{d t}-T \frac{d S}{d t}+P \frac{d V}{d t} \leq\left(T \frac{d S}{d t}-P \frac{d V}{d t}\right)-T \frac{d S}{d t}+P \frac{d V}{d t}=0, \tag{1.43}
\end{equation*}
$$

[^798]so that the thermal equilibrium now corresponds to the minimum of $G$ rather than $F$. One can argue very convincingly that the difference, $G-F=P V$ between these two potentials (also equal to $H-E$ ) has very little to do with thermodynamics at all, because this difference exists (although not much advertised) in classical mechanics as well. ${ }^{28}$ Indeed, the difference may be generalized as $G-F=-\mathcal{Z}_{j} q_{j}$, where $q_{j}$ is any generalized coordinate and $z_{j}$ is the corresponding generalized force - see Eq. (1) and its discussion. In this case the minimum of $F$ corresponds to the equilibrium of an autonomous system (with $\mathcal{F}_{j}=0$ ), while the equilibrium position of the same system under the action of external force $z_{j}$ is given by the minimum of $G$. Thus the external force "wants" the system to subdue to its effect, "rewarding" it by lowering its $G$. (The analogy with the "disorder pressure" by a heat bath, discussed in the last paragraph, is evident.)

For two remaining thermodynamic potentials, $E$ and $H$, the calculations similar to Eqs. (42) and (43) make less sense, because that would require taking $S=$ const (with $V=$ const for $E$, and $P=$ const for $H$ ), but it is hard to prevent the entropy from growing if initially it had been lower than its equilibrium value, at least on the long-term basis. ${ }^{29}$ Thus the circular diagram is not so symmetric after all: $G$ and/or $F$ are somewhat more useful for most practical calculations than $E$ and $H$.

One more important conceptual question is why the main task of statistical physics should be the calculation of thermodynamic potentials, rather than just a relation between $P, V$, and $T$. (Such relation is called the equation of state of the system.) Let us explore this issue on the example of an ideal classical gas in thermodynamic equilibrium, for which the equation of state should be well known to the reader from undergraduate physics (in Chapter 3, we will be derived from statistics):

$$
\begin{equation*}
P V=N T, \tag{1.44}
\end{equation*}
$$

where $N$ is the number of particles in volume $V .{ }^{30}$ Let us try to use it for the calculation of all thermodynamic potentials, and all other thermodynamic variables discussed above. We may start, for example, from the calculation of the free energy $F$. Indeed, solving Eq. (44) for pressure, $P=N T / V$, and integrating the second of Eqs. (35), we get

$$
\begin{equation*}
F=-\left.\int P d V\right|_{T}=-N T \int \frac{d V}{V}=-N T \int \frac{d(V / N)}{(V / N)}=-N T \ln \frac{V}{N}+N f(T), \tag{1.45}
\end{equation*}
$$

where I have divided $V$ by $N$ in both instances just to present $F$ as a manifestly extensive variable, in this uniform system proportional to $N$. The integration "constant" $f(T)$ is some function of temperature that cannot be recovered from the equation of state. This function also affects all other thermodynamic potentials, and entropy. Indeed, using the first of Eqs. (35) together with Eq. (45), we get

[^799]\[

$$
\begin{equation*}
S=-\left(\frac{\partial F}{\partial T}\right)_{V}=N\left[\ln \frac{V}{N}-\frac{d f}{d T}\right] \tag{1.46}
\end{equation*}
$$

\]

and now can combine Eqs. (33) and (46) to calculate the (internal) energy,

$$
\begin{equation*}
E=F+T S=\left(-N T \ln \frac{V}{N}+N f\right)+T\left(N \ln \frac{V}{N}-N \frac{d f}{d T}\right)=N\left(f-T \frac{d f}{d T}\right) \tag{1.47}
\end{equation*}
$$

then use Eqs. (27), (44) and (47) to calculate enthalpy,

$$
\begin{equation*}
H=E+P V=E+N T=N\left(f-T \frac{d f}{d T}+T\right) \tag{1.48}
\end{equation*}
$$

and, finally, plug Eqs. (44), and (45) into Eq. (37) to calculate the Gibbs energy

$$
\begin{equation*}
G=F+P V=N\left(-T \ln \frac{V}{N}+f+T\right) \tag{1.49}
\end{equation*}
$$

In particular, Eq. (47) describes a very important property of the ideal classical gas: its energy depends only on temperature, but not on volume or pressure. One might question whether function $f(T)$ may be physically insignificant, just like the arbitrary constant that may be always added to the potential energy in non-relativistic mechanics. In order to address this concern, let us calculate, from Eqs. (24) and (28), both heat capacities, that are readily measurable quantities:

$$
\begin{gather*}
C_{V}=\left(\frac{\partial E}{\partial T}\right)_{V}=-N T \frac{d^{2} f}{d T^{2}},  \tag{1.50}\\
C_{P}=\left(\frac{\partial H}{\partial T}\right)_{P}=N\left(-T \frac{d^{2} f}{d T^{2}}+1\right)=C_{V}+N . \tag{1.51}
\end{gather*}
$$

We see that function $f(T)$, or at least its second derivative, is measurable. ${ }^{31}$ (In Chapter 3, we will calculate this function for two simple "microscopic" models of the ideal classical gas.) The meaning of this function is evident from the physical picture of the ideal gas: pressure $P$ exerted on the walls of the containing volume is produced only by the translational motion of the gas molecules, while their internal energy $E$ (and hence other thermodynamic potentials) may be also contributed by the internal motion of the molecules - their rotations, vibrations, etc. Thus, the equation of state does not give the full thermodynamic description of a system, while the thermodynamic potentials do.

### 1.5. Systems with variable number of particles

Now we have to consider one more important case when the number $N$ of particles in a system is not rigidly fixed, but may change as a result of a thermodynamic process. Typical examples of such a system is a gas sample separated from the environment by a penetrable partition (Fig. 7), and a gas in a contact with the liquid of the same molecules.

[^800]environment


Fig. 1.7. Example of a system with variable number of particles.

Let us analyze this situation for the simplest case when all the particles are similar (though the analysis may be readily extended to systems with particle of several sorts). In this case we can consider $N$ as an independent thermodynamic variable whose variation may change energy $E$ of the system, so that (for a slow, reversible process) Eq. (17) should be now generalized as

$$
\begin{equation*}
d E=T d S-P d V+\mu d N \tag{1.52}
\end{equation*}
$$

Chemical potential: definition
where $\mu$ is a new function of state, called the chemical potential. ${ }^{32}$ Keeping the definitions of other thermodynamic potentials, given by Eqs. (27), (33), and (37) intact, we see that expressions for their differentials should be generalized as

$$
\begin{align*}
& d H=T d S+V d P+\mu d N  \tag{1.53a}\\
& d F=-S d T-P d V+\mu d N  \tag{1.53b}\\
& d G=-S d T+V d P+\mu d N \tag{1.53c}
\end{align*}
$$

so that the chemical potential may be calculated as either of the following derivatives: ${ }^{33}$

$$
\begin{equation*}
\mu=\left(\frac{\partial E}{\partial N}\right)_{S, V}=\left(\frac{\partial H}{\partial N}\right)_{S, P}=\left(\frac{\partial F}{\partial N}\right)_{T, V}=\left(\frac{\partial G}{\partial N}\right)_{T, P} \tag{1.54}
\end{equation*}
$$

Despite their similarity, one of Eqs. (53)-(54) is more consequential than the others. Indeed, the Gibbs energy $G$ is the only thermodynamic potential that is a function of two intensive parameters, $T$ and $P$. However, as all thermodynamic potentials, $G$ has to be extensive, so that in a system of similar particles it has to be proportional to $N$ :

$$
\begin{equation*}
G=N f(T, P) . \tag{1.55}
\end{equation*}
$$

Plugging this expression into the last of Eqs. (54), we see that $\mu$ equals $f(T, P)$. In other words,

$$
\begin{equation*}
\mu=\frac{G}{N} \tag{1.56}
\end{equation*}
$$

so that the chemical potential is just the Gibbs energy per particle.

[^801]In order to demonstrate how vital the notion of chemical potential may be, let us consider the situation (parallel to that shown in Fig. 2) when a system consists of two parts, with equal pressure and temperature, that can exchange particles at a relatively slow rate (much slower than the speed of internal relaxation inside each of the parts). Then we can write two equations similar to Eq. (5):

$$
\begin{equation*}
N=N_{1}+N_{2}, \quad G=G_{1}+G_{2}, \tag{1.57}
\end{equation*}
$$

where $N=$ const, and Eq. (56) may be used to describe each component of $G$ :

$$
\begin{equation*}
G=\mu_{1} N_{1}+\mu_{2} N_{2} . \tag{1.58}
\end{equation*}
$$

Plugging $N_{2}$ expressed from the first of Eqs. (57), $N_{2}=N-N_{1}$, into Eq. (58), we see that

$$
\begin{equation*}
\frac{d G}{d N_{1}}=\mu_{1}-\mu_{2} \tag{1.59}
\end{equation*}
$$

so that the minimum of $G$ is achieved at $\mu_{1}=\mu_{2}$. Hence, in the conditions of fixed temperature and pressure, i.e. when $G$ is the appropriate thermodynamic potential, the chemical potentials of the system parts should be equal - the so-called chemical equilibrium.

Later we will also run into cases when volume $V$ of a system, its temperature $T$, and the chemical potential $\mu$ are all fixed. (The last condition may be readily implemented by allowing the system of interest to exchange particles with a reservoir so large that its $\mu$ stays constant.) A thermodynamic potential appropriate for this case may be obtained from the free energy $F$ by subtraction of the product $\mu N$, resulting is the so-called grand thermodynamic potential (or the "Landau potential")

Grand potential: definition and full differential

Indeed, for a reversible process, the full differential of this potential is

$$
\begin{equation*}
d \Omega=d F-d(\mu N)=(-S d T-P d V+\mu d N)-(\mu d N+N d \mu)=-S d T-P d V-N d \mu \tag{1.61}
\end{equation*}
$$

so that if $\Omega$ has been calculated as a function of $T, V$ and $\mu$, other thermodynamic variables may be found as

$$
\begin{equation*}
S=-\left(\frac{\partial \Omega}{\partial T}\right)_{V, \mu}, \quad P=-\left(\frac{\partial \Omega}{\partial V}\right)_{T, \mu}, \quad N=-\left(\frac{\partial \Omega}{\partial \mu}\right)_{T, V} \tag{1.62}
\end{equation*}
$$

For an irreversible process, acting exactly as we have done with other potentials, it is straightforward to prove that in the conditions of fixed $T, V$, and $\mu, d \Omega / d t \leq 0$, so that system's equilibrium indeed corresponds to the minimum of the grand potential $\Omega$.

### 1.6. Thermal machines

In order to complete this brief review of thermodynamics, I cannot pass the topic of thermal machines - not because it will be used much in this course, but mostly because of its practical and historic significance. (Indeed, the whole field of thermodynamics was spurred by the famous 1824 work by S. Carnot, which in particular gave an alternative, indirect form of the $2^{\text {nd }}$ law of thermodynamics see below.)

Figure 8a shows the generic scheme of a thermal machine that may perform mechanical work on the environment (in the notation of Eq. (1), equal to $-\mathscr{W}$ ) during each cycle of the expansion/compression of the "working gas", by transferring different amounts of heat from a high-temperature heat bath $\left(Q_{H}\right)$ and to the low-temperature bath $\left(Q_{L}\right)$. One relation between three amounts $Q_{H}, Q_{L}$, and $\mathcal{W}$ is immediately given by the energy conservation (i.e. by "the $1^{\text {st }}$ law of thermodynamics"):

$$
\begin{equation*}
Q_{H}-Q_{L}=-w . \tag{1.63}
\end{equation*}
$$

From Eq. (1), the mechanical work during the cycle may be calculated as

$$
\begin{equation*}
-w=\oint P d V \tag{1.64}
\end{equation*}
$$

i.e. equals the area circumvented by the representing point on the $[P, V]$ plane - see Fig. $8 b .{ }^{34}$ Hence, the work depends on the exact form of the cycle, which in turn depends not only on $T_{H}$ and $T_{L}$, but also on working gas' properties.


Fig. 1.8. (a) The simplest implementation of a thermal machine, and (b) the graphic presentation of the mechanical work it performs. On panel (b), solid arrow indicates the heat engine cycle direction, while the dashed arrow, the refrigerator cycle direction.

An exception from this rule is the famous Carnot cycle, consisting of two isothermal and two adiabatic processes (all reversible!). In its heat engine's form, the cycle starts from an isothermic expansion of the gas in contact with the hot bath (i.e. at $T=T_{H}$ ), followed by its additional adiabatic expansion until $T$ drops to $T_{\mathrm{L}}$. Then an isothermal compression of the gas is performed in its contact with the cold bath (at $T=T_{L}$ ), followed by its additional adabatic compression to raise its temberature to $T_{H}$ again, after which the cycle is repeated again and again. (Note that during this cycle the working gas is never in contact with both heat baths simultaneously, thus avoiding the irreversible heat transfer between them.) The cycle's shape on the $[V, P]$ plane depends on exact properties of the working gas and may be rather complicated. However, since the entropy is constant at any adabatic process, the Carnot cycle shape on the [ $S, T]$ plane is always rectangular - see Fig. 9. ${ }^{35}$

[^802]

(b)

Fig. 1.9. Representation of the Carnot cycle (a) on the [ $S, T]$ plane and (b) the $[V, P]$ plane (schematically). The meaning of arrows is the same as in Fig. 8.

Since during each isotherm, the working gas is brought into thermal contact only with the corresponding heat bath, Eq. (19), $d Q=T d S$ may be immediately integrated to yield

$$
\begin{equation*}
Q_{H}=T_{H}\left(S_{2}-S_{1}\right), \quad Q_{L}=T_{L}\left(S_{2}-S_{1}\right) . \tag{1.65}
\end{equation*}
$$

Hence the ratio of these two heat flows is completely determined by their temperature ratio:

$$
\begin{equation*}
\frac{Q_{H}}{Q_{L}}=\frac{T_{H}}{T_{L}}, \tag{1.66}
\end{equation*}
$$

regardless of the working gas properties. Equations (63) and (66) are sufficient to find the ratio of work $-w$ to any of $Q_{H}$ and $Q_{L}$. For example, the main figure-of-merit of a thermal machine used as a heat engine $\left(Q_{H}>0, Q_{L}>0,-\mathcal{W}=|\mathcal{W}|>0\right)$, is its efficiency
engine efficiency: definition

$$
\begin{equation*}
\eta \equiv \frac{|w|}{Q_{H}}=\frac{Q_{H}-Q_{L}}{Q_{H}}=1-\frac{Q_{L}}{Q_{H}} \leq 1 \tag{1.67}
\end{equation*}
$$

For the Carnot cycle, Eq. (66) immediately yields the famous relation,

Carnot cycle's
efficiency

$$
\begin{equation*}
\eta_{\text {Carnot }}=1-\frac{T_{L}}{T_{H}} \tag{1.68}
\end{equation*}
$$

which shows that at given $T_{L}$ (that is typically the ambient temperature $\sim 300 \mathrm{~K}$ ), the efficiency may be increased, ultimately to 1 , by raising temperature of the heat source.

On the other hand, if the cycle is reversed (see the dashed arrows in Figs. 8 and 9), the same thermal machine may serve as a refrigerator, providing the heat removal from the low-temperature bath $\left(Q_{L}<0\right)$ for the cost of consuming external work: $w>0$. This reversal does not affect the basic relation (63) that may be used to calculate the relevant figure-of-merit, called the cooling coefficient of performance ( $\mathrm{COP}_{\text {cooling }}$ )

$$
\begin{equation*}
\mathrm{COP}_{\text {cooling }} \equiv \frac{\left|Q_{L}\right|}{w}=\frac{Q_{L}}{Q_{H}-Q_{L}} . \tag{1.69}
\end{equation*}
$$

Notice that this coefficient may readily be above unity; in particular, for the Carnot cycle we may use Eq. (66) (which is also unaffected by the cycle reversal) to get
nuclear spins by external magnetic field. In such refrigerators (to be further discussed in the next chapter), the role of the $\{-P, V\}$ pair of variables is played by the $\{\mathcal{H}, B\}$ pair - see Eq. (3).

$$
\begin{equation*}
\left(\mathrm{COP}_{\text {cooling }}\right)_{\text {Carnot }}=\frac{T_{L}}{T_{H}-T_{L}} \tag{1.70}
\end{equation*}
$$

so that the $\mathrm{COP}_{\text {cooling }}$ is larger than 1 at $T_{H}<2 T_{L}$, and even may be very large when the temperature difference $\left(T_{H}-T_{L}\right)$, sustained by the refrigerator, tends to zero. For example, in a typical airconditioning system, $T_{H}-T_{L} \sim T_{L} / 30$, so that the Carnot value of $\mathrm{COP}_{\text {cooling }}$ is as high as $\sim 30$, while in the state-of-the-art commercial HVAC systems it is the range for 3 to 4 . This is why the term "cooling efficiency", used in some textbooks instead of (COP) $)_{\text {cooling, }}$, may be misleading.

Since in the reversed cycle $Q_{H}=-w+Q_{L}<0$, the system also provides heat flow into the hotter heat bath, and thus may be used as a heat pump. However, the figure-of-merit appropriate for this application is different:

$$
\begin{equation*}
\mathrm{COP}_{\text {heating }} \equiv \frac{\left|Q_{H}\right|}{w}=\frac{Q_{H}}{Q_{H}-Q_{L}} \tag{1.71}
\end{equation*}
$$

so that for the Carnot cycle

$$
\begin{equation*}
\left(\mathrm{COP}_{\text {heating }}\right)_{\text {Carnot }}=\frac{T_{H}}{T_{H}-T_{L}} . \tag{1.72}
\end{equation*}
$$

Note that this COP is always larger than 1, meaning that the Carnot heat pump is always more efficient than the direct conversion of work into heat (where $Q_{H}=-\mathcal{W}$, and $\mathrm{COP}_{\text {heating }}=1$ ), though practical electricity-driven heat pumps are substantially more complex (and hence more expensive) than, say, simple electric heaters. Such heat pumps, with typical $\mathrm{COP}_{\text {heating }}$ values around 4 in summer and 2 in winter, are frequently used for heating large buildings.

I have dwelled so long on the Carnot cycle, because it has a remarkable property: the highest possible efficiency of all heat-engine cycles. Indeed, in the Carnot cycle the transfer of heat between any heat bath and the working gas is performed reversibly, when their temperatures are equal. If this is not so, heat might flow from a hotter to colder system without performing any work. Hence the result (68) also yields the maximum efficiency of any heat engine. In particular, it shows that $\eta_{\max }=0$ at $T_{H}=T_{L}$, i.e., no heat engine can perform any mechanical work in the absence of temperature gradients. ${ }^{36}$ In some alternative axiomatic systems of thermodynamics, this fact, i.e. the impossibility of the direct conversion of heat to work, is postulated, and serves the role of the $2^{\text {nd }}$ law.

Note also that according to Eq. (70), $\mathrm{COP}_{\text {cooling }}$ of the Carnot cycle tends to zero at $T_{\mathrm{L}} \rightarrow 0$, making it impossible to reach the absolute zero of temperature, and hence illustrating the meaningful (Nernst's) formulation of the $3^{\text {rd }}$ law of thermodynamics. Indeed, let us prescribe a certain (but very large) heat capacity $C(T)$ to the low-temperature bath, and use the definition of this variable to write the following evident expression for the (very small) change of its temperature as a result of a relatively large number $d n$ of similar refrigeration cycles:

$$
\begin{equation*}
C\left(T_{L}\right) d T_{L}=Q_{L} d n . \tag{1.73}
\end{equation*}
$$

[^803]Together with Eq. (66), this relation yields

$$
\begin{equation*}
C\left(T_{L}\right) d T_{L}=-\frac{\left|Q_{H}\right|}{T_{H}} T_{L} d n, \tag{1.74}
\end{equation*}
$$

so that if we perform many $(n)$ cycles (with constant $Q_{H}$ and $T_{H}$ ), the initial and final values of $T_{L}$ obey the following equation

$$
\begin{equation*}
\int_{T_{\mathrm{ini}}}^{T_{\mathrm{fin}}} \frac{C(T) d T}{T}=-\frac{\left|Q_{H}\right|}{T_{H}} n . \tag{1.75}
\end{equation*}
$$

For example, if $C(T)$ is a constant, Eq. (75) yields an exponential law,

$$
\begin{equation*}
T_{\mathrm{fin}}=T_{\mathrm{ini}} \exp \left\{-\frac{\left|Q_{H}\right|}{C T_{H}} n\right\}, \tag{1.76}
\end{equation*}
$$

with the absolute zero not reached as any finite $n$. Relation (75) proves the Nernst theorem if $C(T)$ does not vanish at $T \rightarrow 0$, but for such metastable systems as glasses the situation is more complicated. ${ }^{37}$ Fortunately, this issue does not affect other aspects of statistical physics - at least those to be discussed in this course.

### 1.7. Exercise problems

1.1. Two bodies, with negligible thermal expansion coefficients and constant heat capacities $C_{1}$ and $C_{2}$, are placed into a weak thermal contact, at different initial temperatures $T_{1}$ and $T_{2}$. Calculate the full change of entropy of the system before it reaches the full thermal equilibrium.
1.2. A gas has the following properties:
(i) $C_{V}=a T^{b}$, and
(ii) the work $w_{T}$ needed for its isothermal compression from $V_{2}$ to $V_{1}$ equals $c T \ln \left(V_{2} / V_{1}\right)$,
where $a, b$, and $c$ are constants. Find the equation of state of the gas, and calculate the temperature dependences of its entropy $S$, and thermodynamic potentials $E, H, F, G$ and $\Omega$.
1.3. A vessel with an ideal classical gas of indistinguishable molecules is separated by a partition so that the number $N$ of molecules in both parts is the same but their volumes are different. The gas is in thermal equilibrium, and its pressure in one part is $P_{1}$, and in another, $P_{2}$. Calculate the change of entropy caused by a fast removal of the partition. Analyze the result.
1.4. An ideal classical gas of $N$ particles, is initially confined to volume $V$, and let alone to reach the thermal equilibrium with a heat bath of temperature $T$. Then the gas is allowed to expand to volume $V^{\prime}>V$ in one the following ways:

[^804](i) The expansion slow, so that due to the thermal contact with the heat bath, the gas temperature remains equal to $T$ all the time.
(ii) The partition separating volumes $V$ and $\left(V^{\prime}-V\right)$ is removed very fast, allowing the gas to expand rapidly.

For each process, calculate the changes of pressure, temperature, energy, and entropy of the gas during its expansion.
1.5. For an ideal classical gas with temperature-independent specific heat, derive the relation between $P$ and $V$ at the adiabatic expansion/compression.
1.6. Calculate the speed and wave impedance of acoustic waves in an ideal classical gas with temperature-independent $C_{P}$ and $C_{V}$, in the limits when that the wave propagation may be treated as:
(i) an isothermal process,
(ii) an adiabatic process.

Which of these limits corresponds to higher wave frequencies?
1.7. As will be discussed in Sec. 3.5, the so-called "hardball" models of classical particle interaction yield the following equation of state of a gas of such particles:

$$
P=T \varphi(n)
$$

where $n=N / V$ is the particle density, and function $\varphi(n)$ is generally different from that $\left(\varphi_{\text {ideal }}(n)=n\right)$ of the ideal gas. For such a gas, with temperature-independent $c_{V}$, calculate:
(i) the energy of the gas, and
(ii) its pressure as a function of $n$ at adiabatic compression.
1.8. For an arbitrary thermodynamic system with a fixed number of particles, prove the following Maxwell relations (already mentioned in Sec. 1.4):

$$
\text { (i): }\left(\frac{\partial S}{\partial V}\right)_{T}=\left(\frac{\partial P}{\partial T}\right)_{V}, \quad \text { (ii): }\left(\frac{\partial V}{\partial S}\right)_{P}=\left(\frac{\partial T}{\partial P}\right)_{S}, \quad \text { (iii): }\left(\frac{\partial S}{\partial P}\right)_{T}=-\left(\frac{\partial V}{\partial T}\right)_{P}, \quad \text { (iv): }\left(\frac{\partial P}{\partial S}\right)_{V}=-\left(\frac{\partial T}{\partial V}\right)_{S} .
$$

1.9. A process, performed with a fixed portion of an ideal gas, may be represented with a straight line on the $[P, V]$ plane - see Fig. on the right. Find the point at which the heat flow into/out of the gas changes its direction.

1.10. Two bodies have equal and constant heat capacities $C$, but different temperatures, $T_{1}$ and $T_{2}$. Calculate the maximum mechanical work obtainable from this system, using a heat engine.
1.11. Express the efficiency of a heat engine that uses the "Joule cycle" consisting of two adiabatic and two isobaric processes (see Fig. on the right), via the minimum and maximum values of pressure, and compare the result with that for the Carnot cycle. Assume an ideal classical working gas with constant $C_{P}$ and $C_{V}$.

1.12. Calculate the efficiency of a heat engine using the "Otto cycle", ${ }^{38}$ which consists of two adiabatic and two isochoric (constantvolume) processes - see Fig. on the right. Explore how does the efficiency depend on the ratio $r \equiv V_{\max } / V_{\min }$, and compare it with Carnot cycle's efficiency. Assume an ideal working gas with temperature-independent specific heat.

1.13. A heat engine's cycle consists of two isothermal ( $T=$ const) and two isochoric ( $V=$ const) reversible processes - see Fig. on the right.
(i) Assuming that the working gas is an ideal classical gas of $N$ particles, calculate the mechanical work performed by the engine during one cycle.
(ii) Are the specified conditions sufficient to calculate engine's efficiency?


[^805]

## Chapter 2. Principles of Physical Statistics

This chapter is the key part of this course. It is started with a brief discussion of such basic notions of statistical physics as statistical ensembles, probability, and ergodicity. Then the so-called microcanonical distribution postulate is formulated in parallel with the statistical definition of entropy. The next step is the derivation of the Gibbs distribution, which is frequently considered the summit of the statistical physics, and one more, grand canonical distribution, which is more convenient for some tasks - in particular for the derivation of the Boltzmann, Fermi-Dirac, and Bose-Einstein statistics for systems of independent particles.

### 2.1. Statistical ensembles and probability

As has been already discussed in Sec. 1.1, statistical physics deals with systems in conditions when either the unknown initial conditions, or the system complexity, or the laws of motion (as in the case of quantum mechanics) do not allow a definite prediction of measurement results. The main formalism for the analysis of such systems is the probability theory, so let me start with a very brief review of its basic concepts using informal "physical" language - less rigorous but (hopefully) more transparent than a standard mathematical treatment. ${ }^{1}$

Consider $N \gg 1$ independent similar experiments carried out with apparently similar systems (i.e. systems with identical macroscopic parameters such as volume, pressure, etc.), but still giving, by any of the reasons outlined above, different results of measurements. Such a collection of experiments, together with the fixed method of result processing, is a good example of a statistical ensemble. Let us start from the case when the experiments may have $M$ different discrete outcomes, and the number of experiments giving the corresponding different results is $N_{1}, N_{2}, \ldots, N_{M}$, so that

$$
\begin{equation*}
\sum_{m=1}^{M} N_{m}=N . \tag{2.1}
\end{equation*}
$$

The probability of each outcome, for the given statistical ensemble, is then defined as

$$
\begin{equation*}
W_{m} \equiv \lim _{N \rightarrow \infty} \frac{N_{m}}{N} . \tag{2.2}
\end{equation*}
$$

Though this definition is so close to our everyday experience that it is almost self-evident, a few remarks may still be relevant.

First, probabilities $W_{m}$ depend on the exact statistical ensemble they are defined for, notably including the method of result processing. As an example, consider the standard coin tossing. For the ensemble of all tossed coins, the probabilities of both the heads and tails outcomes equal $1 / 2$. However, nothing prevents us from defining another statistical ensemble as a set of coin-tossing experiments with the heads-up outcome. Evidently, the probability of finding coins with tails up in this new ensemble is not $1 / 2$ but 0 . Still, this set of experiments is not only legitimate but also a rather meaningful statistical

[^806]ensemble; for example, the exact position and orientation of the tossed coins on the floor, within this restricted ensemble, may be rather random.

Second, a statistical ensemble does not necessarily require $N$ different physical systems, e.g., $N$ different coins. It is intuitively clear that tossing the same coin $N$ times constitutes an ensemble with similar statistical properties. More generally, a set of $N$ experiments with the same system provides a statistical ensemble equivalent to the set of experiments with $N$ different systems, provided that the experiments are kept independent, i.e. that outcomes of past experiments do not affect those of the experiments to follow. Moreover, for most physical systems of interest any special preparation is unnecessary, and $N$ different experiments, separated by sufficiently long time intervals, form a "good" statistical ensemble - the property called ergodicity. ${ }^{2}$

Third, the reference to infinite $N$ in Eq. (2) does not strip the notion of probability from its practical relevance. Indeed, it is easy to prove (see Chapter 5) that, at very general conditions, at finite but sufficiently large $N$, numbers $N_{m}$ are approaching their average (or expectation) values ${ }^{3}$

$$
\begin{equation*}
\left\langle N_{m}\right\rangle \equiv W_{m} N \tag{2.3}
\end{equation*}
$$

with the relative deviation scale decreasing as $1 /\left\langle N_{m}\right\rangle^{1 / 2}$.
Now let me list those properties of probabilities that we will immediately need. First, dividing Eq. (1) by $N$ and following the limit $N \rightarrow \infty$, we get the well-known normalization condition

$$
\begin{equation*}
\sum_{m=1}^{M} W_{m}=1 \tag{2.4}
\end{equation*}
$$

just remember that it is true only if each experiment definitely yields one of outcomes $N_{1}, N_{2}, \ldots, N_{M}$. Next, if we have an additive function of results,

$$
\begin{equation*}
f=\frac{1}{N} \sum_{m=1}^{M} N_{m} f_{m}, \tag{2.5}
\end{equation*}
$$

where $f_{m}$ are some definite (deterministic) coefficients, we may define the statistical average (also called the expectation value) of the function as

$$
\begin{equation*}
\langle f\rangle \equiv \lim _{N \rightarrow \infty} \frac{1}{N} \sum_{m=1}^{M}\left\langle N_{m}\right\rangle f_{m}, \tag{2.6}
\end{equation*}
$$

[^807]so that using Eq. (3) we get
\[

$$
\begin{equation*}
\langle f\rangle=\sum_{m=1}^{M} W_{m} f_{m} \tag{2.7}
\end{equation*}
$$

\]

Notice that Eq. (3) may be considered as the particular form of this general result, for all $f_{m}=1$.
Next, the spectrum of possible experimental outcomes is frequently continuous. (Think, for example, about the positions of the marks left by bullets fired into a target from a far.) The above formulas may be readily generalized to this case; let us start from the simplest situation when all different outcomes may be described by one continuous variable $q$, which replaces the discrete index $m$ in Eqs. (1)-(7). The basic relation for this case is the self-evident fact that the probability $d W$ of having an outcome within a very small interval $d q$ near point $q$ is proportional to the magnitude of that interval:

$$
\begin{equation*}
d W=w(q) d q \tag{2.8}
\end{equation*}
$$

Function $w(q)$, which does not depend on $d q$, is called the probability density. Now all the above formulas may be recast by replacing probabilities $W_{m}$ by products (8), and the summation over $m$, by integration over $q$. In particular, instead of Eq. (4) the normalization condition now becomes

$$
\begin{equation*}
\int w(q) d q=1 \tag{2.9}
\end{equation*}
$$

where the integration should be extended over the whole range of possible values of $q$. Similarly, instead by Eq. (5), it is natural to consider a function $f(q)$. Then instead of Eq. (7), the expectation value of the function may be calculated as

$$
\begin{equation*}
\langle f\rangle=\int w(q) f(q) d q \tag{2.10}
\end{equation*}
$$

It is straightforward to generalize these formulas to the case of more variables. For example, results of measurements of a particle with 3 degrees of freedom may be described by the probability density $w$ defined in the 6D space of its generalized radius-vector $\mathbf{q}$ and momentum $\mathbf{p}$. As a result, the expectation value of a function of these variables may be expressed as a 6D integral

$$
\begin{equation*}
\langle f\rangle=\int w(\mathbf{q}, \mathbf{p}) f(\mathbf{q}, \mathbf{p}) d^{3} q d^{3} p \tag{2.11}
\end{equation*}
$$

Some systems considered in this course consist of components whose quantum properties cannot be ignored, so let us discuss how $\langle f\rangle$ should be calculated in this case. If by $f_{m}$ we mean measurement results, Eq. (7) (and its generalizations) of course remains valid, but since these numbers themselves may be affected by the intrinsic quantum-mechanical uncertainty, it may make sense to have a bit deeper look into this situation. Quantum mechanics tells us ${ }^{4}$ that the most general expression for the expectation value of an observable $f$ in a certain ensemble of macroscopically similar systems is

$$
\begin{equation*}
\langle f\rangle=\sum_{m, m^{\prime}} W_{m m^{\prime}} f_{m^{\prime} m} \equiv \operatorname{Tr}(\mathrm{Wf}) \tag{2.12}
\end{equation*}
$$

Here $f_{m m}$, are the matrix elements of the quantum-mechanical operator $\hat{f}$ corresponding to the observable $f$, in a full basis of orthonormal states $m$,

$$
\begin{equation*}
f_{m m^{\prime}}=\langle m| \hat{f}\left|m^{\prime}\right\rangle, \tag{2.13}
\end{equation*}
$$

[^808]while coefficients $W_{m m}$ are elements of the so-called density matrix W , which represents, in the same basis, a density operator $\hat{W}$ describing properties of this ensemble. Equation (12) is evidently more general than Eq. (7), and is reduced to it only if the density matrix is diagonal:
\[

$$
\begin{equation*}
W_{m m^{\prime}}=W_{m} \delta_{m m^{\prime}}, \tag{2.14}
\end{equation*}
$$

\]

(where $\delta_{m m}$, is the Kronecker symbol), when the diagonal elements $W_{m}$ play the role of probabilities of the corresponding states.

Thus the largest difference between the quantum and classical description is the presence, in Eq. (12), of the off-diagonal elements of the density matrix. They have largest values in the pure (also called "coherent") ensemble, in which the state of the system may be described with state vectors, e.g., the ketvector

$$
\begin{equation*}
|\alpha\rangle=\sum_{m} \alpha_{m}|m\rangle \tag{2.15}
\end{equation*}
$$

where $\alpha_{m}$ are some complex coefficients. In this simple case, the density matrix elements are merely

$$
\begin{equation*}
W_{m m^{\prime}}=\alpha_{m}^{*} \alpha_{m^{\prime}}, \tag{2.16}
\end{equation*}
$$

so that the off-diagonal elements are of the same order as the diagonal elements. For example, in the very important particular case of a two-level system, the pure-state density matrix is

$$
\mathrm{W}=\left(\begin{array}{ll}
\alpha_{1}^{*} \alpha_{1} & \alpha_{1}^{*} \alpha_{2}  \tag{2.17}\\
\alpha_{2}^{*} \alpha_{1} & \alpha_{2}^{*} \alpha_{2}
\end{array}\right)
$$

so that the product of its off-diagonal components is as large as that of the diagonal components. In the most important basis of stationary states, i.e. eigenstates of system's time-independent Hamiltonian, coefficients $\alpha_{m}$ oscillate in time as ${ }^{5}$

$$
\begin{equation*}
\alpha_{m}(t)=\alpha_{m}(0) \exp \left\{-i \frac{E_{m}}{\hbar} t\right\}=\left|\alpha_{m}\right| \exp \left\{-i \frac{E_{m}}{\hbar} t+i \varphi_{m}\right\}, \tag{2.18}
\end{equation*}
$$

where $E_{m}$ are the corresponding eigenenergies, and $\varphi_{m}$ are constant phase shifts. This means that while the diagonal terms of the density matrix (16) remain constant, its off-diagonal components are oscillating functions of time:

$$
\begin{equation*}
W_{m m^{\prime}}=\alpha_{m^{\prime}}^{*} \alpha_{m}=\left|\alpha_{m^{\prime}} \alpha_{m}\right| \exp \left\{i \frac{E_{m}-E_{m^{\prime}}}{\hbar} t\right\} \exp \left\{i\left(\varphi_{m^{\prime}}-\varphi_{m}\right)\right\} . \tag{2.19}
\end{equation*}
$$

Due to the extreme smallness of the Planck constant (on the human scale of things), a miniscule random perturbations of eigenenergies are equivalent to substantial random changes of the phase multiplier, so that the time average of any off-diagonal matrix element tends to zero. Moreover, even if our statistical ensemble consists of systems with exactly the same $E_{m}$, but different values $\varphi_{m}$ (which are typically hard to control at the initial preparation of the system), the average values of all $W_{m m^{\prime}}$ (with $m \neq m^{\prime}$ ) vanish again.

[^809]This is why, besides some very special cases, typical statistical ensembles of quantum particles are far from being pure, and in most cases (certainly including the thermodynamic equilibrium), a good approximation for their description is given by the opposite limit of the so-called classical mixture in which all off-diagonal matrix elements of the density matrix equal zero, and its diagonal elements $W_{m m}$ are merely the probabilities $W_{m}$ of the corresponding eigenstates. In this case, for observables compatible with energy, Eq. (12) is reduced to Eq. (7), with $f_{m}$ being the eigenvalues of variable $f$.

### 2.2. Microcanonical ensemble and distribution

Let us start with the discussion of physical statistics with the simplest, microcanonical statistical ensemble ${ }^{6}$ that is defined a set of macroscopically similar closed (isolated) systems with virtually the same total energy $E$. Since in quantum mechanics the energy of a closed system is quantized, it is convenient to include into the ensemble all systems with energies $E_{m}$ within a narrow interval $\Delta E \ll E$, that is nevertheless much larger than the average distance $\delta E$ between the energy levels, so that the number $M$ of different quantum states within interval $\Delta E$ is large, $M \gg 1$. Such choice of $\Delta E$ is only possible if $\delta E \ll E$; however, the reader should not worry too much about this condition, because the most important applications of the microcanonical ensemble are for very large systems (or very high energies) when the energy spectrum is very dense. ${ }^{7}$


Fig. 2.1. Very schematic image of the microcanonical ensemble. (Actually, the ensemble deals with quantum states rather than energy levels. An energy level may be degenerate, i.e. correspond to several states.)

This ensemble serves as the basis for the formulation of a postulate which is most frequently called the microcanonical distribution (or sometimes the "main statistical hypothesis"): in the thermodynamic equilibrium, all possible states of the microcanonical ensemble have equal probability,

$$
\begin{equation*}
W_{m}=\frac{1}{M}=\text { const. } \tag{2.20}
\end{equation*}
$$

Though in some constructs of statistical mechanics this equality is derived from other axioms, which look more plausible to their authors, I believe that Eq. (20) may be taken as the starting point of the statistical physics, supported "just" by the compliance of all its corollaries with experimental observations. ${ }^{8}$

Note that postulate (20) sheds a light on the nature of the macroscopic irreversibility of microscopically reversible (closed) systems: if such a system was initially in a certain state, its time

[^810]evolution with just miniscule interactions with environment (which is necessary for reaching the thermodynamic equilibrium) would eventually lead to the uniform distribution of its probability among all states with the essentially same energy. Each of these states is not "better" than the initial one; rather, in a macroscopic system, there are just so many of these states that the chance to find the system in the initial state is practically nil - again, think about the ink drop diffusion into a glass of water.

Now let us find a suitable definition of entropy $S$ of a microcanonical ensemble member - for now, in the thermodynamic equilibrium only. Since $S$ is a measure of disorder, it should be related to the amount of information lost when the system goes from the full order to the full disorder, i.e. into the microcanonical distribution (20), or, in other words, the amount of information ${ }^{9}$ necessary to find the exact state of your system in a microcanonical ensemble.

In the information theory, the amount of information necessary to make a definite choice between two options with equal probabilities (Fig. 2a) is defined as

$$
\begin{equation*}
I(2) \equiv \log _{2} 2=1 \tag{2.21}
\end{equation*}
$$

This unit of information is called a bit. Now, if we need to make a choice between 4 equally probable opportunities, it can be made in two similar steps (Fig. 2b), each requiring one bit of information, so that the total amount of information necessary for the choice is

$$
\begin{equation*}
I(4)=2 I(2)=2=\log _{2} 4 . \tag{2.22}
\end{equation*}
$$

An obvious extension of this process to the choice between $M=2^{m}$ states gives

$$
\begin{equation*}
I(M)=m I(2)=m=\log _{2} M . \tag{2.23}
\end{equation*}
$$


(b)

Fig. 2.2. "Logarithmic trees" of binary decisions for making a choice between (a) 2 and (b) 4 opportunities with equal probabilities.

This measure, if extended naturally to any integer $M$, is quite suitable for the definition of entropy at equilibrium, with the only difference that, following tradition, the binary logarithm is replaced with the natural one: ${ }^{10}$

[^811]\[

$$
\begin{equation*}
S \equiv \ln M \tag{2.24a}
\end{equation*}
$$

\]

Using Eq. (20), we may recast this definition in the most frequently used form

$$
\begin{array}{r}
\text { Entropy } \\
\text { in }  \tag{2.24b}\\
\text { equilibrium }
\end{array}
$$

$$
S=\ln \frac{1}{W_{m}}=-\ln W_{m}
$$

(Again, please note that Eq. (24) is valid in the thermodynamic equilibrium only!)
Equation (24) satisfies the major condition for the entropy definition in thermodynamics, i.e. to be a unique characteristics of disorder. Indeed, according to Eq. (20), number $M$ (and hence any function of $M$ ) are the only possible measures characterizing the microcanonical distribution. We also need this function of $M$ to satisfy another requirement to the entropy, of being an extensive thermodynamic variable, and Eq. (24) does satisfy this requirement as well. Indeed, mathematics says that for two independent systems the joint probability is just a product of their partial probabilities, and hence, according to Eq. (24b), their entropies just add up.

Now let us see whether Eqs. (20) and (24) are compatible with the $2^{\text {nd }}$ law of thermodynamics. For that, we need to generalize Eq. (24) for $S$ to an arbitrary state of the system (generally, out of thermodynamic equilibrium), with arbitrary state probabilities $W_{m}$. For that, let us first recognize that $M$ in Eq. (24) is just the number of possible ways to commit a particular system to a certain state $m$ ( $m=1$, $2, \ldots M)$, in a statistical ensemble where each state is equally probable. Now let us consider a more general ensemble, still consisting of a large number $N \gg 1$ of similar systems, but with a certain number $N_{m}=W_{m} N \gg 1$ of systems in each of $M$ states, with $W_{m}$ not necessarily equal. In this case the evident generalization of Eq. (24) is that the entropy $S_{N}$ of the whole ensemble is

$$
\begin{equation*}
S_{N} \equiv \ln M\left(N_{1}, N_{2}, . .\right), \tag{2.25}
\end{equation*}
$$

where $M\left(N_{1}, N_{2}, \ldots\right)$ is the number of ways to commit a particular system to a certain state $m$, while keeping all numbers $N_{m}$ fixed. Such number $M\left(N_{1}, N_{2}, \ldots\right)$ is clearly equal to the number of ways to distribute $N$ distinct balls between $M$ different boxes, with the fixed number $N_{m}$ of balls in each box, but in no particular order within it. Comparing this description with the definition of the so-called multinomial coefficients, ${ }^{11}$ we get

$$
\begin{equation*}
M\left(N_{1}, N_{2}, \ldots\right)={ }^{N} C_{N_{1}, N_{2}, \ldots, N_{M}} \equiv \frac{N!}{N_{1}!N_{2}!\ldots N_{M}!}, \quad \text { with } N=\sum_{m=1}^{M} N_{m} \tag{2.26}
\end{equation*}
$$

In order to simplify the resulting expression for $S_{N}$, we can use the famous Stirling formula in its crudest, de Moivre's form ${ }^{12}$ whose accuracy is suitable for most purposes of statistical physics:

$$
\begin{equation*}
\ln (N!)_{\mid N \rightarrow \infty} \rightarrow N(\ln N-1) . \tag{2.27}
\end{equation*}
$$

When applied to our current problem, this gives the following average entropy per system, ${ }^{13}$

[^812]\[

$$
\begin{align*}
S \equiv & \frac{S_{N}}{N}=\frac{1}{N} \ln \left({ }^{N} C_{N_{1}, N_{2}, \ldots, N_{M}}\right)=\frac{1}{N}\left[\ln (N!)-\sum_{m=1}^{M} \ln \left(N_{m}!\right)\right] \\
& \rightarrow \frac{1}{N}\left[N(\ln N-1)-\sum_{m=1}^{M} N_{m}\left(\ln N_{m}-1\right)\right]=\ln N-\frac{1}{N} \sum_{m=1}^{M} N_{m} \ln N_{m}=-\sum_{m=1}^{M} \frac{N_{m}}{N} \ln \frac{N_{m}}{N} . \tag{2.28}
\end{align*}
$$
\]

and since this result is only valid in the limit $N_{m} \rightarrow \infty$ anyway, we may use Eq. (2) to present it as

$$
\begin{equation*}
S=-\sum_{m=1}^{M} W_{m} \ln W_{m}=\sum_{m=1}^{M} W_{m} \ln \frac{1}{W_{m}} . \tag{2.29}
\end{equation*}
$$

Entropy
out of equilibrium

This extremely important formula ${ }^{14}$ may be interpreted as the average of the entropy values given by Eq. (24), weighed with specific probabilities $W_{m}$ in accordance with the general formula (7). ${ }^{15}$

Now let us find what distribution of probabilities $W_{m}$ provides the largest value of entropy (29). The answer is almost evident from a single glance at Eq. (29). For example, if coefficients $W_{m}$ are constant (and hence equal to $1 / M^{\prime}$ ) for a subgroup of $M^{\prime} \leq M$ states and equal zero for all others, all $M^{\prime}$ nonvanishing terms in the sum (29) are equal to each other, so that

$$
\begin{equation*}
S=M^{\prime} \frac{1}{M^{\prime}} \ln M^{\prime}=\ln M^{\prime} \tag{2.30}
\end{equation*}
$$

so that the closer $M^{\prime}$ to its maximum number $M$ the larger $S$. Hence, the maximum of $S$ is reached at the uniform distribution given by Eq. (24).

In order to prove this important fact more strictly, let us find the maximum of function given by Eq. (29). If its arguments $W_{1}, W_{2}, \ldots W_{M}$ were completely independent, this could be done by finding the point (in the $M$-dimensional space of coefficients $W_{m}$ ) where all partial derivatives $\partial S / \partial W_{m}$ are equal to zero. However, since the probabilities are constrained by condition (4), the differentiation has to be carried out more carefully, taking into account this interdependence:

$$
\begin{equation*}
\left[\frac{\partial}{\partial W_{m}} S\left(W_{1}, W_{2}, \ldots\right)\right]_{\mathrm{cond}}=\frac{\partial S}{\partial W_{m}}+\sum_{m^{\prime} \neq m} \frac{\partial S}{\partial W_{m^{\prime}}} \frac{\partial W_{m^{\prime}}}{\partial W_{m}} . \tag{2.31}
\end{equation*}
$$

At the maximum of function $S$, all such expressions should be equal to zero simultaneously. This condition may be presented as $\partial S / \partial W_{m}=\lambda$, where the so-called Lagrange multiplier $\lambda$ is independent of $m$. Indeed, at such point Eq. (31) becomes

$$
\begin{equation*}
\left[\frac{\partial}{\partial W_{m}} S\left(W_{1}, W_{2}, \ldots\right)\right]_{\mathrm{cond}}=\lambda+\sum_{m^{\prime} \neq m} \lambda \frac{\partial W_{m^{\prime}}}{\partial W_{m}}=\lambda\left(\frac{\partial W_{m}}{\partial W_{m}}+\sum_{m^{\prime} \neq m} \frac{\partial W_{m^{\prime}}}{\partial W_{m}}\right)=\lambda \frac{\partial}{\partial W_{m}}(1)=0 . \tag{2.32}
\end{equation*}
$$

[^813]For the particular expression (29), condition $\partial S / \partial W_{m}=\lambda$ yields

$$
\begin{equation*}
\frac{\partial S}{\partial W_{m}} \equiv \frac{d}{d W_{m}}\left[-W_{m} \ln W_{m}\right]=-\ln W_{m}-1=\lambda . \tag{2.33}
\end{equation*}
$$

Equation (33) may hold for all $m$ (and hence the entropy reach its maximum value) only if $W_{m}$ is independent on $m$. Thus entropy (29) indeed reaches its maximum value (24) at equilibrium.

To summarize, we see that definition (24) of entropy in statistical physics does fit all the requirements imposed on this variable by thermodynamics. ${ }^{16}$ In particular, we have been able to prove the $2^{\text {nd }}$ law of thermodynamics, starting from that definition and a more fundamental postulate (20). Now let me discuss one possible point of discomfort with that definition: it depends on the accepted energy interval of the microcanonical ensemble, for whose width $\Delta E$ no exact guidance is offered. However, if the interval $\Delta E$ contains many states, $M \gg 1$, then with a very small relative error (vanishing in the limit $M \rightarrow \infty$ ), $M$ may be presented as

$$
\begin{equation*}
M=g(E) \Delta E \tag{2.34}
\end{equation*}
$$

where $g(E)$ is the density of states of the system:

$$
\begin{equation*}
g(E) \equiv \frac{d \Sigma(E)}{d E} \tag{2.35}
\end{equation*}
$$

$\Sigma(E)$ being the total number of states with energies below $E$. (Note that the average interval $\delta E$ between energy levels, mentioned in the beginning of this section, is just $\delta E=\Delta E / M=1 / g$.) Plugging Eq. (34) into Eq. (24), we get

$$
\begin{equation*}
S=\ln M=\ln g(E)+\ln \Delta E \tag{2.36}
\end{equation*}
$$

so that the only effect of a particular choice of $\Delta E$ is an offset of entropy by a constant, and in Chapter 1 we have seen that such a shift does not affect any measurable quantity. Of course, Eq. (34), and hence Eq. (36) are only precise in the limit when density of states $g(E)$ is so large that the range available for the appropriate choice of $\Delta E$,

$$
\begin{equation*}
g^{-1}(E) \ll \Delta E \ll E, \tag{2.37}
\end{equation*}
$$

is sufficiently broad: $g(E) E=E / \delta E \gg 1$.
In order to get some feeling of the functions $g(E)$ and $S(E)$ and the feasibility of condition (37), and also to see whether the microcanonical distribution may be directly used for calculations of thermodynamic variables in particular systems, let us apply it to a microcanonical ensemble of many sets of $N \gg 1$ independent, similar harmonic oscillators with eigenfrequency $\omega$. (Please note that the requirement of a virtually fixed energy is applied, in this case, the total energy $E_{N}$ of the set, rather to a single oscillator - whose energy $E$ may be virtually arbitrary, though certainly less than $E_{N} \sim N E$.) Basic quantum mechanics ${ }^{17}$ teaches us that the eigenenergies of such an oscillator form a discrete, equidistant spectrum:

[^814]\[

$$
\begin{equation*}
E_{m}=\hbar \omega\left(m+\frac{1}{2}\right), \quad \text { where } m=0,1,2, \ldots \tag{2.38}
\end{equation*}
$$

\]

If $\omega$ is kept constant, the zero-point energy $\hbar \omega / 2$ does not contribute to any thermodynamic properties of the system and may be ignored, ${ }^{18}$ so that for the sake of simplicity we may take that point as the energy origin, and replace Eq. (38) with $E_{m}=m \hbar \omega$. Let us carry out an approximate analysis of the system for the case when its average energy per oscillator,

$$
\begin{equation*}
E=\frac{E_{N}}{N}, \tag{2.39}
\end{equation*}
$$

is much larger than the energy quantum $\hbar \omega$. For one oscillator, the number of states with energy $\varepsilon_{1}$ below certain value $=E_{1} \gg \hbar \omega$ is evidently $\Sigma\left(E_{1}\right) \approx E_{1} / \hbar \omega$ (Fig. 3a). For two oscillators, all possible values of the total energy $\left(\varepsilon_{1}+\varepsilon_{2}\right)$ below some level $E_{2}$ correspond to the points of a 2D square grid within the right triangle shown in Fig. 3b, giving $\Sigma\left(E_{2}\right) \approx(1 / 2)\left(E_{2} / \hbar \omega\right)^{2}$. For three oscillators, the possible values of the total energy $\left(\varepsilon_{1}+\varepsilon_{2}+\varepsilon_{3}\right)$ correspond to those points of the 3D cubic mesh, that fit inside the right pyramid shown in Fig. 3c, giving $\Sigma\left(E_{3}\right) \approx(1 / 2)(1 / 3)\left(E_{3} / \hbar \omega\right)^{3}=(1 / 3!)\left(E_{3} / \hbar \omega\right)^{3}$, etc.


Fig. 2.3. Calculating functions $\Sigma\left(\mathrm{E}_{N}\right)$ for the systems of (a) one, (b) two and (c) three quantum oscillators.
An evident generalization of these formulas to arbitrary $N$ gives the number of states

$$
\begin{equation*}
\Sigma\left(E_{N}\right) \approx \frac{1}{N!}\left(\frac{E_{N}}{\hbar \omega}\right)^{N} \tag{2.40}
\end{equation*}
$$

where coefficient $1 / N$ ! has the geometrical meaning of the (hyper)volume of the $N$-dimensional right pyramid with unit sides. Differentiating Eq. (40), we get

$$
\begin{equation*}
g\left(E_{N}\right)=\frac{d \Sigma\left(E_{N}\right)}{d E_{N}}=\frac{1}{(N-1)!} \frac{E_{N}^{N-1}}{(\hbar \omega)^{N}} \tag{2.41}
\end{equation*}
$$

so that

[^815]\[

$$
\begin{equation*}
S_{N}\left(E_{N}\right)=\ln g\left(E_{N}\right)+\text { const }=-\ln [(N-1)!]+(N-1) \ln E_{N}-N \ln (\hbar \omega)+\text { const. } \tag{2.42}
\end{equation*}
$$

\]

For $N \gg 1$ we can ignore the difference between $N$ and $(N-1)$ in both instances, and use the Stirling formula (27) to simplify this result as

$$
\begin{equation*}
S_{N}(E)-\text { const } \approx N\left(\ln \frac{E_{N}}{N \hbar \omega}+1\right) \approx N\left(\ln \frac{E}{\hbar \omega}\right)=\ln \left[\left(\frac{E}{\hbar \omega}\right)^{N}\right] \tag{2.43}
\end{equation*}
$$

(The second approximation is only valid at very high $E / \hbar \omega$ ratios, when the logarithm in Eq. (43) is substantially larger than 1 , i.e. is rather crude. ${ }^{19}$ ) Returning for a second to the density of states, we see that in the limit $N \rightarrow \infty$, it is exponentially large:

$$
\begin{equation*}
g\left(E_{N}\right)=e^{S_{N}} \approx\left(\frac{E}{\hbar \omega}\right)^{N} \tag{2.44}
\end{equation*}
$$

so that both conditions (37) may be satisfied within a very broad range of $\Delta E$.
Now we can use Eq. (43) to find all thermodynamic properties of the system, though only in the limit $E \gg \hbar \omega$. Indeed, according to thermodynamics (see Sec. 1.2), if the system volume and number of particles are fixed, the derivative $d S / d E$ is nothing more than the reciprocal temperature - see Eqs. (1.9) or (1.15). In our current case, we imply that the harmonic oscillators are distinct, for example by their spatial positions. Hence, even if we can speak of some volume of the system, it is certainly fixed. ${ }^{20}$ Differentiating Eq. (43) over energy $E$, we get

## Average energy of a classical

 oscillator$$
\begin{equation*}
\frac{1}{T}=\frac{d S_{N}}{d E_{N}}=\frac{N}{E_{N}}=\frac{1}{E} \tag{2.45}
\end{equation*}
$$

Reading this result backwards, we see that the average energy $E$ of a harmonic oscillator equals $T$ (i.e. $k_{\mathrm{B}} T_{\mathrm{K}}$ is SI units). As we will show in Sec. 5 below, this is the correct asymptotic form of the exact result, valid in our current limit $E \gg \hbar \omega$.

Result (45) may be readily generalized. Indeed, in quantum mechanics a harmonic oscillator with eigenfrequency $\omega$ may by described by Hamiltonian

$$
\begin{equation*}
\hat{H}=\frac{\hat{p}^{2}}{2 m}+\frac{\kappa \hat{q}^{2}}{2} \tag{2.46}
\end{equation*}
$$

where $q$ is some generalized coordinate, and $p$ the corresponding generalized momentum, $m$ is oscillator's mass, ${ }^{21}$ and $\kappa$ is the spring constant, so that $\omega=(\kappa / m)^{1 / 2}$. Since in thermodynamic equilibrium the density matrix is always diagonal (see Sec. 1 above) in basis of stationary states $m$, quantum-mechanical averages of the kinetic and potential energies may be found from Eq. (7):

[^816]\[

$$
\begin{equation*}
\left\langle\frac{p^{2}}{2 m}\right\rangle=\sum_{m=0}^{\infty} W_{m}\langle m| \frac{\hat{p}^{2}}{2 m}|m\rangle, \quad\left\langle\frac{\kappa q^{2}}{2}\right\rangle=\sum_{m=0}^{\infty} W_{m}\langle m| \frac{\kappa \hat{q}^{2}}{2}|m\rangle, \tag{2.47}
\end{equation*}
$$

\]

where $W_{m}$ is the probability to occupy $m$-th energy level, and bra- and ket-vectors describe the stationary state corresponding to that level. ${ }^{22}$ However, both classical and quantum mechanics teach us that for any $m$, the bra-kets under the sums in Eqs. (47), which present the average kinetic and mechanical energies of the oscillator on its $m^{\text {th }}$ energy level, are equal to each other, and hence each of them is equal to $E_{m} / 2$. Hence, even though we do not know the probability distribution $W_{m}$ yet (it will be calculated in Sec. 5 below), we may conclude that in the "classical limit" $T \gg \hbar \omega$,

$$
\begin{equation*}
\left\langle\frac{p^{2}}{2 m}\right\rangle=\left\langle\frac{\kappa q^{2}}{2}\right\rangle=\frac{T}{2} \tag{2.48}
\end{equation*}
$$

Now let us consider a system with an arbitrary number of degrees of freedom, described by a more general Hamiltonian: ${ }^{23}$

$$
\begin{equation*}
\hat{H}=\sum_{j} \hat{H}_{j}, \quad \hat{H}_{j}=\frac{\hat{p}_{j}^{2}}{2 m_{j}}+\frac{\kappa_{j} \hat{q}_{j}^{2}}{2} \tag{2.49}
\end{equation*}
$$

with (generally, different) eigenfrequencies $\omega_{j}=\left(\kappa_{j} / m_{j}\right)^{1 / 2}$. Since the "modes" (effective harmonic oscillators), contributing into this Hamiltonian, are independent, result (48) is valid for each of the modes. This is the famous equipartition theorem: at thermal equilibrium with $T \gg \hbar \omega_{j}$, the average energy of each so-called half-degree of freedom (which are defined as variables $p_{j}$ or $q_{j}$, giving a quadratic term to the system's Hamiltonian), is equal to $T / 2 .{ }^{24}$ In particular, for each Cartesian coordinate $q_{j}$ of a free-moving, non-interacting particle this theorem is valid for any temperature, because such coordinates may be considered as 1D harmonic oscillators with vanishing potential energy, i.e. $\omega_{j}=0$, so that condition $T \gg \hbar \omega_{j}$ is fulfilled at any temperature.

At this point, a first-time student of thermodynamics should be very much relieved to see that the counter-intuitive thermodynamic definition (1.9) of temperature does indeed correspond to what we all have known about this notion from our kindergarten physics courses.

I believe that our case study of quantum oscillator systems has been a fair illustration of both the strengths and weaknesses of the microcanonical ensemble approach. ${ }^{25}$ On one hand, we could calculate virtually everything we wanted in the classical limit $T \gg \hbar \omega$, but calculations for arbitrary $T \sim \hbar \omega$, though possible, are difficult, because for that, all vertical steps of function $\Sigma\left(E_{N}\right)$ have to be carefully

[^817]counted. In Sec. 4, we will see that other statistical ensembles are much more convenient for such calculations.

Let me conclude this discussion of entropy with a short notice on deterministic classical systems with a few degrees of freedom (and even simpler mathematical objects called "maps") that may exhibit essentially disordered behavior, called the deterministic chaos. ${ }^{26}$ Such chaotic system may be approximately characterized by an entropy defined similarly to Eq. (29), where $W_{m}$ are probabilities to find it in different small regions of phase space, at well separated time intervals. On the other hand, one can use an equation slightly more general than Eq. (29) to define the so-called Kolmogorov (or "Kolmogorov-Sinai") entropy $K$ that characterizes the speed of loss of information about the initial state of the system, and hence what is called the "chaos' depth". In the definition of $K$, the sum over $m$ is replaced with the summation over all possible permutations $\{m\}=m_{0}, m_{1}, \ldots, m_{N-1}$ of small space regions, and $W_{m}$ is replaced with $W_{\{m\}}$, the probability of finding the system in the corresponding regions $m$ at time moment $t_{m}$, with $t_{m}=m \tau$, in the limit $\tau \rightarrow 0$, with $N \tau=$ const. For chaos in the simplest objects, 1D maps, $K$ is equal to the Lyapunov exponent $\lambda>0 .{ }^{27}$ For systems of higher dimensionality, which are characterized by several Lyapunov exponents $\lambda$, the Kolmogorov entropy is equal to the phase-space average of the sum of all positive $\lambda$. These facts provide a much more practicable way of (typically, numerical) calculation of the Kolmogorov entropy than the direct use of its definition. ${ }^{28}$

### 2.3. Maxwell's Demon, information, and computation

Before proceeding to other statistical distributions, I would like to address one more popular concern about Eq. (24), the direct relation between the entropy and information. Some physicists are still uneasy with entropy being nothing else than the (deficit of) information, ${ }^{29}$ though to the best of my knowledge, nobody has yet been able to suggest any experimentally verifiable difference between these two notions. Let me give one example of their direct relation, that is essentially a development of the thought experiment suggested by Maxwell as early as in 1867.

Consider a volume containing just one molecule (considered as a point particle), and separated to two equal halves by a movable partition with a door that may be opened and closed at will, at no energy cost (Fig. 4a). If the door is open and the system is in thermodynamic equilibrium, we do not know on which side of the door partition the molecule is. Here the disorder (and hence entropy) are largest, and there is no way to get, from a large ensemble of such systems, any useful mechanical energy.

Now, let us consider that we (as instructed by, in Lord Kelvin's formulation, an omniscient Maxwell's Demon) know which side of the partition the molecule is currently located. Then we may

[^818]close the door, so that molecule's impacts on the partition create, on the average, a pressure force 7 directed toward the empty part of the volume (in Fig. 4b, the right one). Now we can get from the molecule some mechanical work, say by allowing force $\boldsymbol{7}$ to move the partition to the right, and picking up the resulting mechanical energy by some deterministic external mechanism. After the partition has been moved to the right end of the volume, we can open the door again (Fig. 4c), equalizing the molecule's average pressure on both sides of the partition, and then slowly move the partition back to the middle of the volume, without doing any substantial work. With the kind help by Maxwell's Demon, we can repeat the cycle again and again, and hence make the system to do unlimited mechanical work, fed "only" by information and thermal motion, and thus implementing the perpetual motion machine of the $2^{\text {nd }}$ kind - see Sec. 1.6. The fact that such heat engines do not exist means that the Maxwell's Demon does not either: getting any new information, at nonvanishing temperature (i.e. at thermal agitation of particles) has a finite energy cost.


Fig. 2.4. The Maxwell's Demon paradox: the volume with a single molecule (a) before and (b) after closing the door, and (c) after opening the door in the end of the expansion stage.

In order to evaluate this cost, let us calculate the maximum work per cycle made by the Maxwell's heat engine (Fig. 4), assuming that it is constantly in thermal equilibrium with a heat bath of temperature $T$. Formula (21) tells us that the information supplied by the demon (what exactly half of the volume contains the molecule) is exactly one bit, $I(2)=1$. According to Eq. (24), this means that by getting this information we are changing the entropy by

$$
\begin{equation*}
\Delta S_{I}=-\ln 2 \tag{2.50}
\end{equation*}
$$

Now, it would be a mistake to plug this (negative) entropy change into Eq. (1.19). First, that relation is only valid for slow, reversible processes. Moreover (and more importantly), this equation, as well as its irreversible version (1.41), is only valid for a fixed statistical ensemble. The change $\Delta S_{I}$ does not belong to this category, and may be formally described by the change of the statistical ensemble - from the one consisting of all similar systems (experiments) with an unknown location of the molecule, to the new ensemble consisting of the systems with the molecule in its certain (in Fig. 4, left) half. ${ }^{30}$

Now let us consider the slow expansion of the "gas" after the door had been closed. At this stage, we do not need the demon's help any longer (i.e. the statistical ensemble is fixed), and we can use relation (1.19). At the assumed isothermal conditions ( $T=$ const), this relation may be integrated over the whole expansion process, getting $\Delta Q=T \Delta S$. At the final position, the system's entropy should be the same as initially, i.e. before the door had been opened, because we again do not know where in the volume the molecule is. This means that the entropy was replenished, during the reversible expansion,

[^819]from the heat bath, by $\Delta S=-\Delta S_{\mathrm{I}}=+\ln 2$, so that $\Delta Q=T \Delta S=T \ln 2$. Since by the end of the whole cycle the internal energy $E$ of the system is the same as before, all this heat should have gone into the mechanical energy obtained during the expansion. Thus the obtained work per cycle (i.e. for each obtained information bit) is $T \ln 2\left(k_{\mathrm{B}} T_{\mathrm{K}} \ln 2\right.$ in SI units), about $4 \times 10^{-21}$ Joule at room temperature. This is exactly the minimum energy cost of getting one bit of new information about a system at temperature $T$.

The smallness of that amount on the everyday human scale has left the Maxwell's Demon paradox an academic exercise for almost a century. However, its discussion resumed in the 1960s in the context of energy consumption at numerical calculations, motivated by the exponential (Moore's-law) progress of the digital integrated circuits, which leads in particular, to a fast reduction of energy $\Delta E$ "spent" (turned into heat) per one binary logic operation. In the current generations of semiconductor digital integrated circuits, $\Delta E$ is of the order of $\sim 10^{-16} \mathrm{~J},{ }^{31}$ i.e. still exceeds the room-temperature value of $T \ln 2=k_{\mathrm{B}} T_{\mathrm{K}} \ln 2 \approx 3 \times 10^{-21} \mathrm{~J}$ by more than 4 orders of magnitude. Still, some engineers believe that thermodynamics imposes an important lower limit on $\Delta E$ and hence presents an insurmountable obstacle to the future progress of computation, ${ }^{32}$ so that the issue deserves a discussion.

Let me believe that the reader of these notes understands that, in contrast to naïve popular thinking, computers do not create any new information; all they can do it to reshape (process) it, loosing most of input information on the go. Indeed, any digital computation algorithm may be decomposed into simple, binary logical operations, each of them performed by a certain logic circuit called the logic gate. Some of these gates (e.g., logical NOT performed by inverters, as well as memory READ and WRITE operations) do not change the amount of information in the computer. On the other hand, such information-irreversible logic gates as two-input NAND (or NOR, or XOR, etc.) actually erase one bit at each operation, because they turn two input bits into one output bit (Fig. 5a).

(b)

Fig. 2.5. Simple examples of (a) irreversible and (b) potentially reversible logic circuits. Each rectangle presents a circuit storing one bit of information.

In 1961, R. Landauer arrived at the conclusion that each logic operation should turn into heat at least energy

[^820]\[

$$
\begin{equation*}
\Delta E_{\min }=T \ln 2 \equiv k_{\mathrm{B}} T_{\mathrm{K}} \ln 2 \tag{2.51}
\end{equation*}
$$

\]

This result may be illustrated with the Maxwell's Demon machine shown in Fig. 4, operating as heat pump. At the first stage, with the door closed, it uses external mechanical work $\Delta E=T \ln 2$ to reduce the volume in which of the molecule is confined from $V$ to $V / 2$, pumping heat $-\Delta Q=\Delta E$ into the heat bath. To model a logically-irreversible logic gate, let us now open the door in the partition, and thus loose 1 bit of information about molecule's position. Then we will never get work $T \ln 2$ back, because moving the partition back to the right, with door open, takes place at zero average pressure. Hence, Eq. (51) gives a fundamental limit for energy loss (per bit) at the logically irreversible computation.

However, in 1973 C. Bennett came up with convincing arguments that it is possible to avoid such energy loss by using only operations that are reversible not only physically, but also logically. ${ }^{33}$ For that, one has to avoid any loss of information, i.e. any erasure of intermediate results, for example in the way shown in Fig. 5b. (For that, gate F should be physically reversible, with no substantial static power consumption.) In the end of all calculations, after the result has been copied into a memory, the intermediate results may be "rolled back" through reversible gate to be eventually merged into a copy of input data, again without erasing a single bit. The minimal energy dissipation at such reversible calculation tends to zero as the operation speed is decreased, so that the average energy loss per bit may be less than the perceived "fundamental thermodynamic limit" (51). ${ }^{34}$ The price to pay for this ultralow dissipation is an enormous (exponential) complexity of hardware necessary for storage of all intermediate results. However, using irreversible gates sparely, it may be possible to reduce the complexity dramatically, so that in future the mostly reversible computation may be able to reduce energy consumption in practical digital electronics. ${ }^{35}$

Before we leave Maxwell's Demon behind, let me use it to discuss, for one more time, the relation between the reversibility of the classical and quantum mechanics of Hamiltonian systems and the irreversibility possible in thermodynamics and statistical physics. In our (or rather Lord Kelvin's :-) gedanken experiment shown in Fig. 4, the laws of mechanics governing the motion of the molecule are reversible all times. Still, at partition's motion to the right, driven by molecule's impacts, the entropy grows, because the molecule picks up heat $\Delta Q>0$, and hence entropy $\Delta S=\Delta Q / T>0$, from the heat bath. The physical mechanism of this irreversible entropy (read: disorder) growth is the interaction of the molecule with uncontrollable components of the heat bath, and the resulting loss of information about the motion of the molecule. Philosophically, the emergence of irreversibility in large systems is a strong argument against the reductionism - a naïve belief that knowing the exact laws of Nature at one level of its complexity, we can readily understand all the phenomena on the higher levels of its organization. In reality, the macroscopic irreversibility of large systems is a wonderful example of a new law (in this case, the $2^{\text {nd }}$ law of thermodynamics) that becomes relevant on the substantially new level of complexity - without defying the lower-level laws. Without such new laws, very little of the higher level organization of Nature may be understood.

[^821]
### 2.4. Canonical ensemble and the Gibbs distribution

As we have seen in Sec. 2, the microcanonical distribution may be directly used for solving some simple problems, ${ }^{36}$ but a further development of this approach (also due to J. Gibbs) turns out to be much more convenient for calculations. Let us consider that a statistical ensemble of similar systems we are studying, each in thermal equilibrium with a much larger heat bath of temperature $T$ (Fig. 6a). Such an ensemble is called canonical.
(a)

(b)


Fig. 2.6. (a) System in a heat bath (a canonical ensemble member) and (b) energy spectrum of the composite system (including the heat bath).

Next, it is intuitively evident that if the heat bath is sufficiently large, any thermodynamic variables characterizing the system under study should not depend on heat bath's environment. In particular, we may assume that the heat bath is thermally insulated; then the total energy $E_{\Sigma}$ of the composite system (consisting of the system of our interest, plus the heat bath) does not change in time. For example, if our system of interest is in its certain (say, $m^{\text {th }}$ ) quantum state, then the sum

$$
\begin{equation*}
E_{\Sigma}=E_{m}+E_{\mathrm{HB}} \tag{2.52}
\end{equation*}
$$

is time-independent. Now let us partition the canonical ensemble of such systems into much smaller sub-ensembles, each being a microcanonical ensemble of composite systems whose time-independent total energy $E_{\Sigma}$ is the same - as discussed in Sec. 2, within a certain very small energy interval $\Delta E_{\Sigma} \ll$ $E_{\Sigma}$. According to the microcanonical distribution, probabilities to find the composite system, within this new ensemble, in any state are equal. Still, heat bath energies $E_{\mathrm{HB}}=E_{\Sigma}-E_{m}$ (Fig. 6b) of members of this microcanonical sub-ensemble may be different due to the difference in $E_{m}$.

The probability $W\left(E_{m}\right)$ to find the system of our interest (within the selected sub-ensemble) in a state with energy $E_{m}$ is proportional to the number $\Delta M$ of such systems in the sub-ensemble. Due to the very large size of the heat bath in comparison with that of the system under study, the heat bath' density of states $g_{\mathrm{HB}}$ is very high, and $\Delta E_{\Sigma}$ may be selected so that

$$
\begin{equation*}
\frac{1}{g_{\mathrm{HB}}} \ll \Delta E_{\Sigma} \ll\left|E_{m}-E_{m^{\prime}}\right| \ll E_{\mathrm{HB}}, \tag{2.53}
\end{equation*}
$$

where $m$ and $m$ ' are any states of the system of our interest. As Fig. 6b shows, in this case we may write $\Delta M=g_{\mathrm{HB}}\left(E_{\mathrm{HB}}\right) \Delta E_{\Sigma}$. As a result, within the microcanonical ensemble with the total energy $E_{\Sigma}$,

[^822]\[

$$
\begin{equation*}
W_{m} \propto \Delta M=g_{\mathrm{HB}}\left(E_{\mathrm{HB}}\right) \Delta E_{\Sigma}=g_{\mathrm{HB}}\left(E_{\Sigma}-E_{m}\right) \Delta E_{\Sigma} . \tag{2.54}
\end{equation*}
$$

\]

Let us simplify this expression further, using the Taylor expansion with respect to relatively small $E_{m} \ll E_{\Sigma}$. However, here we should be careful. As we have seen in Sec. 2, the density of states of a large system is an extremely rapidly growing function of energy, so that if we applied the Taylor expansion directly to Eq. (54), the Taylor series would converge for very small $E_{m}$ only. A much broader applicability range may be obtained by taking logarithm of both parts of Eq. (54) first:

$$
\begin{equation*}
\ln W_{m}=\mathrm{const}+\ln \left[g_{\mathrm{HB}}\left(E_{\Sigma}-E_{m}\right)\right]+\ln \Delta E_{\Sigma}=\mathrm{const}+S_{\mathrm{HB}}\left(E_{\Sigma}-E_{m}\right), \tag{2.55}
\end{equation*}
$$

where the second equality results from application of Eq. (36) to the heat bath, and $\ln \Delta E_{\Sigma}$ has been incorporated into the constant. Now, we can Taylor-expand the (much more smooth) function of energy in the right-hand part, and limit ourselves to the two leading terms of the series:

$$
\begin{equation*}
\ln W_{m} \approx \mathrm{const}+\left.S_{\mathrm{HB}}\right|_{E_{m}=0}-\left.\frac{d S_{\mathrm{HB}}}{d E_{\mathrm{HB}}}\right|_{E_{m}=0} E_{m} . \tag{2.56}
\end{equation*}
$$

But according to Eq. (1.9), the derivative participating in this expression is nothing else than the reciprocal heat bath temperature that (due to the large bath size) does not depend on whether $E_{m}$ is equal to zero or not. Since our system of interest is in the thermal equilibrium with the bath, this is also the temperature $T$ of the system - see Eq. (1.8). Hence Eq. (56) is merely

$$
\begin{equation*}
\ln W_{m}=\text { const }-\frac{E_{m}}{T} . \tag{2.57}
\end{equation*}
$$

This equation describes a substantial decrease of $W_{m}$ as $E_{m}$ is increased by several $T$, and hence our linear approximation (56) is virtually exact as soon as $E_{\mathrm{HB}}$ is much larger than $T$ - the condition that is rather easy to satisfy, because as we have seen in Sec. 2, the average energy of each particle is of the order of $T$.

Now we should be careful again, because so far we have only derived Eq. (57) for a subensemble with fixed $E_{\Sigma}$. However, since the right-hand part of Eq. (57) includes only $E_{m}$ and $T$ that are independent of $E_{\Sigma}$, this relation is valid for all sub-ensembles of the canonical ensemble, and hence for the later ensemble as the whole. ${ }^{37}$ Hence for the total probability to find our system of interest in state with energy $E_{m}$, in the canonical ensemble with temperature $T$, we can write

$$
\begin{equation*}
W_{m}=\text { const } \times \exp \left\{-\frac{E_{m}}{T}\right\} \equiv \frac{1}{Z} \exp \left\{-\frac{E_{m}}{T}\right\} . \tag{2.58}
\end{equation*}
$$

This is the famous Gibbs distribution (sometimes called the "canonical distribution"), ${ }^{38}$ which is frequently arguably the summit of statistical physics, ${ }^{39}$ because it may be used for a straightforward (or at least conceptually straightforward :-) calculation of all statistical and thermodynamic variables.

[^823]Before I illustrate this, let me first calculate the coefficient $Z$ participating in Eq. (58) for the general case. Requiring, in accordance with Eq. (4), the sum of all $W_{m}$ to be equal 1, we get

Statistical
sum

$$
\begin{equation*}
Z=\sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\} \tag{2.59}
\end{equation*}
$$

where the summation is formally extended to all quantum states of the system, though in practical calculations, the sum may be truncated to include only the states that are noticeably occupied. This apparently humble normalization coefficient $Z$ turns out to be so important for the relation between the Gibbs distribution (i.e. statistics) and thermodynamics that it has a special name - or actually, two names: either the statistical sum or the partition function. To demonstrate how important $Z$ is, let us use the general Eq. (29) for entropy to calculate its value for the particular case of the canonical ensemble, i.e. the Gibbs distribution of probabilities $W_{n}$ :

$$
\begin{equation*}
S=-\sum_{m} W_{m} \ln W_{m}=\frac{\ln Z}{Z} \sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\}+\frac{1}{Z T} \sum_{m} E_{m} \exp \left\{-\frac{E_{m}}{T}\right\} . \tag{2.60}
\end{equation*}
$$

According to the general rule (7), the thermodynamic (i.e. ensemble-average) value $E$ of the internal energy of the system is

$$
\begin{equation*}
E=\sum_{m} W_{m} E_{m}=\frac{1}{Z} \sum_{m} E_{m} \exp \left\{-\frac{E_{m}}{T}\right\}, \tag{2.61a}
\end{equation*}
$$

so that the second term in the right-hand part of Eq. (60) is just $E / T$, while the first term equals just $\ln Z$, due to the normalization condition (59). (As a parenthetic remark, using the notion of reciprocal temperature $\beta \equiv 1 / T$, Eq. (61a), with account of Eq. (59), may be also rewritten as

$$
\begin{equation*}
E=-\frac{\partial(\ln Z)}{\partial \beta} \tag{2.61b}
\end{equation*}
$$

This formula is very convenient for calculations if our prime interest is the average energy $E$ rather than $F$ or $W_{n}$.) With these substitutions, Eq. (60) yields a very simple relation between the statistical sum and entropy:

$$
\begin{equation*}
S=\frac{E}{T}+\ln Z . \tag{2.62}
\end{equation*}
$$

Using Eq. (1.33), we see that Eq. (62) gives a straightforward way to calculate the free energy $F$ of the system from nothing else than its statistical sum:

$$
\begin{equation*}
F \equiv E-T S=T \ln \frac{1}{Z} \tag{2.63}
\end{equation*}
$$

[^824]Now, using the general thermodynamic relations (see especially the circular diagram shown in Fig. 1.7b, and its discussion) we can calculate all thermodynamic potentials of the system, and all other variables of interest. Let me only note that in order to calculate pressure $P$ - e.g., from the second of Eqs. (1.35) - we would need to know the explicit dependence of $F$, and hence of the statistical sum $Z$ on the system volume $V$. This would require the calculation, by appropriate methods of either classical or quantum mechanics, of the volume dependence of eigenenergies $E_{m}$. I will give numerous examples of such calculations later in the course. ${ }^{40}$

As the final note of this section, Eqs. (59) and (63) may be combined to give a very elegant expression,

$$
\begin{equation*}
\exp \left\{-\frac{F}{T}\right\}=\sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\} \tag{2.64}
\end{equation*}
$$

which offers a convenient interpretation of free energy as a (rather specific) average of eigenenergies of the system. One more convenient formula may be obtained by using Eq. (64) to rewrite the Gibbs distribution (58) in the form

$$
\begin{equation*}
W_{m}=\exp \left\{\frac{F-E_{m}}{T}\right\} . \tag{2.65}
\end{equation*}
$$

In particular, this expression shows that that since all probabilities $W_{m}$ are below $1, F$ is always lower than the lowest energy level. Also, note that probabilities $W_{m}$ do not depend on the energy reference choice, i. e. on an arbitrary constant added to all $E_{m}$ (and hence to $E$ and $F$ ).

### 2.5. Harmonic oscillator statistics

The last property may be immediately used in our first example of the Gibbs distribution application to a particular, but very important system - the harmonic oscillator, for the more general case then was done in Sec. 2, namely for a "quantum oscillator" with an arbitrary relation between $T$ and $\hbar \omega .{ }^{41}$ Let us consider a canonical ensemble of similar oscillators, each in a contact with a heat bath of temperature $T$. Selecting the zero-point energy $\hbar \omega / 2$ for the origin of $E$, oscillator eigenenergies (38) become $E_{m}=m \hbar \omega(m=0,1, \ldots)$, so that the Gibbs distribution for probabilities of these states is

$$
\begin{equation*}
W_{m}=\frac{1}{Z} \exp \left\{-\frac{E_{m}}{T}\right\}=\frac{1}{Z} \exp \left\{-\frac{m \hbar \omega}{T}\right\} \tag{2.66}
\end{equation*}
$$

[^825]with the statistical sum
\[

$$
\begin{equation*}
Z \equiv \sum_{m=0}^{\infty} \exp \left\{-\frac{m \hbar \omega}{T}\right\}=\sum_{m=0}^{\infty} \lambda^{m}, \quad \text { where } \lambda \equiv \exp \left\{-\frac{\hbar \omega}{T}\right\} \leq 1 \tag{2.67}
\end{equation*}
$$

\]

This is just the well-known infinite geometric progression (the "geometric series"), ${ }^{42}$ with the sum

$$
\begin{equation*}
Z=\frac{1}{1-\lambda}=\frac{1}{1-e^{-\hbar \omega / T}} \tag{2.68}
\end{equation*}
$$

Quantum oscillator's statistics

(a)

(b)

Fig. 2.7. Statistical and thermodynamic parameters of a harmonic oscillator, as functions of temperature.

This average energy may be calculated in any of two ways: either using Eq. (7):

$$
\begin{equation*}
E=\sum_{m=0}^{\infty} E_{m} W_{m}=\left(1-e^{-\hbar \omega / T}\right) \sum_{m=0}^{\infty} m \hbar \omega e^{-m \hbar \omega / T}, \tag{2.70}
\end{equation*}
$$

or (simpler) using Eq. (61b), as

[^826]\[

$$
\begin{equation*}
E=-\frac{\partial}{\partial \beta} \ln Z=\frac{\partial}{\partial \beta} \ln (1-\exp \{-\beta \hbar \omega\}), \quad \beta \equiv \frac{1}{T} . \tag{2.71}
\end{equation*}
$$

\]

Both methods give (of course) the same famous result, ${ }^{43}$

$$
\begin{equation*}
E=E(\omega, T)=\hbar \omega \frac{1}{e^{\hbar \omega / T}-1}, \tag{2.72}
\end{equation*}
$$

Quantum
which is valid for arbitrary temperature and plays the key role in many fundamental problems of physics. The red line in Fig. 7b shows this $E$ as a function of normalized temperature. At low temperatures, $T \ll \hbar \omega$, the oscillator is predominantly in its lowest (ground) state, and its energy (on top of the constant zero-point energy $\hbar \omega / 2$ !) is exponentially small: $E \approx \hbar \omega \exp \{-\hbar \omega / T\} \ll T$, $\hbar \omega$. On the other hand, in the high-temperature limit the energy tends to $T$. This is exactly the result (a particular case of the equipartition theorem) that was obtained in Sec. 2 from the microcanonical distribution. Please note how much simpler is the calculation starting from the Gibbs distribution, even for an arbitrary ratio $T / \hbar \omega$.

To complete the discussion of thermodynamic properties of the harmonic oscillator, we can calculate its free energy using Eq. (63):

$$
\begin{equation*}
F=T \ln \frac{1}{Z}=T \ln \left(1-e^{-\hbar \omega / T}\right) \tag{2.73}
\end{equation*}
$$

Now entropy may be found from thermodynamics: either from the first of Eqs. (1.35), $S=-(\partial F / \partial T)_{V}$, or (even more easily) from Eq. (1.33): $S=(E-F) / T$. Both relations give, of course, the same result:

$$
\begin{equation*}
S=\frac{\hbar \omega}{T} \frac{1}{e^{\hbar \omega / T}-1}-\ln \left(1-e^{-\hbar \omega / T}\right) \tag{2.74}
\end{equation*}
$$

Finally, since in the general case the dependence of the oscillator properties (essentially, $\omega$ ) on volume $V$ in this problem is not specified, such variables as $P, \mu, G, W$, and $\Omega$ are not defined, and we may calculate only the average heat capacity $C$ per one oscillator:

$$
\begin{equation*}
C=\frac{\partial E}{\partial T}=\left(\frac{\hbar \omega}{T}\right)^{2} \frac{e^{\hbar \omega / T}}{\left(e^{\hbar \omega / T}-1\right)^{2}}=\left[\frac{\hbar \omega / 2 T}{\sinh (\hbar \omega / 2 T)}\right]^{2} \tag{2.75}
\end{equation*}
$$

The calculated thermodynamic variables are shown in Fig. 7b. In the low-temperature limit ( $T$ $\ll \hbar \omega$ ), they all tend to zero. On the other hand, in the high temperature limit ( $T \gg \hbar \omega$ ), $F \rightarrow-T$ $\ln (T / \hbar \omega) \rightarrow-\infty, S \rightarrow \ln (T / \hbar \omega) \rightarrow+\infty$, and $C \rightarrow 1$ (in SI units, $C \rightarrow k_{\mathrm{B}}$ ). Note that the last limit is the direct corollary of the equipartition theorem: each of two "half-degrees of freedom" of the oscillator gives, in the classical limit, a contribution $C=1 / 2$ into its heat capacity.

Now let us use Eq. (69) to discuss the statistics of the quantum oscillator described by Hamiltonian (46), in the coordinate representation. Again using density matrix' diagonality at thermodynamic equilibrium, we may use a relation similar to Eqs. (47) to calculate the probability density to find the oscillator at coordinate $q$ :

[^827]\[

$$
\begin{equation*}
w(q)=\sum_{m=0}^{\infty} W_{m} w_{m}(q)=\sum_{m=0}^{\infty} W_{m}\left|\psi_{m}(q)\right|^{2}=\left(1-e^{-\hbar \omega / T}\right) \sum_{m=0}^{\infty} e^{-m \hbar \omega / T}\left|\psi_{m}(q)\right|^{2}, \tag{2.76}
\end{equation*}
$$

\]

where $\psi_{m}(q)$ is the eigenfunction of $m$-th stationary state of the oscillator. Since each $\psi_{m}(q)$ is proportional to the Hermite polynomial ${ }^{44}$ that requires at least $m$ elementary functions for its representation, working out the sum in Eq. (76) is a bit tricky, ${ }^{45}$ but the final result is rather simple: $w(q)$ is just a normalized Gaussian distribution (the "bell curve"),

$$
\begin{equation*}
w(q)=\frac{1}{(2 \pi)^{1 / 2} \delta q} \exp \left\{-\frac{q^{2}}{2(\delta q)^{2}}\right\}, \tag{2.77}
\end{equation*}
$$

with $\langle q\rangle=0$, and

$$
\begin{equation*}
\left\langle q^{2}\right\rangle=\frac{\hbar}{2 m \omega} \operatorname{coth} \frac{\hbar \omega}{2 T} . \tag{2.78}
\end{equation*}
$$

Since coth $\xi$ tends to 1 at $\xi \rightarrow \infty$, and diverges as $1 / \xi$ at $\xi \rightarrow 0$, Eq. (78) shows that the width of coordinate distribution is constant (and equal to that, $\hbar / 2 m \omega$, of the ground-state wavefunction $\psi_{0}$ ) at $T$ $\ll \hbar \omega$, and grows as $T / m \omega^{2}$ at $T / \hbar \omega \rightarrow \infty$.

As a sanity check, we may use Eq. (78) to write the following expression,

$$
\langle U\rangle \equiv\left\langle\frac{\kappa q^{2}}{2}\right\rangle=\frac{\hbar \omega}{4} \operatorname{coth} \frac{\hbar \omega}{2 T} \rightarrow \begin{cases}\hbar \omega / 4, & \text { at } T \ll \hbar \omega  \tag{2.79}\\ T / 2, & \text { at } \hbar \omega \ll T\end{cases}
$$

for the average potential energy of the oscillator. In order to comprehend this result, let us notice that Eq. (72) for the average full energy $E$ was obtained by counting it from the ground state energy $\hbar \omega / 2$ of the oscillator. ${ }^{46}$ If we add this energy to the result, we get


$$
\begin{equation*}
E=\frac{\hbar \omega}{e^{\hbar \omega / T}-1}+\frac{\hbar \omega}{2}=\frac{\hbar \omega}{2} \operatorname{coth} \frac{\hbar \omega}{2 T} \tag{2.80}
\end{equation*}
$$

We see that for arbitrary temperature, $\langle U\rangle=E / 2$, as we already concluded from Eq. (47). This means that the average kinetic energy, equal to $E-\langle U\rangle$, is also the same:

$$
\begin{equation*}
\left\langle\frac{p^{2}}{2 m}\right\rangle=\left\langle\frac{\kappa q^{2}}{2}\right\rangle=\frac{E}{2}=\frac{\hbar \omega}{4} \operatorname{coth} \frac{\hbar \omega}{2 T} . \tag{2.81}
\end{equation*}
$$

In the classical limit $T \gg \hbar \omega$, both energies equal $T / 2$, reproducing the equipartition theorem result (48).

### 2.6. Two important applications

The results of the previous section, especially Eq. (72), have enumerable applications in physics, but I will have time for a brief discussion of only two of them.

[^828](i) Blackbody radiation. Let us consider a free-space volume $V$ limited by non-absorbing (i.e. ideally reflecting) walls. Electrodynamics tells us ${ }^{47}$ that electromagnetic field in such a cavity may be presented as a sum of "modes" with time evolution similar to that of the usual harmonic oscillator, and quantum mechanics says ${ }^{48}$ that the energy of such electromagnetic oscillator is quantized in accordance with Eq. (38), so that at thermal equilibrium the average energy is described by Eq. (72). If volume $V$ is large enough, ${ }^{49}$ the number of these modes within a small range $d k$ of the wavevector magnitude $k$ is ${ }^{50}$
\[

$$
\begin{equation*}
d N=\frac{g V}{(2 \pi)^{3}} d^{3} k=\frac{g V}{(2 \pi)^{3}} 4 \pi k^{2} d k \tag{2.82}
\end{equation*}
$$

\]

where for electromagnetic waves, the degeneracy factor $g=2$, due to their two different (e.g., linear) polarizations for the same wave vector $\mathbf{k}$. With the isotropic dispersion relation for waves in vacuum, $k$ $=\omega / c$, the elementary volume $d^{3} k$ corresponding to a small interval $d \omega$ is a spherical shell of small thickness $d k=d \omega / c$, and Eq. (82) yields

$$
\begin{equation*}
d N=\frac{2 V}{(2 \pi)^{3}} 4 \pi \frac{\omega^{2} d \omega}{c^{3}}=V \frac{\omega^{2}}{\pi^{2} c^{3}} d \omega . \tag{2.83}
\end{equation*}
$$

Using Eq. (72), we see that the spectral density of electromagnetic wave energy, per unit volume, is

$$
\begin{equation*}
u(\omega) \equiv \frac{E}{V} \frac{d N}{d \omega}=\frac{\hbar \omega^{3}}{\pi^{2} c^{3}} \frac{1}{e^{\hbar \omega / T}-1} \tag{2.84}
\end{equation*}
$$

This is the famous Planck's blackbody radiation law. ${ }^{51}$ To understand why its name mentions radiation, let us consider a small planar part, of area $d A$, of a surface that completely absorbs electromagnetic waves incident from any direction. (Such "perfect black body" approximation may be closely approached in special experimental structures, especially in limited frequency intervals.) Figure 8 shows that if the arriving wave was planar, with the incidence angle $\theta$, then power $d \mathcal{P}_{d}(\omega)$ absorbed by the surface within a small frequency interval $d \omega$ (i.e. energy arriving at the surface within unit time interval), would be equal to the radiation energy within the same frequency interval and inside a cylinder of height $c$, base area $d A \cos \theta$, and hence volume $d V=c d A \cos \theta$ :

$$
\begin{equation*}
d P_{\theta}(\omega)=u(\omega) d \omega d V=u(\omega) d \omega c d A \cos \theta \tag{2.85}
\end{equation*}
$$

Since the thermally-induced field is isotropic, i.e. propagates equally in all directions, this results should be averaged over all solid angles within the polar angle interval $0 \leq \theta \leq \pi / 2$ :

$$
\begin{equation*}
\frac{d \mathcal{P}(\omega)}{d A d \omega}=\frac{1}{4 \pi} \int \frac{d P_{\theta}(\omega)}{d A d \omega} d \Omega=c u(\omega) \frac{1}{4 \pi} \int_{0}^{\pi / 2} \sin \theta d \theta \int_{0}^{2 \pi} d \varphi \cos \theta=\frac{c}{4} u(\omega) \tag{2.86}
\end{equation*}
$$

[^829]Hence the Planck's expression (84), multiplied by $c / 4$, gives the power absorbed by such "blackbody" surface. But at thermal equilibrium, this absorption has to be exactly balanced by the surface's own radiation, due to its finite temperature $T$.


Fig. 2.8. Calculating the relation between $d \mathcal{P}(\omega)$ and $u(\omega) d \omega$.

I am confident that the reader is familiar with the main features of the Planck law (84), including its general shape (Fig. 9), with the low-frequency asymptote $u(\omega) \propto \omega^{2}$ (due to its historic significance bearing the special name of the Rayleigh-Jeans law), the exponential drop at high frequencies (the Wien law), and the resulting maximum of function $u(\omega)$, reached at frequency $\omega_{\max }$,

$$
\begin{equation*}
\hbar \omega_{\max } \approx 2.82 T \tag{2.87}
\end{equation*}
$$

i.e. at wavelength $\lambda_{\max }=2 \pi / k_{\max }=2 \pi c / \omega_{\max } \approx 2.22 c \hbar / T$. Still, I cannot help mentioning two particular values corresponding to visible light ( $\lambda_{\text {max }} \sim 500 \mathrm{~nm}$ ) for Sun's surface temperature $T_{\mathrm{K}} \approx 6,000 \mathrm{~K}$, and to mid-infrared range $\left(\lambda_{\max } \sim 10 \mu \mathrm{~m}\right)$ for the Earth's surface temperature $T_{\mathrm{K}} \approx 300 \mathrm{~K}$. The balance of these two radiations, absorbed and emitted by the Earth, determines its surface temperature, and hence has the key importance for all life on our planet. As one more example, the cosmic microwave background (CMB) radiation, closely following the Planck law with $T_{\mathrm{K}}=2.726 \mathrm{~K}$ (and hence having maximum density at $\lambda_{\max } \approx 1.9 \mathrm{~mm}$ ), and in particular its weak anisotropy, is a major source of data for all modern cosmology. ${ }^{52}$


Fig. 2.9. Frequency dependence of the blackbody radiation density, normalized by $u_{0} \equiv$ $T^{3} / \pi^{2} \hbar^{2} c^{3}$, according to the Planck law (red line) and the Rayleigh-Jeans law (blue line).

[^830]Now let us calculate the total energy $E$ of this radiation in some volume $V$. It may be found from Eq. (72) by integration its over all frequencies: ${ }^{53}$

$$
\begin{equation*}
E=V \int_{0}^{\infty} u(\omega) d \omega=V \int_{0}^{\infty} \frac{\hbar \omega^{3}}{\pi^{2} c^{3}} \frac{d \omega}{e^{\hbar \omega / T}-1}=\frac{V T^{4}}{\pi^{2} \hbar^{3} c^{3}} \int_{0}^{\infty} \frac{\xi^{3} d \xi}{e^{\xi}-1}=V \frac{\pi^{2}}{15 \hbar^{3} c^{3}} T^{4} . \tag{2.88}
\end{equation*}
$$

(The last transition in Eq. (88) uses a table integral equal to $\left.\Gamma(4) \zeta(4)=(3!)\left(\pi^{4} / 90\right)=\pi^{4} / 15 .{ }^{54}\right)$ Using Eq. (86) to recast Eq. (88) into the total power radiated by a blackbody surface, we get the well-known Stefan (or "Stefan-Boltzmann") law

$$
\begin{equation*}
\frac{d \mathcal{P}}{d A}=\frac{\pi^{2}}{60 \hbar^{3} c^{2}} T^{4}=\sigma T_{\mathrm{K}}^{4}, \tag{2.89a}
\end{equation*}
$$

where $\sigma$ is the Stefan-Boltzmann constant

$$
\begin{equation*}
\sigma \equiv \frac{\pi^{2}}{60 \hbar^{3} c^{2}} k_{\mathrm{B}}^{4} \approx 5.67 \times 10^{-8} \frac{\mathrm{~W}}{\mathrm{~m}^{2} \mathrm{~K}^{4}} \tag{2.89b}
\end{equation*}
$$

By this time, the thoughtful reader should have an important concern ready: Eq. (84) and hence Eq. (88) are based on Eq. (72) for the average energy of each oscillator, counted from its ground energy $\hbar \omega / 2$. However, the radiation power should not depend on the energy origin; why have not we included the ground energy of each oscillator into integration (88), as we have done in Eq. (80)? The answer is that usual radiation detectors only measure the difference between power $\mathcal{P}_{\text {in }}$ of the incident radiation (say, that of a blackbody surface with temperature $T$ ) and their own back-radiation $P_{\text {out }}$ with power corresponding to some effective temperature $T_{d}$ of the detector (Fig. 10). But however low $T_{d}$ is, the temperature-independent ground state energy contribution $\hbar \omega / 2$ to the back radiation is always there. Hence, the $\hbar \omega / 2$ drops out from the difference, and cannot be detected - at least in this simple way. This is the reason why we had the right to ignore this contribution in Eq. (88) - very fortunately, because it would lead to the integral's divergence at its upper limit. However, let me repeat again that the groundstate energy of the electromagnetic field oscillators is physically real - and important.


Fig. 2.10. Generic scheme of the electromagnetic radiation power measurement.

[^831]One more interesting result may be deduced from the free energy $F$ of the electromagnetic radiation, which may be also calculated by integration of Eq. (73) over all the modes, with the appropriate weight:

$$
\begin{equation*}
F=\sum_{\omega} T \ln \left(1-e^{-\hbar \omega / T}\right) \rightarrow \int_{0}^{\infty} T \ln \left(1-e^{-\hbar \omega / T}\right) \frac{d N}{d \omega} d \omega=\int_{0}^{\infty} T \ln \left(1-e^{-\hbar \omega / T}\right)\left(V \frac{\omega^{2}}{\pi^{2} c^{3}}\right) d \omega \tag{2.90}
\end{equation*}
$$

Presenting $\omega^{2} d \omega$ as $d\left(\omega^{3}\right) / 3$, this integral may be readily worked out by parts, and reduced to a table integral similar to that in Eq. (88), yielding a surprisingly simple result:

$$
\begin{equation*}
F=-V \frac{\pi^{2}}{45 \hbar^{3} c^{3}} T^{4}=-\frac{E}{3} \tag{2.91}
\end{equation*}
$$

Now we can use the second of general thermodynamic equations (1.35) to calculate pressure:

$$
\begin{equation*}
P=-\left(\frac{\partial F}{\partial V}\right)_{T}=\frac{\pi^{2}}{45 \hbar^{3} c^{3}} T^{4}=\frac{E}{3 V} . \tag{2.92a}
\end{equation*}
$$

This result might be, of course, derived by the integration of the expression for the forces exerted by each mode of the electromagnetic on confining the walls confining it to volume $V,{ }^{55}$ but notice how much simpler the thermodynamic calculation is. Rewritten in the form,


$$
\begin{equation*}
P V=\frac{E}{3} \tag{2.92b}
\end{equation*}
$$

this result may be considered as the equation of state of the electromagnetic field, i.e. from the quantummechanical point of view, the photon gas. As we will prove in the next chapter, the equation of state (1.44) of the ideal classical gas may be presented in a similar form, but with a coefficient generally different from Eq. (92). In particular, according to the equipartition theorem, for an ideal gas of nonrelativistic atoms whose internal degrees of freedom are in their ground state, whose whole energy is that of three translational "half-degrees of freedom", $E=3 N(T / 2)$, the factor before $E$ is twice larger than in Eq. (92). On the other hand, a relativistic treatment of the classical gas shows that Eq. (92) is valid for any gas in the ultra-relativistic limit, $T \gg m c^{2}$, where $m$ is the rest mass of the gas particle. Evidently, photons (i.e. particles with $m=0$ ) satisfy this condition. ${ }^{56}$

Finally, let me note that Eq. (92) allows the following interesting interpretation. The last of Eqs. (1.60), being applied to Eq. (92), shows that in this particular case the grand potential $\Omega$ equals ( $-E / 3$ ). But according to the definition of $\Omega$, the first of Eqs. (1.60), this means that the chemical potential of the electromagnetic field excitations vanishes:

$$
\begin{equation*}
\mu=\frac{F-\Omega}{N}=0 . \tag{2.93}
\end{equation*}
$$

In Sec. 8 below, we will see that the same result follows from Eq. (72) and the Bose-Einstein distribution, and discuss its physical sense.

[^832](ii) Specific heat of solids. The heat capacity of solids is readily measurable, and in the early 1900s its experimentally observed temperature dependence served as an important test for emerging quantum theories. However, theoretical calculation of $C_{V}$ is not simple, ${ }^{57}$ even for isolators whose specific heat is due to thermally-induced vibrations of their crystal lattice alone. ${ }^{58}$ Indeed, a solid may be treated as an elastic continuum only at low relatively frequencies. Such continuum supports three different modes of mechanical waves with the same frequency $\omega$, that obey similar, linear dispersion laws, $\omega=v k$, but velocity $v=v_{l}$ for one of these modes (the longitudinal sound) is higher than that $\left(v_{t}\right)$ of two other modes (the transverse sound). ${ }^{59}$ At such frequencies the wave mode density may be described by an evident modification of Eq. (83):
\[

$$
\begin{equation*}
d N=V \frac{1}{(2 \pi)^{3}}\left(\frac{1}{v_{l}^{3}}+\frac{2}{v_{t}^{3}}\right) 4 \pi \omega^{2} d \omega . \tag{2.94a}
\end{equation*}
$$

\]

For what follows, it is convenient to rewrite this relation in a form similar to Eq. (83):

$$
\begin{equation*}
d N=\frac{3 V}{(2 \pi)^{3}} 4 \pi \frac{\omega^{2} d \omega}{v^{3}}, \quad \text { with } v \equiv\left[\frac{1}{3}\left(\frac{1}{v_{l}^{3}}+\frac{2}{v_{t}^{3}}\right)\right]^{-1 / 3} . \tag{2.94b}
\end{equation*}
$$

However, wave theory shows ${ }^{60}$ that as frequency $\omega$ of a sound wave in a periodic structure is increased so that its half-wavelength $\pi / k$ approaches the crystal period $d$, the dispersion law $\omega(k)$ becomes nonlinear before the frequency reaches a maximum at $k=\pi / d$. To make the things even more complex, 3D crystals are generally anisotropic, so that the dispersion law is different in different directions of wave propagation. As a result, the exact statistics of thermally excited sound waves, and hence the heat capacity of crystals, is rather complex and specific for each particular crystal type.

In 1912, P. Debye suggested an approximate theory of the temperature dependence of the specific heat, which is in a surprisingly good agreement with experiment for many insulators, including polycrystalline and amorphous materials. In his model, the linear (acoustic) dispersion law $\omega=v k$, with the effective sound velocity $v$, defined by the latter of Eqs. (94b), is assumed to be exact all the way up to some cutoff frequency $\omega_{\mathrm{D}}$, the same for all three wave modes. This cutoff frequency may be defined by the requirement that the total number of acoustic modes, calculated within this model from Eq. (94b),

$$
\begin{equation*}
N=V \frac{1}{(2 \pi)^{3}} \frac{3}{v^{3}} \int_{0}^{\omega_{D}} 4 \pi \omega^{2} d \omega=\frac{V \omega_{D}^{3}}{2 \pi^{2} v^{3}}, \tag{2.95}
\end{equation*}
$$

is equal to the universal number $N=3 n V$ of degrees of freedom (and hence of independent oscillation modes) in a system of $n V$ elastically coupled particles, where $n$ is the atomic density of the crystal, i.e. the number of atoms per unit volume. Within this model, Eq. (72) immediately yields the following expression for the average energy and specific heat (in thermal equilibrium at temperature $T$ ):

[^833]Debye law

$$
\begin{gather*}
E=V \frac{1}{(2 \pi)^{3}} \frac{3}{v^{3}} \int_{0}^{\omega_{\mathrm{D}}} \frac{\hbar \omega}{e^{\hbar \omega / T}-1} 4 \pi \omega^{2} d \omega=3 n V T \cdot D(x)_{x=T_{\mathrm{D}} / T},  \tag{2.96}\\
c_{V} \equiv \frac{C_{V}}{n V}=\frac{1}{n V}\left(\frac{\partial E}{\partial T}\right)_{V}=3\left[D(x)-x \frac{d D(x)}{d x}\right]_{x=T_{\mathrm{D}} / T}, \tag{2.97}
\end{gather*}
$$

where $T_{\mathrm{D}} \equiv \hbar \omega_{\mathrm{D}}$ is called the Debye temperature, ${ }^{61}$ and

$$
D(x) \equiv \frac{3}{x^{3}} \int_{0}^{x} \frac{\xi^{3} d \xi}{e^{\xi}-1} \rightarrow \begin{cases}1, & \text { at } x \rightarrow 0  \tag{2.98}\\ \pi^{4} / 5 x^{3}, & \text { at } x \rightarrow \infty\end{cases}
$$

the Debye function. Red lines in Fig. 11 show the temperature dependence of the specific heat $c_{V}$ (per atom) within the Debye model. At high temperatures, it approaches a constant value of 3, corresponding to energy $E=3 n V T$, in accordance with the equipartition theorem for each of 3 degrees of freedom of each atom. (This model-insensitive value of $c_{V}$ is known as the Dulong-Petit law.) In the opposite limit of low temperatures, the specific heat is much smaller:

$$
\begin{equation*}
c_{V} \approx \frac{12 \pi^{4}}{5}\left(\frac{T}{T_{D}}\right)^{3} \ll 1 \tag{2.99}
\end{equation*}
$$

reflecting the reduction of the number of excited waves with $\hbar \omega<T$ as the temperature is decreased.


Fig. 2.11. Temperature dependence of the specific heat in the Debye (red lines) and Einstein (blue lines) models.

As a historic curiosity, P. Debye's work followed one by A. Einstein, who had suggested (in 1907) a simpler model of crystal vibrations. In this model, all $3 n V$ independent oscillatory modes of $n V$ atoms of the crystal have approximately the same frequency, say $\omega_{\mathrm{E}}$, and Eq. (72) immediately yields

[^834]\[

$$
\begin{equation*}
E=3 n V \frac{\hbar \omega_{\mathrm{E}}}{e^{\hbar \omega_{\mathrm{E}} / T}-1}, \tag{2.100}
\end{equation*}
$$

\]

so that the specific heat is functionally similar to Eq. (75):

$$
\begin{equation*}
c_{V} \equiv \frac{1}{n V}\left(\frac{\partial E}{\partial T}\right)_{V}=3\left[\frac{\hbar \omega_{\mathrm{E}} / 2 T}{\sinh \left(\hbar \omega_{\mathrm{E}} / 2 T\right)}\right]^{2} \tag{2.101}
\end{equation*}
$$

This dependence $c_{V}(T)$ is shown with blue lines in Fig. 11 (assuming, for the sake of simplicity, $\hbar \omega_{\mathrm{E}}=T_{\mathrm{D}}$ ). At high temperatures, this result does satisfy the universal Dulong-Petit law ( $c_{V}=3$ ), but at low temperatures the Einstein's model predicts a much faster (exponential) drop of the specific heart as the temperature is reduced. (The difference between the Debye and Einstein models is not too spectacular on the linear scale, but in the log-log plot, shown on the right panel of Fig. 11, it is rather dramatic. ${ }^{62}$ ) The Debye model is in a much better agreement with experimental data for simple, monoatomic crystals, thus confirming the conceptual correctness of his wave-based approach.

Note, however, that when a genius such as A. Einstein makes an error, there is probably some deep and important reason behind it. Indeed, crystals with the basic cell consisting of atoms of two or more types (such as NaCl , etc.), feature two or more separate branches of the dispersion law $\omega(k)$ - see, e.g., Fig. $12 .{ }^{63}$


Fig. 2.12. Dispersion relation for longitudinal waves in a simple 1D model of a solid, with similar interparticle distances $d$, but alternating particle masses, plotted for a particular mass ratio $r=5$.

While the lower "acoustic" branch is virtually similar to those for monoatomic crystals, and may be approximated by the Debye model, $\omega=v k$, reasonably well, the upper ("optical" ${ }^{64}$ ) branch does approach $\omega=0$ at any $k$. Moreover, for large values of the atom mass ratio $r$, the optical branches are almost flat, with virtually $k$-independent frequencies $\omega_{0}$ that correspond to simple oscillations of each light atom between its heavy counterparts. For thermal excitations of such oscillations, and their

[^835]contribution to the specific heat, the Einstein model (with $\omega_{\mathrm{E}}=\omega_{0}$ ) gives a very good approximation, so that the specific heat may be well described by a sum of the Debye and Einstein laws (97) and (101), with appropriate weights.

### 2.7. Grand canonical ensemble and distribution

As we have seen, the Gibbs distribution is a very convenient way to calculate statistical and thermodynamic properties of systems with a fixed number $N$ of particles. However, for systems in which $N$ may vary, another distribution is preferable for some applications. Several examples of such situations (as well as the basic thermodynamics of such systems) have already been discussed in Sec. 1.5. Perhaps even more importantly, statistical distributions for systems with variable $N$ are also applicable to the ensembles of independent particles on a certain single-particle energy level - see the next section.

With this motivation, let us consider what is called the grand canonical ensemble (Fig. 13). It is similar to the canonical ensemble discussed in the previous section (Fig. 6) in all aspects, besides that now the system under study and the heat bath (in this case typically called the environment) may exchange not only heat but also particles. In all system members of the ensemble, the environments are in both the thermal and chemical equilibrium, and their temperatures $T$ and chemical potentials $\mu$ are equal.


Fig. 2.13. Member of a grand canonical ensemble.

Now let us assume that the system of interest is also in the chemical and thermal equilibrium with its environment. Then using exactly the same arguments as in Sec. 4 (including the specification of a microcanonical sub-ensemble with fixed $E_{\Sigma}$ and $N_{\Sigma}$ ), we may generalize Eq. (55), taking into account that entropy $S_{\text {env }}$ of the environment is now a function of not only its energy $E_{\text {env }}=E_{\Sigma}-E_{m, N},{ }^{65}$ but also the number of particles $N_{\mathrm{E}}=N_{\Sigma}-N$, with $E_{\Sigma}$ and $N_{\Sigma}$ fixed:

$$
\begin{align*}
\ln W_{m, N} & \propto \ln M=\ln g_{\mathrm{env}}\left(E_{\Sigma}-E_{m, N}, N_{\Sigma}-N\right)+\ln \Delta E_{\Sigma}=S_{\mathrm{env}}\left(E_{\Sigma}-E_{m, N}, N_{\Sigma}-N\right)+\mathrm{const} \\
& \approx S_{\mathrm{env}}\left|E_{\Sigma}, N_{\Sigma}-\frac{\partial S_{\mathrm{env}}}{\partial E_{\mathrm{env}}}\right| E_{\Sigma}, \left.N_{\Sigma} E_{m, N}-\frac{\partial S_{\mathrm{env}}}{\partial N_{\mathrm{env}}} \right\rvert\, E_{\Sigma}, N_{\Sigma} N+\mathrm{const} . \tag{2.102}
\end{align*}
$$

In order to simplify this relation, we may rewrite Eq. (1.52) in the equivalent form

[^836]\[

$$
\begin{equation*}
d S=\frac{1}{T} d E+\frac{P}{T} d V-\frac{\mu}{T} d N \tag{2.103}
\end{equation*}
$$

\]

Hence, if entropy $S$ of a system is expressed as a function of $E, V$, and $N$, then

$$
\begin{equation*}
\left(\frac{\partial S}{\partial E}\right)_{V, N}=\frac{1}{T}, \quad\left(\frac{\partial S}{\partial V}\right)_{E, N}=\frac{P}{T}, \quad\left(\frac{\partial S}{\partial N}\right)_{E, V}=-\frac{\mu}{T} \tag{2.104}
\end{equation*}
$$

Applying the first one and the last one of these relations to Eq. (102), and using the equality, of the temperatures $T$ and chemical potentials $\mu$ of the system under study and its environment, at their equilibrium, discussed in Sec. 1.5, we get

$$
\begin{equation*}
\ln W_{m, N}=S_{\mathrm{env}}\left(E_{\Sigma}, N_{\Sigma}\right)-\frac{1}{T} E_{m, N}+\frac{\mu}{T} N+\text { const } . \tag{2.105}
\end{equation*}
$$

Again, exactly as at the derivation of the Gibbs distribution in Sec. 4, we may argue that since $E_{m, N}, T$ and $\mu$ do not depend on the choice of environment's size, i.e. on $E_{\Sigma}$ and $N_{\Sigma}$, the probability $W_{m, N}$ for a system to have $N$ particles and be in $m$-th quantum state in the whole grand canonical ensemble should also obey a relation similar to Eq. (105). As a result, we get the so-called grand canonical distribution:

$$
\begin{equation*}
W_{m, N}=\frac{1}{Z_{G}} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\} \tag{2.106}
\end{equation*}
$$

Just as in the case of the Gibbs distribution, constant $Z_{G}$ (most often called the grand statistical sum, but sometimes the "grand partition function") should be determined from the probability normalization condition, now with the summation of probabilities $W_{m, N}$ over all possible values of both $m$ and $N$ :

$$
\begin{equation*}
Z_{G}=\sum_{m, N} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\} \tag{2.107}
\end{equation*}
$$

Now, using the general Eq. (29) to calculate entropy for distribution (106) (exactly like we did it for the canonical ensemble), we get the following expression,

$$
\begin{equation*}
S=-\sum_{m, N} W_{m, N} \ln W_{m, N}=\ln Z_{G}+\frac{E}{T}-\frac{\mu\langle N\rangle}{T}, \tag{2.108}
\end{equation*}
$$

which is evidently a generalization of Eq. (62). ${ }^{66} \mathrm{We}$ see that now the grand thermodynamic potential $\Omega$ (rather than the free energy $F$ ) may be expressed directly via the normalization coefficient $Z_{G}$ :

$$
\begin{equation*}
\Omega \equiv F-\mu\langle N\rangle=E-T S-\mu\langle N\rangle=T \ln \frac{1}{Z_{G}}=-T \ln \sum_{m, N} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\} . \tag{2.109}
\end{equation*}
$$

Finally, solving the last equality for $Z_{G}$, and plugging the result back into Eq. (106), we can rewrite the grand canonical distribution in the form

[^837]Grand
canonical
sum

$$
\begin{equation*}
W_{m, N}=\exp \left\{\frac{\Omega+\mu N-E_{m, N}}{T}\right\}, \tag{2.110}
\end{equation*}
$$

similar to Eq. (65) for the Gibbs distribution. Indeed, in the particular case when the number $N$ of particles is fixed, $N=\langle N\rangle$, so that $\Omega+\mu N=\Omega+\mu\langle N\rangle \equiv F$, Eq. (110) is reduced right to Eq. (65).

### 2.8. Systems of independent particles

Now we will use the general statistical distributions discussed above to a simple but very important case when each system we are considering consists of many similar particles whose explicit (physical) interaction is negligible. As a result, each particular energy value $E_{m, N}$ of such a system may be presented as a sum of energies $\varepsilon_{k}$ of its particles, where index $k$ numbers single-particle energy levels (rather than of the whole system, as index $m$ does).

Let us start with the classical limit. In classical mechanics, the quantization effects are negligible, i.e. there is a virtually infinite number of states $k$ within each finite energy interval. However, it is convenient to keep, for the time being, the discrete-state language, with understanding that the average number $\left\langle N_{k}\right\rangle$ of particles in each of these states, frequently called the state occupancy, is very small. In this case, we may apply the Gibbs distribution to the canonical ensemble of single particles, and hence use it with the substitution $E_{m, N} \rightarrow \varepsilon_{k}$, so that Eq. (58) becomes

$$
\begin{equation*}
\left\langle N_{k}\right\rangle=c \exp \left\{-\frac{\varepsilon_{k}}{T}\right\} \ll 1 \tag{2.111}
\end{equation*}
$$

where constant $c$ should be found from the normalization condition:

$$
\begin{equation*}
\sum_{k}\left\langle N_{k}\right\rangle=1 . \tag{2.112}
\end{equation*}
$$

This is the famous Boltzmann distribution. ${ }^{67}$ Despite its superficial similarity to the Gibbs distribution (58), let me emphasize the conceptual difference between these two results. The Gibbs distribution describes the probability to find the whole system on energy level $E_{m}$, and it is always valid more exactly, for a canonical ensemble of systems in thermodynamic equilibrium. On the other hand, the Boltzmann distribution describes occupancy of an energy level of a single particle, and for systems of identical particles is valid only in the classical limit $\left\langle N_{k}\right\rangle \ll 1$, even if the particles do not interact directly.

The last fact may be surprising, because it may seem that as soon as particles of the system are independent, nothing prevents us from using the Gibbs distribution to derive Eq. (111), regardless of the value of $\left\langle N_{k}\right\rangle$. This is indeed true if the particles are distinguishable, i.e. may be distinguished from each other - say by their fixed spatial positions, or by the states of certain internal degrees of freedom (say, spin), or any other "pencil mark". However, it is an experimental fact that elementary particles of each particular type (say, electrons) are identical to each other, i.e. cannot be "pencil-marked". For such particles we have to be more careful: even if they do not interact explicitly, there is still some implicit

[^838]dependence in their behavior, which is especially evident for the so-called fermions (fundamental particles with semi-integer spin) they obey the Pauli exclusion principle that forbids two identical particles to be in the same quantum state, even if they do not interact explicitly. ${ }^{68}$

Note that here the term "the same quantum state" carries a heavy meaning load here. For example, if two particles are confined to stay in different spatial positions (say, reliably locked in different boxes), they are distinguishable even if they are internally identical. Thus the Pauli principle, as well as other identity effects such as Bose-Einstein condensation, to be discussed in the next chapter, are important only when identical particles may move in the same spatial region. In order to describe this case, instead of "identical", it is much better to use a more precise (though ugly) term indistinguishable particles. ${ }^{69}$

In order to take these effects into account, let us examine the effects of nonvanishing occupancy $\left\langle N_{k}\right\rangle \sim 1$ on statistical properties of a system of many non-interacting but indistinguishable particles (at the first stage of calculation, either fermions or bosons) in equilibrium, and apply the grand canonical distribution (109) to a very interesting particular grand canonical ensemble: a subset of particles in the same quantum state $k$ (Fig. 14).
single-particle energy levels:


Fig. 2.14. Grand canonical ensemble of particles in the same quantum state (with eigenenergy $\varepsilon_{k}$ ).

In this ensemble, the role of the environment is played by the particles in all other states $k^{\prime} \neq k$, because due to infinitesimal interactions, the particles may change their states. In equilibrium, the chemical potential $\mu$ and temperature $T$ of the system should not depend on the state number $k$, but the grand thermodynamic potential $\Omega_{k}$ of the chosen particle subset may. Replacing $N$ with $N_{k}$ - the particular (not average!) number of particles in $k^{\text {th }}$ state, and the particular energy value $E_{m, N}$ with $\varepsilon_{k} N_{k}$, we may reduce Eq. (109) to

$$
\begin{equation*}
\Omega_{k}=-T \ln \left(\sum_{N_{k}} \exp \left\{\frac{\mu N_{k}-\varepsilon_{k} N_{k}}{T}\right\}\right)=-T \ln \left[\sum_{N_{k}}\left(\exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\}\right)^{N_{k}}\right] \tag{2.113}
\end{equation*}
$$

[^839]where the summation should be carried out over all possible values of $N_{k}$. For the final calculation of this sum, the elementary particle type becomes essential.

In particular, for fermions, obeying the Pauli principle, numbers $N_{k}$ in Eq. (113)may take only two values, either 0 (state $k$ is unoccupied) or 1 (the state is occupied), and the summation gives

$$
\begin{equation*}
\Omega_{k}=-T \ln \left[\sum_{N_{k}=0,1}\left(\exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\}\right)^{N_{k}}\right]=-T \ln \left(1+\exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\}\right) . \tag{2.114}
\end{equation*}
$$

Now the average occupancy may be calculated from the last of Eqs. (1.62) - in this case, with $N$ replaced with $\left\langle N_{k}\right\rangle$ :

$$
\begin{equation*}
\left\langle N_{k}\right\rangle=-\left(\frac{\partial \Omega_{k}}{\partial \mu}\right)_{T, V}=\frac{1}{e^{\left(\varepsilon_{k}-\mu\right) / T}+1} \tag{2.115}
\end{equation*}
$$

This is the famous Fermi-Dirac distribution, derived in 1926 independently by E. Fermi and P. Dirac.
On the other hand, bosons do not obey the Pauli principle, and for them numbers $N_{k}$ can take any non-negative integer values. In this case, Eq. (113) turns into the following equality:

$$
\begin{equation*}
\Omega_{k}=-T \ln \sum_{N_{k}=0}^{\infty}\left(\exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\}\right)^{N_{k}}=-T \ln \sum_{N_{k}=0}^{\infty} \lambda^{N_{k}}, \quad \text { with } \lambda \equiv \exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\} \tag{2.116}
\end{equation*}
$$

This sum is just the usual geometric progression again, which converges if $\lambda<1$, giving

$$
\begin{equation*}
\Omega_{k}=-T \ln \frac{1}{1-\lambda}=-T \ln \frac{1}{1-e^{\left(\mu-\varepsilon_{k}\right) / T}}, \quad \text { for } \mu<\varepsilon_{k} . \tag{2.117}
\end{equation*}
$$

In this case the average occupancy, again calculated using Eq. (1.62) with $N$ replaced with $\left\langle N_{k}\right\rangle$, obeys the Bose-Einstein distribution,

Bose-
Einstein distribution

$$
\begin{equation*}
\left\langle N_{k}\right\rangle=-\left(\frac{\partial \Omega_{k}}{\partial \mu}\right)_{T, V}=\frac{1}{e^{\left(\varepsilon_{k}-\mu\right) / T}-1}, \quad \text { for } \mu<\varepsilon_{k} \tag{2.118}
\end{equation*}
$$

which was derived in 1924 by S. Bose (for the particular case $\mu=0$ ) and generalized in 1925 by A. Einstein for an arbitrary chemical potential. In particular, comparing Eq. (118) with Eq. (72), we see that harmonic oscillator excitations, ${ }^{70}$ each with energy $\hbar \omega$, may be considered as bosons, with zero chemical potential. We have already obtained this result $(\mu=0)$ in a different way - see Eq. (93). Its physical interpretation is that the oscillator excitations may be created inside the system, so that there is no energy cost $\mu$ of moving them into the system from its environment.

The simple form of Eqs. (115) and (118), and their similarity (besides "only" the difference of the signs before unity in their denominators), is one of most beautiful results of physics. This similarity should not disguise the facts that the energy dependences of $\left\langle N_{k}\right\rangle$, given by these two formulas, are rather different - see Fig. 15. In the Fermi-Dirac statistics, the average level occupancy is finite (and

[^840]below 1) at any energy, while in the Bose-Einstein it may be above 1 , and even diverges at $\varepsilon_{k} \rightarrow \mu$. However, for any of these distributions, as temperature is increased, it eventually becomes much larger than the difference $\left(\varepsilon_{k}-\mu\right)$ for all $k$. In this limit, $\left\langle N_{k}\right\rangle \ll 1$, both distributions coincide with each other, as well as with the Boltzmann distribution (111) with $c=\exp \{\mu / T\}$. The last distribution, therefore, serves as the high-temperature limit for quantum particles of both sorts.

A natural question now is how to find the chemical potential $\mu$ participating in Eqs. (115) and (118). In the grand canonical ensemble as such (Fig. 13), with number of particles variable, the value of $\mu$ is imposed by system's environment. However, both the Fermi-Dirac and Bose-Einstein distributions are also applicable to equilibrium systems with a fixed but large number $N$ of particles. In these conditions, the role of the environment for some subset of $N^{\prime} \ll N$ particles is played by the remaining $N-N^{\prime}$ particles. In this case, $\mu$ may be found by calculation of $\langle N\rangle$ from the corresponding distribution, and then requiring it to be equal to the genuine number of particles in the system. In the next section, we will perform such calculations for several particular systems.


Fig. 2.15. Fermi-Dirac (blue line) and Bose-Einstein (red line) distributions, and the Boltzmann distribution with $c=\exp \{\mu / T\}$ (black line).

$$
\left(\varepsilon_{k}-\mu\right) / T
$$

For those and other applications, it will be convenient for us to have ready expressions for entropy $S$ of a general (i.e. not necessarily equilibrium) state of systems of independent Fermi or Bose particles, expressed not as a function of $W_{m}$ of the whole system - as Eq. (29) does, but as a function of the average occupancy numbers $\left\langle N_{k}\right\rangle$. For that, let us consider a composite system, each consisting of $M$ $\gg 1$ similar but distinct component systems, numbered by index $m=1,2, \ldots M$, with independent (i.e. not explicitly interacting) particles. We will assume that though in each of $M$ component systems, the number $N_{k}^{(m)}$ of particles in its $k$-th quantum state may be different (Fig. 16), but their total number $N_{k}^{(\Sigma)}$ in the composite system is fixed:

$$
\begin{equation*}
\sum_{m=1}^{M} N_{k}^{(m)}=N_{k}^{(\Sigma)} \tag{2.119}
\end{equation*}
$$



Fig. 2.16. Composite system with a certain distribution of $N_{k}^{(2)}$ particles in $k$-th state between $M$ component systems.

As a result, the total energy of the composite system is fixed as well,

$$
\begin{equation*}
\sum_{m=1}^{M} N_{k}^{(m)} \varepsilon_{k}=N_{k}^{(\Sigma)} \varepsilon_{k}=\text { const } \tag{2.120}
\end{equation*}
$$

so that an ensemble of many such composite systems (with the same $k$ ), in equilibrium, is microcanonical. According to Eq. (24a), the average entropy $S_{k}$ per component system may be calculated as

$$
\begin{equation*}
S_{k}=\lim _{M, N_{k} \rightarrow \infty} \frac{\ln M_{k}}{M}, \tag{2.121}
\end{equation*}
$$

where $M_{k}$ is the number of possible different ways such composite system (with fixed $N_{k}^{(\Sigma)}$ ) may be implemented.

Let us start the calculation of $M_{k}$ with Fermi particles - for which the Pauli principle is valid. Here the level occupancies $N_{k}{ }^{(m)}$ may be only equal 0 or 1 , so that the distribution problem is solvable only if $N_{k}^{(\Sigma)} \leq M$, and evidently equivalent to the choice of $N_{k}^{(\Sigma)}$ balls (in arbitrary order) from the total number of $M$ distinct balls. Comparing this formulation with the binomial coefficient definition, ${ }^{71}$ we immediately have

$$
\begin{equation*}
M_{k}={ }^{M} C_{N_{k}^{(\Sigma)}}=\frac{M!}{\left(M-N_{k}^{(\Sigma)}\right)!N_{k}^{(\Sigma)}!} . \tag{2.122}
\end{equation*}
$$

From here, using the Stirling formula (again, in its simplest form (27)), we get

$$
\begin{equation*}
S_{k}=-\left\langle N_{k}\right\rangle \ln \left\langle N_{k}\right\rangle-\left(1-\left\langle N_{k}\right\rangle\right) \ln \left(1-\left\langle N_{k}\right\rangle\right) \tag{2.123}
\end{equation*}
$$

where

$$
\begin{equation*}
\left\langle N_{k}\right\rangle \equiv \lim _{M, N_{k} \rightarrow \infty} \frac{N_{k}^{(\Sigma)}}{M} \tag{2.124}
\end{equation*}
$$

is exactly the average occupancy of the $k$-th single-particle level in each system that was discussed earlier in this section. Since for a Fermi system, $\left\langle N_{k}\right\rangle$ is always somewhere between 0 and 1 , so that entropy (123) is always positive.

In the Bose case, where the Pauli limitation is not valid, the number $N_{k}{ }^{(m)}$ of particles on the $k$-th level in each of the systems is an arbitrary (positive) integer. Let us consider $N_{k}{ }^{(\Sigma)}$ particles and ( $M-1$ ) partitions (shown by vertical lines in Fig. 16) between $M$ systems as $\left(M-1+N_{k}^{(\Sigma)}\right)$ similar mathematical objects ordered along one axis. Then $M_{k}$ may be calculated as the number of possible ways to distribute the $(M-1)$ indistinguishable partitions among these $\left(M-1+N_{k}^{(\Sigma)}\right)$ distinct objects, i.e. as the following binomial coefficient: ${ }^{72}$

$$
\begin{equation*}
M_{k}={ }^{M+N_{k}-1} C_{M-1}=\frac{\left(M-1+N_{k}^{(\Sigma)}\right)!}{(M-1)!N_{k}^{(\Sigma)}!} . \tag{2.125}
\end{equation*}
$$

[^841]Applying the Stirling formula (27) again, we get the following result,

$$
\begin{equation*}
S_{k}=-\left\langle N_{k}\right\rangle \ln \left\langle N_{k}\right\rangle+\left(1+\left\langle N_{k}\right\rangle\right) \ln \left(1+\left\langle N_{k}\right\rangle\right) \tag{2.126}
\end{equation*}
$$

which again differs from the Fermi case (123) "only" by the signs in the second term, and is valid for any positive $\left\langle N_{k}\right\rangle$.

Expressions (123) and (126) are valid for an arbitrary (possibly non-equilibrium) case; they may be also used for an alternative derivation of the Fermi-Dirac (115) and Bose-Einstein (118) distributions valid in equilibrium. For that, we may use the method of Lagrange multipliers, requiring (just like it was done in Sec. 2) the total entropy of a system of $N$ independent, similar particles,

$$
\begin{equation*}
S=\sum_{k} S_{k} \tag{2.127}
\end{equation*}
$$

as a function of state occupancies $\left\langle N_{k}\right\rangle$, to attain its maximum, with the conditions of fixed total number of particles $N$ and the total energy $E$ :

$$
\begin{equation*}
\sum_{k}\left\langle N_{k}\right\rangle=N=\text { const }, \quad \sum_{k}\left\langle N_{k}\right\rangle \varepsilon_{k}=E=\mathrm{const} . \tag{2.128}
\end{equation*}
$$

The completion of this calculation is left for reader's exercise.
In the classical limit, when the average occupancies $\left\langle N_{k}\right\rangle$ of all states are small, both the Fermi and Bose expressions for $S_{k}$ tend to the same limit

$$
\begin{equation*}
S_{k}=-\left\langle N_{k}\right\rangle \ln \left\langle N_{k}\right\rangle, \quad \text { for }\left\langle N_{k}\right\rangle \ll 1 . \tag{2.129}
\end{equation*}
$$

This expression, frequently referred to as the Boltzmann (or "classical") entropy, might be also obtained, for arbitrary $\left\langle N_{k}\right\rangle$, directly from Eq. (29) by considering an ensemble of systems, each consisting of just one classical particle, so that $E_{m} \rightarrow \varepsilon_{k}$ and $W_{m} \rightarrow\left\langle N_{k}\right\rangle$. Let me emphasize again that for indistinguishable particles, such identification is generally (i.e. at $\left\langle N_{k}\right\rangle \sim 1$ ) illegitimate even if they do not interact explicitly. As we will see in the next chapter, the indistinguishability affects statistical properties of even classical particles.

### 2.9. Exercise problems

2.1. A famous example of the macroscopic irreversibility was suggested in 1907 by P. Ehrenfest. Two dogs share $2 N \gg 1$ fleas. Each flea may jump to another dog, and the rate (i.e. the probability of jumping per unit time) $\Gamma$ of such an event does not depend on time, and on the location of other fleas. Find the time evolution of the average number of fleas on a dog, and of the flea-related part of dogs' entropy (at arbitrary initial conditions), and prove that the entropy can only grow. ${ }^{73}$
2.2. Use the microcanonical distribution to calculate thermodynamic properties (including entropy, all relevant thermodynamic potentials, and heat capacity), of an ensemble of similar two-level

[^842]Boltzmann entropy
systems, in thermodynamic equilibrium at temperature $T$ that is comparable with the energy gap $\Delta$. For each variable, sketch its temperature dependence, and find its asymptotic values (or trends) in the lowtemperature and high-temperature limits.

Hint: The two-level system is generally defined as any system with just two relevant states whose energies, say $E_{0}$ and $E_{1}$, are separated by a finite gap $\Delta \equiv E_{1}-E_{0}$. Its most popular (but not the only!) example is a spin- $1 / 2$ particle, e.g., an electron, in an external magnetic field.
2.3. Solve the previous problem using the Gibbs distribution. Also, calculate the probabilities of the energy level occupation, and give physical interpretations of your results, in both temperature limits.
2.4. Calculate the low-field magnetic susceptibility $\chi_{m}$ of a dilute set of non-interacting, spontaneous magnetic dipoles $\mathbf{m}$, in thermal equilibrium at temperature $T$, within two models:
(i) the dipole moment $\mathbf{m}$ is a classical vector of fixed magnitude $m_{0}$, but arbitrary orientation, and
(ii) the dipole moment $\mathbf{m}$ belongs to a quantum spin- $1 / 2$ particle, and is described by vector operator $\hat{\mathbf{m}}=\gamma \hat{\mathbf{S}}$, where $\gamma$ is the gyromagnetic ratio, and $\hat{\mathbf{S}}$ is the vector operator of particle's spin. ${ }^{74}$

Hint: The low-field magnetic susceptibility of an isotropic medium is defined ${ }^{75}$ as

$$
\chi_{m} \equiv \frac{\partial M_{z}}{\partial H}
$$

where $\mathbf{M}$ is the (average) magnetization of a unit volume, and axis $z$ is aligned with the direction of the external magnetic field $\mathbb{Z}$.
2.5. Calculate the low-field magnetic susceptibility of a set of non-interacting, distinguishable particles with an arbitrary $\operatorname{spin} s$, neglecting their orbital motion. Compare the result with the solution of the previous problem.

Hint: Quantum mechanics ${ }^{76}$ tells us that the Cartesian component $m_{z}$ of the magnetic moment of such a particle, in the direction of the applied field, may take $(2 s+1)$ values

$$
m_{z}=\gamma \hbar s_{m}, \quad \text { where } s_{m}=-s,-s+1, \ldots, s-1, s,
$$

where $\gamma$ is the gyromagnetic ratio of the particle, and $\hbar$ is the Planck's constant.
2.6. Derive a general expression for the average interaction potential between two similar magnetic dipoles with fixed magnitude $m$ but arbitrary orientation, at thermal equilibrium. Spell out the result in the low-temperature and high-temperature limits.
2.7.* Analyze the possibility of using a system of non-interacting spin-1/2 particles in magnetic field for refrigeration.

Hint: See a footnote in Sec. 1.6.

[^843]2.8. Use the microcanonical distribution to calculate the average entropy, energy, and pressure of a single classical particle of mass $m$, with no internal degrees of freedom, free to move in volume $V$, at temperature $T$.

Hint: Try to make a more accurate calculation than has been done in Sec. 2.2 for the system of $N$ harmonic oscillators. For that you will need to know the volume $V_{d}$ of an $d$-dimensional hypersphere of the unit radius. To avoid being too cruel, I am giving it to you:

$$
V_{d}=\pi^{d / 2} / \Gamma\left(\frac{d}{2}+1\right),
$$

where $\Gamma(\xi)$ is the gamma-function. ${ }^{77}$
2.9. Solve the previous problem starting from the Gibbs distribution.
2.10. Calculate the average energy, entropy, free energy, and the equation of state of a classical 2D particle (without internal degrees of freedom), free to move within area $A$, at temperature $T$, starting from:
(i) the microcanonical distribution, and
(ii) the Gibbs distribution.

Hint: Make the appropriate modification of the notion of pressure.
2.11. A quantum particle of mass $m$ is confined to free motion along a 1 D segment of length $a$. Using any approach you like, find the average force the particle exerts on walls of such a " 1 D quantum well" in thermal equilibrium, and analyze its temperature dependence, focusing on the low-temperature and high-temperature limits.

Hint: You may consider series $\Theta(\xi) \equiv \sum_{n=1}^{\infty} e^{-\xi n^{2}}$ as a known function of $\xi .{ }^{78}$
2.12. Rotational properties of diatomic molecules (such as $\mathrm{N}_{2}, \mathrm{CO}$, etc.) may be reasonably well described using a "dumbbell" model: two point particles, of masses $m_{1}$ and $m_{2}$, with a fixed distance $d$ between them. Ignoring the translational motion of the molecule as the whole, use this model to calculate its heat capacity, and spell out the result in the limits of low and high temperatures. (Quantify the conditions.)
2.13. Calculate the heat capacity of a diatomic molecule, using the simple model described in the previous problem, but now assuming that the rotation is confined to one plane. ${ }^{79}$

[^844]2.14. Low-temperature specific heat of some solids has a considerable contribution from thermal excitation of spin waves, whose dispersion law scales as $\omega \propto k^{2}$ at $\omega \rightarrow 0 .{ }^{80}$ Find the temperature dependence of this contribution to $C_{V}$ at low temperatures and discuss conditions of its experimental observation.
2.15. A rudimentary "zipper" model of DNA replication is a chain of $N$ links that may be either open or closed - see Fig. on the right. Opening a link increases system's energy by $\Delta>0$, and a link may change its state (either open or close) only if all links to the left of it are already open.
 Calculate the average number of open links at thermal equilibrium, and analyze its temperature dependence in detail, especially for the case $N \gg 1$.
2.16. An ensemble of classical 1D particles of mass $m$, residing in the potential wells
$$
U(x)=\alpha|x|^{\gamma}, \quad \text { with } \gamma>0
$$
is in thermal equilibrium at temperature $T$. Calculate the average values of its potential energy $U$ and the full energy $E$ using two approaches:
(i) directly from the Gibbs distribution, and
(ii) using the virial theorem of classical mechanics. ${ }^{81}$
2.17. For a thermally-equilibrium ensemble of slightly anharmonic classical 1D oscillators, with mass $m$ and potential energy
$$
U(q)=\frac{\kappa}{2} x^{2}+\alpha x^{3},
$$
with small coefficient $\alpha$, calculate $\langle x\rangle$ in the first approximation in low temperature $T$.
2.18.* A small conductor (in this context, usually called the single-electron $b o x)$ is placed between two conducting electrodes, with voltage $V$ applied between them. The gap between one of the electrodes and the island is so narrow that electrons may tunnel quantum-mechanically through this gap ("weak tunnel junction") - see Fig. on the right. Calculate the average charge of the island as a function of $V$.

Hint: The quantum-mechanical tunneling of electrons through weak junctions ${ }^{82}$ between macroscopic conductors, and its subsequent energy relaxation
 inside the conductor, may be considered as a single inelastic (energy-dissipating) event, so that the only energy relevant for the thermal equilibrium of the system is its electrostatic potential energy.

[^845]2.19. An $L C$ circuit (see Fig. on the right) is at thermodynamic equilibrium with the environment. Find the r.m.s. fluctuation $\delta \mathscr{V} \equiv\left\langle V^{2}\right\rangle^{1 / 2}$ of the voltage across it, for an arbitrary ratio $T / \hbar \omega$, where $\omega=(L C)^{-1 / 2}$ is the
 resonance frequency of this "tank circuit".
2.20. Derive Eq. (92) from simplistic arguments, representing the blackbody radiation as an ideal gas of photons, treated as ultra-relativistic particles. What do similar arguments give for an ideal gas of classical, non-relativistic particles?
2.21. Calculate the enthalpy, the entropy, and the Gibbs energy of the blackbody electromagnetic radiation with temperature $T$, and then use these results to find the law of temperature and pressure drop at an adiabatic expansion of the radiation.
2.22. As was mentioned in Sec. 2.6(i) of the lecture notes, the relation between the visible temperatures $T_{\oplus}$ of Sun's surface and Earth's surface $T_{\mathrm{o}}$ follows from the balance of the thermal radiation they emit. Prove that this relation indeed follows, with a good precision, from a simple model in which the surfaces radiate as perfect black bodies with a constant, average temperature.

Hint: You may pick up the experimental values you need from any (reliable :-) source.
2.23. If a surface is not perfectly radiation-absorbing ("black"), the electromagnetic power of its thermal radiation differs from the Stefan law (2.89a) by a frequency-dependent factor $\varepsilon<1$, called emissivity:

$$
\frac{\mathcal{P}}{A}=\varepsilon \sigma T^{4} .
$$

Prove that such surface reflects $(1-\varepsilon)$ part of incident radiation.
2.24. If two black surfaces, facing each other, have different temperatures (see Fig. on the right), then according to the Stefan radiation law (2.89), there is a net flow of thermal radiation, from a warmer surface to the colder one:

$$
\frac{P_{\text {net }}}{A}=\sigma\left(T_{1}^{4}-T_{2}^{4}\right) .
$$



For many applications (including low temperature experiments) this flow is detrimental. One way to reduce it is to reduce the emissivity $e(\omega)$ of both surfaces - say by covering them with shiny metallic films. An alternative way toward the same goal is to place, between the surfaces, a thin layer (usually called the thermal shield), with a low emissivity of both surfaces, and disconnected from any heat bath see dashed line in Fig. above. Assuming that the emissivity is the same in both cases, find out which way is more efficient.

Hint: The definition of emissivity may be found, for example, in the previous problem.
2.25. Two parallel, well conducting plates of area $A$ are separated by a free-space gap of a constant thickness $t \ll A^{1 / 2}$. Calculate the energy of the spontaneous electromagnetic field inside the gap
at thermal equilibrium with temperature $T$. Specify the validity limits of your result. Does the radiation push the plates apart?
2.26. Use the Debye theory to estimate the specific heat of aluminum at room temperature (say, 300 K ), and express the result in the following popular units:
(i) $\mathrm{eV} / \mathrm{K}$ per atom,
(ii) $J / K$ per mole, and
(iii) $\mathrm{J} / \mathrm{K}$ per gram.

Compare the last number with the experimental value (from a reliable book or online source).
2.27. Use the general Eq. (123) to re-derive the Fermi-Dirac distribution (115) for a system in equilibrium.
2.28. Each of two similar particles, not interacting directly, may take two quantum states, with single-particle energies $\varepsilon$ equal to 0 and $\Delta$. Write down the statistical sum $Z$ of the system, and use it to calculate its average total energy $E$ of the system, for the cases when the particles are:
(i) distinguishable;
(ii) indistinguishable fermions;
(iii) indistinguishable bosons.

Analyze and interpret the temperature dependence of $\langle E\rangle$ for each case, assuming that $\Delta>0$.
2.29. Calculate the chemical potential of a system of $N \gg 1$ independent fermions, kept at fixed temperature $T$, provided that each particle has two non-degenerate energy levels, separated by gap $\Delta$.

## This page is

## Chapter 3. Ideal and Not-So-Ideal Gases

In this chapter, the general approaches discussed in the previous chapters are applied to calculate statistical and thermodynamic properties of gases, i.e. collections of identical particles (say, atoms or molecules) that are free to move inside a certain volume, either not interacting or weakly interacting with each other.

### 3.1. Ideal classical gas

Interactions of typical atoms and molecules are well localized, i.e. rapidly decreasing with distance $r$ between them, becoming negligible at certain distance $r_{0}$. In a gas of $N$ particles inside volume $V$, the average distance $\langle r\rangle$ between the particles is of the order of $(V / N)^{1 / 3}$. As a result, if the gas density $n \equiv N / V \sim\langle r\rangle^{-3}$ is much lower than $r_{0}{ }^{-3}$, i.e. if $n r_{0}{ }^{3} \ll 1$, the chance for its particles to approach each other and interact is rather small. The model in which such interactions are completely ignored is called the ideal gas.

Let us start with a classical ideal gas, which may be defined as the gas in whose behavior the quantum effects are negligible. As we saw in Sec. 2.8 , the condition of that is to have the average occupancy of each quantum state low:

$$
\begin{equation*}
\left\langle N_{k}\right\rangle \ll 1 . \tag{3.1}
\end{equation*}
$$

It may seem that we have already found properties of such a system, in particular the equilibrium occupancy of its states - see Eq. (2.111):

$$
\begin{equation*}
\left\langle N_{k}\right\rangle=\text { const } \times \exp \left\{-\frac{\varepsilon_{k}}{T}\right\} . \tag{3.2}
\end{equation*}
$$

In some sense it is true, but we still need, first, to see what exactly does Eq. (2) means for the gas, i.e. a system with an essentially continuous energy spectrum, and, second, to show that, rather surprisingly, particles' indistinguishability affects some properties of even classical gases.

The first of these tasks is evidently the easiest for a gas out of external fields, and with no internal degrees of freedom. ${ }^{1}$ In this case $\varepsilon_{k}$ is just the kinetic energy of the particle obeys the isotropic and parabolic dispersion law

$$
\begin{equation*}
\varepsilon_{k}=\frac{p^{2}}{2 m}=\frac{p_{x}^{2}+p_{y}^{2}+p_{z}^{2}}{2 m} . \tag{3.3}
\end{equation*}
$$

Now we have to use two facts from other fields of physics. First, in quantum mechanics, momentum $\mathbf{p}$ is associated with wavevector $\mathbf{k}$ of the de Broglie wave, $\mathbf{p}=\hbar \mathbf{k} .{ }^{2}$ Second, eigenvalues of $\mathbf{k}$ for any waves (including de Broglie waves) in free space are uniformly distributed in the momentum space, with a constant density of states, given by Eq. (2.82)

[^846]\[

$$
\begin{equation*}
\frac{d N_{\text {states }}}{d^{3} k}=\frac{g V}{(2 \pi)^{3}}, \quad \text { i.e. } \frac{d N_{\text {states }}}{d^{3} p}=\frac{g V}{(2 \pi \hbar)^{3}}, \tag{3.4}
\end{equation*}
$$

\]

where $g$ is the degeneracy of particle's internal states (say, for electrons, the spin degeneracy $g=2$ ).
Even regardless of the exact proportionality coefficient between $d N_{\text {states }}$ and $d^{3} p$, the very fact of this proportionality means that the probability $d W$ to find the particle in a small region $d^{3} p=d p_{1} d p_{2} d p_{3}$ of the momentum space is proportional to the right-hand part of Eq. (2), with $\varepsilon_{k}$ given by Eq. (3):

$$
\begin{equation*}
d W=C \exp \left\{-\frac{p^{2}}{2 m T}\right\} d^{3} p=C \exp \left\{-\frac{p_{1}^{2}+p_{2}^{2}+p_{3}^{2}}{2 m T}\right\} d p_{1} d p_{2} d p_{3} . \tag{3.5}
\end{equation*}
$$

Maxwell distribution

This is the famous Maxwell distribution. ${ }^{3}$ The normalization constant $C$ may be readily found from the last form of Eq. (5), by requiring that the integral of $d W$ over all the momentum space to equal 1 , and using the equality of all 1D integrals over the each Cartesian component $p_{j}$ of the momentum $(j=$ $1,2,3$ ), which may be reduced to the well-known dimensionless Gaussian integral: ${ }^{4}$

$$
\begin{equation*}
C=\left[\int_{-\infty}^{+\infty} \exp \left\{-\frac{p_{j}^{2}}{2 m T}\right\} d p_{j}\right]^{-3}=\left[(2 m T)^{1 / 2} \int_{-\infty}^{+\infty} e^{-\xi^{2}} d \xi\right]^{-3}=(2 \pi m T)^{-3 / 2} \tag{3.6}
\end{equation*}
$$

As a sanity check, let us use the Maxwell distribution to calculate the average energy corresponding to each half-degree of freedom:

$$
\begin{equation*}
\left\langle\frac{p_{j}^{2}}{2 m}\right\rangle=\int \frac{p_{j}^{2}}{2 m} d W=\left[C^{1 / 3} \int_{-\infty}^{+\infty} \frac{p_{j}^{2}}{2 m} \exp \left\{-\frac{p_{j}^{2}}{2 m T}\right\} d p_{j}\right]\left[C^{1 / 3} \int_{-\infty}^{+\infty} \exp \left\{-\frac{p_{j^{\prime}}^{2}}{2 m T}\right\} d p_{j^{\prime}}\right]^{2}=\frac{T}{\pi^{1 / 2}} \int_{-\infty}^{+\infty} \xi^{2} e^{-\xi^{2}} d \xi . \tag{3.7}
\end{equation*}
$$

The last integral ${ }^{5}$ equals $\sqrt{ } \pi / 2$, so that, finally,

$$
\begin{equation*}
\left\langle\frac{p_{j}^{2}}{2 m}\right\rangle \equiv\left\langle\frac{m v_{j}^{2}}{2}\right\rangle=\frac{T}{2} \tag{3.8}
\end{equation*}
$$

This result is (fortunately :-) in agreement with the equipartition theorem (2.48). It also means that the r.m.s. velocity of the particles is

$$
\begin{equation*}
\delta v \equiv\left\langle v^{2}\right\rangle^{1 / 2}=\left\langle\sum_{j=1}^{3} v_{j}^{2}\right\rangle^{1 / 2}=\left\langle 3 v_{j}^{2}\right\rangle^{1 / 2}=\left(3 \frac{T}{m}\right)^{1 / 2} . \tag{3.9}
\end{equation*}
$$

[^847]For a typical gas (say, $\mathrm{N}_{2}$ ), with $m \approx 28 m_{p} \approx 4.7 \times 10^{-26} \mathrm{~kg}$ at room temperature ( $T=k_{\mathrm{B}} T_{\mathrm{K}} \approx$ $k_{\mathrm{B}} \times 300 \mathrm{~K} \approx 4.1 \times 10^{-21} \mathrm{~J}$ ), this velocity is about $500 \mathrm{~m} / \mathrm{s}$ - comparable with the sound velocity in the same gas (and the muzzle velocity of typical handgun bullets). Still, it is measurable using simple table-top equipment (say, a set of two concentric, rapidly rotating cylinders with a thin slit collimating an atomic beam emitted at the axis) that was available already in the end of the $19^{\text {th }}$ century. Experiments using such equipment gave convincing confirmations of Maxwell's theory.

This is all very simple (isn't it?), but actually the thermodynamic properties of a classical gas, especially its entropy, are more intricate. To show that, let us apply the Gibbs distribution to gas portions consisting of $N$ particles each, rather than just one of them. If the particles are exactly similar, the eigenenergy spectrum $\left\{\varepsilon_{k}\right\}$ of each of them is also exactly the same, and each value $E_{m}$ of the total energy is just the sum of particular energies $\varepsilon_{k(l)}$ of the particles, where $k(l)$, with $l=1,2, \ldots N$, is the number of the energy level of $l^{\text {th }}$ particle. Moreover, since the gas is classical, $\left\langle N_{k}\right\rangle \ll 1$, the probability of having two or more particles in any state may be ignored. As a result, we can use Eq. (2.59) to write

$$
\begin{equation*}
Z=\sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\}=\sum_{k(l)} \exp \left\{-\frac{1}{T} \sum_{l} \varepsilon_{k(l)}\right\}=\sum_{k(1)} \sum_{k(2)} \ldots \sum_{k(N)} \prod_{l} \exp \left\{-\frac{\varepsilon_{k(l)}}{T}\right\} \tag{3.10}
\end{equation*}
$$

where the summation has to be carried over all possible states of each particle. Since the summation over each set $\{k(l)\}$ concerns only one of the operands of the product of exponents under the sum, it is tempting to complete the calculation as follows:

$$
\begin{equation*}
Z \rightarrow Z_{\text {dist }}=\sum_{k(1)} \exp \left\{-\frac{\varepsilon_{k(1)}}{T}\right\} \cdot \sum_{k(2)} \exp \left\{-\frac{\varepsilon_{k(2)}}{T}\right\} \ldots \cdot \sum_{k(N)} \exp \left\{-\frac{\varepsilon_{k(N)}}{T}\right\}=\left(\sum_{k} \exp \left\{-\frac{\varepsilon_{k}}{T}\right\}\right)^{N} \tag{3.11}
\end{equation*}
$$

where the final summation is over all states of one particle. This formula is indeed valid for distinguishable particles. ${ }^{6}$ However, if particles are indistinguishable (again, meaning that they are identical and free to move within the same spatial region), Eq. (11) has to be modified by what is called the correct Boltzmann counting:

Correct Boltzmann counting

$$
\begin{equation*}
Z=\frac{1}{N!}\left(\sum_{k} \exp \left\{-\frac{\varepsilon_{k}}{T}\right\}\right)^{N} \tag{3.12}
\end{equation*}
$$

that considers all quantum states, differing only by particle permutations in the gas portion, as one.
Now let us take into account that the fundamental relation (4) implies the following rule for the replacement of a sum over quantum states with an integral in the classical limit - whose exact conditions are still to be specified: ${ }^{7}$

$$
\begin{equation*}
\sum_{k}(\ldots) \rightarrow \int(\ldots) d N_{\text {states }}=\frac{g V}{(2 \pi)^{3}} \int(\ldots) d^{3} k=\frac{g V}{(2 \pi \hbar)^{3}} \int(\ldots) d^{3} p \tag{3.13}
\end{equation*}
$$

In application to Eq. (12), this rule yields

[^848]\[

$$
\begin{equation*}
Z=\frac{1}{N!}\left(\frac{g V}{(2 \pi \hbar)^{3}}\left[\int_{-\infty}^{+\infty} \exp \left\{-\frac{p_{j}^{2}}{2 m T}\right\} d p_{j}\right]^{3}\right)^{N} \tag{3.14}
\end{equation*}
$$

\]

The integral in square brackets is the same one as in Eq. (6), i.e. equal to $(2 \pi m T)^{1 / 2}$, so that finally

$$
\begin{equation*}
Z=\frac{1}{N!}\left(\frac{g V}{(2 \pi \hbar)^{3}}(2 \pi m T)^{3 / 2}\right)^{N}=\frac{1}{N!}\left[g V\left(\frac{m T}{2 \pi \hbar^{2}}\right)^{3 / 2}\right]^{N} \tag{3.15}
\end{equation*}
$$

Now, assuming that $N \gg 1,{ }^{8}$ and applying the Stirling formula, we can calculate gas' free energy,

$$
\begin{equation*}
F=T \ln \frac{1}{Z}=-N T \ln \frac{V}{N}+N f(T) \tag{3.16a}
\end{equation*}
$$

with

$$
\begin{equation*}
f(T) \equiv-T\left\{\ln \left[g\left(\frac{m T}{2 \pi \hbar^{2}}\right)^{3 / 2}\right]+1\right\} . \tag{3.16b}
\end{equation*}
$$

The first of these relations is exactly Eq. (1.45) which was derived, in Sec. 1.4, from the equation of state $P V=N T$, using thermodynamic identities. At that stage this equation of state was just postulated, but now we can finally derive it by calculating pressure from the second of Eqs. (1.35), and Eq. (16a):

$$
\begin{equation*}
P=-\left(\frac{\partial F}{\partial V}\right)_{T}=\frac{N T}{V} \tag{3.17}
\end{equation*}
$$

So, the equation of state of the ideal classical gas, with density $n \equiv N / V$, is indeed given by Eq. (1.44):

$$
\begin{equation*}
P=\frac{N T}{V} \equiv n T . \tag{3.18}
\end{equation*}
$$

Hence we may use Eqs. (1.46)-(1.51), derived from this equation of state, to calculate all other thermodynamic variables of the gas. As one more sanity check, let us start with energy. Using Eq. (1.47) with $f(T)$ given by Eq. (16b), we immediately get

$$
\begin{equation*}
E=N\left(f-T \frac{d f}{d T}\right)=\frac{3}{2} N T \tag{3.19}
\end{equation*}
$$

in full agreement with Eq. (8) and hence with the equipartition theorem. Much less trivial is the result for entropy, which may be obtained by combining Eqs. (1.46) and (15):

$$
\begin{equation*}
S=-\left(\frac{\partial F}{\partial T}\right)_{V}=N\left[\ln \frac{V}{N}-\frac{d f(T)}{d T}\right] \tag{3.20}
\end{equation*}
$$

[^849]This formula, ${ }^{9}$ in particular, provides the means to resolve the following gas mixing paradox (sometimes called the "Gibbs paradox"). Consider two volumes, $V_{1}$ and $V_{2}$, separated by a partition, each filled with the same gas, with the same density $n$, at the same temperature $T$. Now let us remove the partition and let the gases mix; would the total entropy change? According to Eq. (20), it would not, because the ration $V / N=n$, and hence the expression in square brackets is the same in the initial and the final state, so that the entropy is additive (extensive). This makes full sense if the gas particles in the both parts of the volume are identical, i.e. the partition's removal does not change our information about the system. However, let us assume that all particles are distinguishable; then the entropy should clearly increase, because the mixing would certainly decrease our information about the system, i.e. increase its disorder. A quantitative description of this effect may be obtained using Eq. (11). Repeating for $Z_{\text {dist }}$ all the calculations made above for $Z$, we readily get a different formula for entropy:

$$
\begin{equation*}
S_{\text {dist }}=N\left[\ln V-\frac{d f_{\text {dist }}(T)}{d T}\right], \quad f_{\text {dist }}(T) \equiv-T \ln \left[g\left(\frac{m T}{2 \pi \hbar^{2}}\right)^{3 / 2}\right] \tag{3.21}
\end{equation*}
$$

Notice that in contrast to the $S$ given by Eq. (20), entropy $S_{\text {dist }}$ is not proportional to $N$ (at fixed temperature $T$ and density $N / V$ ). While for distinguishable particles this fact does not present any conceptual problem, for indistinguishable particles it would mean that entropy were not an extensive variable, i.e. would contradict the basic assumptions of thermodynamics. This fact emphasizes again the necessity of the correct Boltzmann counting in the latter case.

Comparing Eqs. (20) and (21), we can calculate the change of entropy due to mixing of distinguishable particles:

$$
\begin{equation*}
\Delta S_{\text {dist }}=\left(N_{1}+N_{2}\right) \ln \left(V_{1}+V_{2}\right)-\left(N_{1} \ln V_{1}+N_{2} \ln V_{2}\right)=N_{1} \ln \frac{V_{1}+V_{2}}{V_{1}}+N_{2} \ln \frac{V_{1}+V_{2}}{V_{2}}>0 . \tag{3.22}
\end{equation*}
$$

Note that for a particular case, $V_{1}=V_{2}=V / 2$, Eq. (22) reduces to the simple result $\Delta S_{\text {dist }}=\left(N_{1}+N_{2}\right) \ln 2$, which may be readily understood from the point of view of information theory. Indeed, allowing each particle of $N=N_{1}+N_{2}$ to spread to twice larger volume, we loose one bit of information per particle, i.e. $\Delta I=\left(N_{1}+N_{2}\right)$ bits for the whole system.

Let me leave it for the reader to show that result (22) is also valid if particles in each sub-volume are indistinguishable from each other, but different from those in another sub-volume, i.e. for mixing of two different gases. ${ }^{10}$ However, it is certainly not applicable to the system where all particles are identical, stressing again that the correct Boltzmann counting (12) does indeed affect entropy, even though it is not essential for either the Maxwell distribution (5), or the equation of state (18), or average energy (19).

In this context, one may wonder whether the change (22) (called the mixing entropy) is experimentally observable. The answer is yes. For example, after free mixing of two different gases one can use a thin movable membrane that is semipermeable, i.e. penetrable by particles of one type only, to

[^850]separate them again, thus reducing the entropy back to the initial value, and measure either the necessary mechanical work $\Delta \mathcal{W}=T \Delta S_{\text {dist }}$ or the corresponding heat discharge into the heat bath. Practically, measurements of this type are easier in weak solutions, ${ }^{11}$ systems with a small concentration $c \ll 1$ of particles of one sort (solute) within much more abundant particles of another sort (solvent). The mixing entropy also affects thermodynamics of chemical reactions in gases and liquids. ${ }^{12}$ It is curious that besides purely thermal measurements, mixing entropy in some conducting solutions (electrolytes) is also measurable by a purely electrical method, called cyclic voltammetry, in which a low-frequency ac voltage, applied between solid-state electrodes embedded in the solution, is used to periodically separate different ions, and then mix them again. ${ }^{13}$

Now let us briefly discuss two generalizations of our results for ideal classical gases. First, let us consider the ideal classical gas in an external field of potential forces. It may be described by replacing Eq. (3) with

$$
\begin{equation*}
\varepsilon_{k}=\frac{p_{k}^{2}}{2 m}+U\left(\mathbf{r}_{k}\right), \tag{3.23}
\end{equation*}
$$

where $\mathbf{r}_{k}$ is the position of the particular particle, and $U(\mathbf{r})$ is the potential energy per particle. In this cases, Eq. (4) is applicable only to small volumes, $V \rightarrow d V=d^{3} r$ whose linear size is much smaller than the spatial scale of variations of macroscopic parameters of the gas- say, pressure. Hence, instead of Eq. (5), we may only write the probability $d W$ of finding the particle in a small volume $d^{3} r d^{3} p$ of the 6dimensional phase space:

$$
\begin{equation*}
d W=w(\mathbf{r}, \mathbf{p}) d^{3} r d^{3} p, \quad w(\mathbf{r}, \mathbf{p})=\text { const } \times \exp \left\{-\frac{p^{2}}{2 m T}-\frac{U(\mathbf{r})}{T}\right\} . \tag{3.24}
\end{equation*}
$$

Hence, the Maxwell distribution of particle velocities is still valid at each point $\mathbf{r}$, and a more interesting issue here is the spatial distribution of the total density,

$$
\begin{equation*}
n(\mathbf{r}) \equiv N \int w(\mathbf{r}, \mathbf{p}) d^{3} p \tag{3.25}
\end{equation*}
$$

of all gas particles, regardless of their momentum. For this variable, Eq. (24) yields ${ }^{14}$

$$
\begin{equation*}
n(\mathbf{r})=n(0) \exp \left\{-\frac{U(\mathbf{r})}{T}\right\} \tag{3.26}
\end{equation*}
$$

[^851]where the potential energy reference is at the origin. As we will see in Chapter 6, in a non-uniform gas the equation of state (18) is valid locally if particles' mean free path $l$ is much smaller than the spatial scale of changes of function $n(\mathbf{r}) .{ }^{15}$ In this case, the local gas pressure may be still calculated from Eq. (18):
\[

$$
\begin{equation*}
P(\mathbf{r})=n(\mathbf{r}) T=P(0) \exp \left\{-\frac{U(\mathbf{r})}{T}\right\} . \tag{3.27}
\end{equation*}
$$

\]

An important example of application of Eq. (27) is an approximate description of the Earth atmosphere. At all heights $h \ll R_{\mathrm{E}} \sim 6 \times 10^{6} \mathrm{~m}$ above the Earth's surface (say, the sea level), we may describe the Earth gravity effect by potential $U=m g h$, and Eq. (27) yields the so-called barometric formula

$$
\begin{equation*}
P(h)=P(0) \exp \left\{-\frac{h}{h_{0}}\right\}, \quad \text { with } h_{0} \equiv \frac{T}{m g}=\frac{k_{\mathrm{B}} T_{\mathrm{K}}}{m g} . \tag{3.28}
\end{equation*}
$$

For the same $\mathrm{N}_{2}$ (the main component of the atmosphere) at $T_{\mathrm{K}}=300 \mathrm{~K}, h_{0} \approx 7 \mathrm{~km}$. This gives the right order of magnitude of the Earth atmosphere's thickness, though the exact law of pressure change differs somewhat from Eq. (28) because of a certain drop of the absolute temperature $T$ with height, by about $20 \%$ at $h \sim h_{0} .{ }^{16}$

The second generalization I would like to mention is to particles with internal degrees of freedom. Ignoring, for simplicity, the potential energy $U(\mathbf{r})$, we may describe them by replacing Eq. (3) for

$$
\begin{equation*}
\varepsilon_{k}=\frac{p^{2}}{2 m}+\varepsilon_{k}^{\prime}, \tag{3.29}
\end{equation*}
$$

where $\varepsilon_{k}$ ' describes the internal energy of the $k$-th particle. If the particles are similar, we may repeat all above calculations, and see that all the results (including the Maxwell distribution) are still valid, with the only exception of Eq. (16) that now becomes

$$
\begin{equation*}
f(T)=-T\left\{\ln \left[g\left(\frac{m T}{2 \pi \hbar^{2}}\right)^{3 / 2} \times \sum_{\varepsilon_{k^{\prime}}} \exp \left\{-\frac{\varepsilon_{k}^{\prime}}{T}\right\}\right]+1\right\} \tag{3.30}
\end{equation*}
$$

As we already know from Eq. (1.51), this change may affect both heat capacities of the gas, $C_{V}$ and $C_{P}$, but not their difference (equal to $N$ ).

### 3.2. Calculating $\mu$

Now let us return to Eq. (3), i.e. neglect the external field effects, as well as thermal activation of the internal degrees of freedom, and discuss properties of ideal gases of indistinguishable quantum

[^852]particles in more detail, paying special attention to the chemical potential $\mu$ - which, as you may recall, was a little bit mysterious aspect of the Fermi and Bose distributions.

Let us start from the classical gas, and recall the conclusion of thermodynamics that $\mu$ is the Gibbs potential per unit particle - see Eq. (1.56). Hence we can calculate $\mu=G / N$ from Eqs. (1.49) and (16b). The result,

$$
\begin{equation*}
\mu=-T \ln \frac{V}{N}+f(T)+T=T \ln \left[\frac{N}{g V}\left(\frac{2 \pi \hbar^{2}}{m T}\right)^{3 / 2}\right] \tag{3.31}
\end{equation*}
$$

which may be rewritten as

$$
\begin{equation*}
\exp \left\{\frac{\mu}{T}\right\}=\frac{N}{g V}\left(\frac{2 \pi \hbar^{2}}{m T}\right)^{3 / 2} \tag{3.32}
\end{equation*}
$$

is very important, because it gives us some information about $\mu$ not only for a classical gas, but for quantum (Fermi and Bose) gases as well. Indeed, we already know that for indistinguishable particles the Boltzmann distribution (2.111) is valid only if $\left\langle N_{k}\right\rangle \ll 1$. Comparing this condition with quantum statistics (2.115) and (2.118), we see that the condition of gas' classicity may be expressed as

$$
\begin{equation*}
\exp \left\{\frac{\mu-\varepsilon_{k}}{T}\right\} \ll 1 \tag{3.33}
\end{equation*}
$$

for all $\varepsilon_{k}$. Since the lowest value of $\varepsilon_{k}$ given by Eq. (3) is zero, Eq. (33) for a gas may be satisfied only if $\exp \{\mu / T\} \ll 1$. This means that the chemical potential of the classical has to be not just negative, but also "strongly negative" in the sense

$$
\begin{equation*}
-\mu \gg T \tag{3.34}
\end{equation*}
$$

According to Eq. (32), this condition may be presented as

$$
\begin{equation*}
T \gg T_{0} \tag{3.35}
\end{equation*}
$$

with $T_{0}$ defined as

$$
\begin{equation*}
T_{0} \equiv \frac{\hbar^{2}}{m}\left(\frac{n}{g}\right)^{2 / 3}=\frac{\hbar^{2}}{g^{2 / 3} m r_{A}^{2}}, \quad \text { with } r_{A} \equiv \frac{1}{n^{1 / 3}}=\left(\frac{V}{N}\right)^{1 / 3} . \tag{3.36}
\end{equation*}
$$

Condition (35) is very transparent physically: disregarding factor $g^{2 / 3}$ (which is typically not much larger than 1), it means that the average thermal energy of a particle (which is of the order of $T$ ) has to be much larger than the energy of quantization of particle's motion at length $r_{A}$ - the average distance between the particles. An alternative form of this condition is ${ }^{17}$

$$
\begin{equation*}
r_{A} \gg g^{-1 / 3} r_{c}, \quad \text { with } r_{c} \equiv \frac{\hbar}{(m T)^{1 / 2}} . \tag{3.37}
\end{equation*}
$$

[^853]For a typical gas (say, $\mathrm{N}_{2}$, with $m \approx 14 m_{p} \approx 2.3 \times 10^{-26} \mathrm{~kg}$ ) at the standard room temperature ( $T=$ $\left.k_{\mathrm{B}} \times 300 \mathrm{~K} \approx 4.1 \times 10^{-21} \mathrm{~J}\right), r_{c} \approx 10^{-11} \mathrm{~m}$, i.e. is significantly smaller than the physical size $a \sim 3 \times 10^{-10} \mathrm{~m}$ of the molecule. This estimate shows that at room temperature, as soon as any practical gas is rare enough to be ideal $\left(r_{A} \gg a\right)$, it is classical, i.e. the only way to observe the quantum effects in the translation motion of molecules is a very deep refrigeration. According to Eq. (36), for the same nitrogen molecule, taking $r_{A} \sim 10^{3} a \sim 10^{-7} \mathrm{~m}$ (to ensure that direct interaction effects are negligible), $T_{0}$ should be well below $1 \mu \mathrm{~K}$.

In order to analyze quantitatively what happens with gases when $T$ is reduced to such low values, we need to calculate $\mu$ for an arbitrary ideal gas of indistinguishable particles. Let us use the lucky fact that the Fermi-Dirac and the Bose-Einstein statistics may be represented with one formula:

$$
\begin{equation*}
\langle N(\varepsilon)\rangle=\frac{1}{e^{(\varepsilon-\mu) / T} \pm 1} \tag{3.38}
\end{equation*}
$$

where (and everywhere in the balance of this section) the top sign stands for fermions and the lower one is for bosons, to discuss the fermionic and bosonic gases on the same breath.

If we deal with a member of the grand canonical ensemble (Fig. 2.13), in which $\mu$ is externally fixed, we may apply Eq. (39) to calculate the average number $N$ of particles in volume $V$. If the volume is so large that $N \gg 1$, we may use the general state counting rule (13):

$$
\begin{equation*}
N=\frac{g V}{(2 \pi)^{3}} \int\langle N(\varepsilon)\rangle d^{3} k=\frac{g V}{(2 \pi \hbar)^{3}} \int \frac{d^{3} p}{e^{[\varepsilon(p)-\mu] / T} \pm 1}=\frac{g V}{(2 \pi \hbar)^{3}} \int_{0}^{\infty} \frac{4 \pi p^{2} d p}{e^{[\varepsilon(p)-\mu] / T} \pm 1} \tag{3.39}
\end{equation*}
$$

In most practical cases, however, the number $N$ of gas particles is fixed by particle confinement (i.e. the gas portion under study is a member of the canonical ensemble - see Fig. 2.6), and hence $\mu$ rather than $N$ should be calculated. Here comes the main trick: if $N$ is very large, the relative fluctuation of the particle number is negligibly small $(\sim 1 / \sqrt{ } N \ll 1)$, and the relation between the average values of $N$ and $\mu$ should not depend which of these variables is exactly fixed. Hence, Eq. (39), with $\mu$ having the sense of the average chemical potential, should be valid even if $N$ is exactly fixed, so that small fluctuations of $N$ are replaced with (equally small) fluctuations of $\mu$. Physically (as was already mentioned in Sec. 2.8), in this case the role of the $\mu$-fixing environment for any gas sub-portion is played by the rest of the gas, and Eq. (39) expresses the condition of self-consistency of such mutual particle exchange.

In this situation, Eq. (39) may be used for calculating the average $\mu$ as a function of two independent parameters: $N$ (i.e. of the gas density $n=N / V$ ) and temperature $T$. For carrying out this calculation, it is convenient to convert the right-hand part of Eq. (39) to an integral over particle's energy $\varepsilon(p)=p^{2} / 2 m$, so that $p=(2 m \varepsilon)^{1 / 2}$, and $d p=(m / 2 \varepsilon)^{1 / 2} d \varepsilon$ :

$$
\begin{equation*}
N=\frac{g V m^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\varepsilon^{1 / 2} d \varepsilon}{e^{(\varepsilon-\mu) / T} \pm 1} \tag{3.40}
\end{equation*}
$$

This key result may be presented in two more convenient forms. First, Eq. (40), derived for our current (3D, isotropic and parabolic-dispersion) approximation (3), is just particular case of a general relation

$$
\begin{equation*}
N=\int_{0}^{\infty} g(\varepsilon)\langle N(\varepsilon)\rangle d \varepsilon, \tag{3.41}
\end{equation*}
$$

where

$$
\begin{equation*}
g(\varepsilon) \equiv \frac{d N_{\text {states }}}{d \varepsilon} \tag{3.42}
\end{equation*}
$$

is the temperature-independent density of all quantum states of a particle - regardless of whether they are occupied or not. Indeed, according to the general Eq. (4), for our simple model (3),

$$
\begin{equation*}
g(\varepsilon)=g_{3}(\varepsilon) \equiv \frac{d N_{\text {states }}}{d \varepsilon}=\frac{d}{d \varepsilon}\left(\frac{g V}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} p^{3}\right)=\frac{4 \pi g V}{3(2 \pi \hbar)^{3}} \frac{d\left(p^{3}\right)}{d \varepsilon}=\frac{g V m^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \varepsilon^{1 / 2} \tag{3.43}
\end{equation*}
$$

so that we return to Eq. (39). On the other hand, for some calculations, it is convenient to introduce a dimensionless energy variable $\xi \equiv \varepsilon / T$ to express Eq. (40) via a dimensionless integral:

$$
\begin{equation*}
N=\frac{g V(m T)^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi-\mu / T} \pm 1} \tag{3.44}
\end{equation*}
$$

As a sanity check, in the classical limit (34), the exponent in the denominator of the fraction under the integral is much larger than 1, and Eq. (44) reduces to

$$
\begin{equation*}
N=\frac{g V(m T)^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi-\mu / T}} \approx \frac{g V(m T)^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \exp \left\{\frac{\mu}{T} \int_{0}^{\infty} \xi^{1 / 2} e^{-\xi} d \xi, \quad \text { at }-\mu \gg T .\right. \tag{3.45}
\end{equation*}
$$

By the definition of gamma-function $\Gamma(\xi),{ }^{18}$ this dimensionless integral is just $\Gamma(3 / 2)=\sqrt{ } \pi / 2$, and we get

$$
\begin{equation*}
\exp \left\{\frac{\mu}{T}\right\}=N \frac{\sqrt{2} \pi^{2} \hbar^{3}}{g V(m T)^{3 / 2}} \frac{2}{\sqrt{\pi}}=\left(2 \pi \frac{T_{0}}{T}\right)^{3 / 2}, \tag{3.46}
\end{equation*}
$$

which is exactly the same result as given by Eq. (34), which has been obtained in a rather different way - from the Boltzmann distribution and thermodynamic identities.

Unfortunately, in the general case of arbitrary $\mu$ the integral in Eq. (44) cannot be worked out analytically. ${ }^{19}$ The best we can do is to use temperature $T_{0}$, defined by Eq. (37), to rewrite Eq. (44) as

$$
\begin{equation*}
\frac{T}{T_{0}}=\left[\frac{1}{\sqrt{2} \pi^{2}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi-\mu / T} \pm 1}\right]^{-2 / 3} \tag{3.47}
\end{equation*}
$$

We may use this relation to calculate ratio $T / T_{0}$, and then ratio $\mu / T_{0} \equiv(\mu / T) \times\left(T / T_{0}\right)$, as functions of $\mu / T$ numerically, and then plot the results versus each other, thinking of the former ratio as the argument.

Figure 1 shows the resulting plot. It shows that at large temperatures, $T \gg T_{0}$, the chemical potential is negative and approaches the classical behavior given by Eq. (46) for both fermions and bosons - just as we could expect. For fermions, the reduction of temperature leads to $\mu$ changing its sign from negative to positive, and then approaching a constant positive value called the Fermi energy, $\varepsilon_{\mathrm{F}} \approx$ $7.595 T_{0}$ at $T \rightarrow 0$. On the contrary, the chemical potential of a gas of bosons stays negative, and turns

[^854]into zero at certain critical temperature $T_{c} \approx 3.313 T_{0}$. Both these limits, which are very important for applications, may (and will be :-) explored analytically, but separately for each statistics.


Fig. 3.1. Chemical potential of an ideal gas of $N \gg 1$ indistinguishable quantum particles, as a function of temperature (at fixed gas density $n \equiv N / V$, which fixes parameter $T_{0} \propto$ $n^{3 / 2}$ ), for two different quantum statistics. The dashed line shows the classical approximation (46) valid at $T \gg T_{0}$.

Before doing that (in the next two sections), let me show that, rather surprisingly, for any (but non-relativistic!) quantum gas, the product $P V$ expressed in terms of energy,

$$
\begin{equation*}
P V=\frac{2}{3} E \tag{3.48}
\end{equation*}
$$

is the same as follows from Eqs. (18) and (19) for the classical gas, and hence does not depend on particle's statistics. In order to prove this, it is sufficient to use Eqs. (2.114) and (2.117) for the grand thermodynamic potential of each quantum state, which may be conveniently represented by a single formula,

$$
\begin{equation*}
\Omega_{k}=\mp T \ln \left(1 \pm e^{\left(\mu-\varepsilon_{k}\right) / T}\right) \tag{3.49}
\end{equation*}
$$

and sum them over all states $k$, using the general summation formula (13). The result for the total grand potential of a 3D gas with the dispersion law (3) is

$$
\begin{equation*}
\Omega=\mp T \frac{g V}{(2 \pi \hbar)^{3}} \int_{0}^{\infty} \ln \left(1 \pm e^{\left(\mu-p^{2} / 2 m\right) / T}\right) 4 \pi p^{2} d p=\mp T \frac{g V m^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \ln \left(1 \pm e^{(\mu-\varepsilon) / T}\right) \varepsilon^{1 / 2} d \varepsilon \tag{3.50}
\end{equation*}
$$

Working out this integral by parts, exactly as we did it with the one in Eq. (2.90), we get

$$
\begin{equation*}
\Omega=-\frac{2}{3} \frac{g V m^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\varepsilon^{3 / 2} d \varepsilon}{e^{(\varepsilon-\mu) / T} \pm 1}=-\frac{2}{3} \int_{0}^{\infty} \varepsilon g_{3}(\varepsilon)\langle N(\varepsilon)\rangle d \varepsilon . \tag{3.51}
\end{equation*}
$$

But the last integral is just the total energy $E$ of the gas:

$$
\begin{equation*}
E=\frac{g V}{(2 \pi \hbar)^{3}} \int_{0}^{\infty} \frac{p^{2}}{2 m} \frac{4 \pi p^{2} d p}{e^{[\varepsilon(p)-\mu] / T} \pm 1}=\frac{g V m^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\varepsilon^{3 / 2} d \varepsilon}{e^{(\varepsilon-\mu) / T} \pm 1}=\int_{0}^{\infty} \varepsilon g_{3}(\varepsilon)\langle N(\varepsilon)\rangle d \varepsilon, \tag{3.52}
\end{equation*}
$$

so that for any temperature and any particle type, $\Omega=-(2 / 3) E$. But since, from thermodynamics, $\Omega=-$ $P V$, we have Eq. (48) proved. This universal relation will be repeatedly used below.

### 3.3. Degenerate Fermi gas

The analysis of low-temperature properties of a Fermi gas is very simple in the limit $T=0$. Indeed, in this limit, the Fermi-Dirac distribution (2.115) is just a step function:

$$
\langle N(\varepsilon)\rangle= \begin{cases}1, & \text { for } \varepsilon<\mu  \tag{3.53}\\ 0, & \text { for } \mu<\varepsilon\end{cases}
$$

- see by the bold line in Fig. 2a. Since $\varepsilon=p^{2} / 2 m$ is isotropic in the momentum space, this means that at $T$ $=0$, in that space the particles fully occupy all possible quantum states within a sphere (frequently called either the Fermi sphere or the Fermi sea) with some radius $p_{\text {F }}$ (Fig. 2b), while all states above the sea surface are empty. Such degenerate Fermi gas is a striking manifestation of the Pauli principle: though at thermodynamic equilibrium at $T=0$ all particles try to lower their energies as much as possible, only $g$ of them may occupy each quantum state within the Fermi sphere. As a result, the sphere's volume is proportional to the particle number $N$, or rather to their density $n=N / V$.


Fig. 3.2. Representation of the Fermi sea: (a) on the energy axis and (b) in the momentum space.

Indeed, radius $p_{\mathrm{F}}$ may be readily related to the number of particles $N$ using Eq. (40) whose integral in this case is just the Fermi sphere volume:

$$
\begin{equation*}
N=\frac{g V}{(2 \pi \hbar)^{3}} \int_{0}^{p_{\mathrm{F}}} 4 \pi p^{2} d p=\frac{g V}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} p_{\mathrm{F}}^{3} . \tag{3.54}
\end{equation*}
$$

Now we can use Eq. (3) to express via $N$ the chemical potential $\mu$ (which is this limit, $T \rightarrow 0$, bears the special name of the Fermi energy $\left.\varepsilon_{\mathrm{F}}\right)^{20}$ :

$$
\begin{equation*}
\left.\varepsilon_{\mathrm{F}} \equiv \mu\right|_{T=0}=\frac{p_{\mathrm{F}}^{2}}{2 m}=\frac{\hbar^{2}}{2 m}\left(6 \pi^{2} \frac{N}{g V}\right)^{2 / 3}=\left(\frac{9 \pi^{4}}{2}\right)^{1 / 3} T_{0} \approx 7.595 T_{0}, \tag{3.55a}
\end{equation*}
$$

where $T_{0}$ is the quantum temperature scale defined by Eq. (36). This formula quantifies the lowtemperature trend of function $\mu(T)$, clearly visible in Fig. 1, and in particular explains the ratio $\varepsilon_{\mathrm{F}} / T$ mentioned in Sec. 2. Note also a useful and simple relation,

$$
\begin{equation*}
\varepsilon_{\mathrm{F}}=\frac{3}{2} \frac{N}{g_{3}\left(\varepsilon_{\mathrm{F}}\right)}, \tag{3.55b}
\end{equation*}
$$

which may be obtained immediately from Eqs. (43) and (54).

[^855]The total energy of the gas may be (equally easily) calculated from Eq. (52):

$$
\begin{equation*}
E=\frac{g V}{(2 \pi \hbar)^{3}} \int_{0}^{p_{\mathrm{F}}} \frac{p^{2}}{2 m} 4 \pi p^{2} d p=\frac{g V}{(2 \pi \hbar)^{3}} \frac{4 \pi}{2 m} \frac{p_{\mathrm{F}}^{5}}{5}=\frac{3}{5} \varepsilon_{\mathrm{F}} N \tag{3.56}
\end{equation*}
$$

showing that the average energy, $\langle\varepsilon\rangle \equiv E / N$, of a particle inside the Fermi sea is equal to $3 / 5=60 \%$ of that $\left(\varepsilon_{\mathrm{F}}\right)$ of the most energetic occupied states, on the Fermi surface. Since, according to the formulas of Chapter 1, at zero temperature $H=G=N \mu$, and $F=E$, the only thermodynamic variable still to be calculated is pressure $P$. For that, we could use any of thermodynamic relations $P=(H-E) / V$ or $P=-$ $(\partial F / \partial V)_{T}$, but it is even easier to use our recent result (48). Together with Eq. (56), it yields

$$
\begin{equation*}
P=\frac{2}{3} \frac{E}{V}=\frac{2}{5} \varepsilon_{F} \frac{N}{V}=\left(\frac{36 \pi^{4}}{125}\right)^{1 / 3} P_{0} \approx 3.035 P_{0}, \quad \text { where } P_{0} \equiv n T_{0}=\frac{\hbar^{2}}{m g^{2 / 3}} n^{5 / 3} \tag{3.57}
\end{equation*}
$$

From here, it is easy to calculate the bulk modulus (reciprocal compressibility), ${ }^{21}$

$$
\begin{equation*}
K \equiv-V\left(\frac{\partial P}{\partial V}\right)_{T}=\frac{2}{3} \varepsilon_{\mathrm{F}} \frac{N}{V} \tag{3.58}
\end{equation*}
$$

which is simpler to measure experimentally.
Perhaps the most important example ${ }^{22}$ of the degenerate Fermi gas are the conduction electrons in metals - the electrons that belong to outer shells of the isolated atoms but become common in solid metals and can move through the crystal lattice almost freely. Though electrons (which are fermions with spin $s=1 / 2$ and hence the spin degeneracy $g=2 s+1=2$ ) are negatively charged, the Coulomb interaction of conduction electrons with each other is substantially compensated by the positively charged ions of the atomic lattice, so that they follow the simple formulas derived above reasonably well. This is especially true for alkali metals (forming Group 1 of the periodic table of elements), whose experimentally measured Fermi surfaces are spherical within $1 \%$ even within $0.1 \%$ for Na. Table 1 lists, in particular, the experimental values of the bulk modulus for such metals, together with the values given by Eq. (58) using $\varepsilon_{\mathrm{F}}$ calculated from Eq. (55) with the experimental density of conduction electrons. Evidently, the agreement is pretty good, taking into account that the simple theory described above completely ignores such factors as the Coulomb and exchange interactions of the electrons. This agreement implies that, surprisingly, the rigidity of solids (or at least metals) is predominantly due to the kinetic energy of conduction electrons, complemented with the Pauli principle, rather than any electrostatic interactions - though, to be fair, these interactions are the crucial factor defining the equilibrium value of $n$. Numerical calculations using more accurate approximations (e.g., the density functional theory ${ }^{23}$ ) that agree with experiment with a few percent accuracy, confirm this conclusion. ${ }^{24}$

[^856]Table 3.1. Experimental and theoretical parameters of electron's Fermi sea in some alkali metals ${ }^{25}$

| Metal | $\mathcal{E}_{\mathrm{F}}(\mathrm{eV})$ <br> Eq. $(55)$ | $K(\mathrm{GPa})$ <br> Eq. (58) | $K(\mathrm{GPa})$ <br> experiment | $\gamma\left(\mathrm{mcal} / \mathrm{mole} \cdot \mathrm{K}^{2}\right)$ <br> Eq. (69) | $\gamma\left(\mathrm{mcal} / \mathrm{mole} \cdot \mathrm{K}^{2}\right)$ <br> experiment |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Na | 3.24 | 923 | 642 | 0.26 | 0.35 |
| K | 2.12 | 319 | 281 | 0.40 | 0.47 |
| Rb | 1.85 | 230 | 192 | 0.46 | 0.58 |
| Cs | 1.59 | 154 | 143 | 0.53 | 0.77 |

Now looking at the values of $\varepsilon_{\mathrm{F}}$ listed in the table, note that room temperatures ( $T_{\mathrm{K}} \sim 300 \mathrm{~K}$ ) correspond to $T \sim 25 \mathrm{meV}$. As a result, virtually all experiments with metals, at least in their solid or liquid form, are performed in the limit $T \ll \mathcal{E}_{\mathrm{F}}$. According to Eq. (39), at such temperatures the occupancy step described by the Fermi-Dirac distribution has a finite but relatively small width $\sim T-$ see the dashed line in Fig. 2a. Calculations in this case are much facilitated by the so-called Sommerfeld expansion formula ${ }^{26}$ for integrals like (40) and (52):

$$
\begin{equation*}
I(T) \equiv \int_{0}^{\infty} \varphi(\varepsilon)\langle N(\varepsilon)\rangle d \varepsilon \approx \int_{0}^{\mu} \varphi(\varepsilon) d \varepsilon+\frac{\pi^{2}}{6} T^{2} \frac{d \varphi(\mu)}{d \mu}, \quad \text { at } T \ll \mu, \tag{3.59}
\end{equation*}
$$

Sommerfeld expansion
where $\varphi(\varepsilon)$ is an arbitrary function that is sufficiently smooth at $\varepsilon=\mu$ and integrable at $\varepsilon=0$. In order to prove this formula, let us introduce another function

$$
\begin{equation*}
f(\varepsilon) \equiv \int_{0}^{\varepsilon} \varphi\left(\varepsilon^{\prime}\right) d \varepsilon^{\prime}, \quad \text { so that } \varphi(\varepsilon)=\frac{d f(\varepsilon)}{d \varepsilon} \tag{3.60}
\end{equation*}
$$

and work out the integral $I(T)$ by parts:

$$
\begin{equation*}
I(T)=\int_{0}^{\infty} \frac{d f(\varepsilon)}{d \varepsilon}\langle N(\varepsilon)\rangle d \varepsilon=\int_{\varepsilon=0}^{\varepsilon=\infty}\langle N(\varepsilon)\rangle d f=[\langle N(\varepsilon)\rangle f]_{\varepsilon=0}^{\varepsilon=\infty}-\int_{\varepsilon=0}^{\varepsilon=\infty} f(\varepsilon) d\langle N(\varepsilon)\rangle=\int_{0}^{\infty} f(\varepsilon)\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon . \tag{3.61}
\end{equation*}
$$

As evident from Eq. (39) and/or Fig. 2a, at $T \ll \mu$, function ( $-\partial\langle N(\varepsilon)\rangle / \partial \varepsilon$ ) approaches zero for all energies, besides a narrow peak, of unit area, at $\varepsilon \approx \mu$. Hence, if we expand function $f(\varepsilon)$ in the Taylor series near this point, just a few leading terms of the expansion should give us a good approximation:

$$
\begin{align*}
I(T) & \approx \int_{0}^{\infty}\left[f(\mu)+\left.\frac{d f}{d \varepsilon}\right|_{\varepsilon=\mu}(\varepsilon-\mu)+\left.\frac{1}{2} \frac{d^{2} f}{d \varepsilon^{2}}\right|_{\varepsilon=\mu}(\varepsilon-\mu)^{2}\right]\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon  \tag{3.62}\\
& =\int_{0}^{\mu} \varphi\left(\varepsilon^{\prime}\right) d \varepsilon^{\prime} \int_{0}^{\infty}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon+\varphi(\mu) \int_{0}^{\infty}(\varepsilon-\mu)\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon+\frac{1}{2} \frac{d \varphi(\mu)}{d \mu} \int_{0}^{\infty}(\varepsilon-\mu)^{2}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon
\end{align*}
$$

[^857]In the last form of this relation, the first integral over $\varepsilon$ equals $\langle N(\varepsilon=0)\rangle-\langle N(\varepsilon=\infty\rangle=1$, the second one vanishes (because the function under it is asymmetric about point $\varepsilon=\mu$ ), and only the last one needs to be dealt with explicitly, by working it out by parts and then using a table integral:27

$$
\begin{equation*}
\int_{0}^{\infty}(\varepsilon-\mu)^{2}\left(-\frac{\partial\left\langle N_{k}\right\rangle}{\partial \varepsilon}\right) d \varepsilon \approx T^{2} \int_{-\infty}^{+\infty} \xi^{2} \frac{d}{d \xi}\left(-\frac{1}{e^{\xi}+1}\right) d \xi=4 T^{2} \int_{0}^{+\infty} \frac{\xi d \xi}{e^{\xi}+1}=4 T^{2} \frac{\pi^{2}}{12} \tag{3.63}
\end{equation*}
$$

Being plugged into Eq. (62), this result proves the Sommerfeld formula (59).
The last preparatory step we need is to take into account a possible small difference (as we will see below, also proportional to $T^{2}$ ) between the temperature-dependent chemical potential $\mu(T)$ and the Fermi energy defined as $\varepsilon_{\mathrm{F}} \equiv \mu(0)$, in the largest (first) term in the right-hand part of Eq. (62), to write

$$
\begin{equation*}
I(T) \approx \int_{0}^{\varepsilon_{\mathrm{F}}} \varphi(\varepsilon) d \varepsilon+\left(\mu-\varepsilon_{\mathrm{F}}\right) \varphi(\mu)+\frac{\pi^{2}}{6} T^{2} \frac{d \varphi(\mu)}{d \mu}=I(0)+\left(\mu-\varepsilon_{\mathrm{F}}\right) \varphi(\mu)+\frac{\pi^{2}}{6} T^{2} \frac{d \varphi(\mu)}{d \mu} . \tag{3.64}
\end{equation*}
$$

Now, applying this formula to Eq. (41) and the last form of Eq. (52), we get the following results (which are valid for any dispersion law $\varepsilon(\mathbf{p})$ and even any dimensionality of the gas):

$$
\begin{gather*}
N(T)=N(0)+\left(\mu-\varepsilon_{\mathrm{F}}\right) g(\mu)+\frac{\pi^{2}}{6} T^{2} \frac{d g(\mu)}{d \mu},  \tag{3.65}\\
E(T)=E(0)+\left(\mu-\varepsilon_{\mathrm{F}}\right) \mu g(\mu)+\frac{\pi^{2}}{6} T^{2} \frac{d}{d \mu}[\mu g(\mu)] . \tag{3.66}
\end{gather*}
$$

However, the number of particles does not change with temperature, $N(T)=N(0)$, so that Eq. (65) gives an equation for finding the temperature-induced change of $\mu$ :

$$
\begin{equation*}
\mu-\varepsilon_{\mathrm{F}}=-\frac{\pi^{2}}{6} T^{2} \frac{1}{g(\mu)} \frac{d g(\mu)}{d \mu} . \tag{3.67}
\end{equation*}
$$

Note that the change is quadratic in $T$ and negative, in agreement with the numerical results shown with the red line in Fig. 1. Plugging this expression (which is only valid when the magnitude of the change is much smaller than $\varepsilon_{\mathrm{F}}$ ) into Eq. (66), we finally get the finite-temperature correction to energy:

$$
\begin{equation*}
E(T)-E(0)=\frac{\pi^{2}}{6} g(\mu) T^{2} \tag{3.68}
\end{equation*}
$$

where within the accuracy of our approximation, $\mu$ may be replaced with $\varepsilon_{\mathrm{F}}$. (Due to the universal relation (48), Eq. (68) also gives the temperature correction to pressure.) Now we may use Eq. (68) to calculate the heat capacity of the degenerate Fermi gas:

$$
\begin{equation*}
C_{V} \equiv\left(\frac{\partial E}{\partial T}\right)_{V}=\gamma T, \quad \gamma=\frac{\pi^{2}}{3} g\left(\varepsilon_{\mathrm{F}}\right) . \tag{3.69}
\end{equation*}
$$

According to Eq. (55b), in the particular case of a 3D gas with the isotropic and parabolic dispersion law (3), Eq. (69) reduces to

[^858]\[

$$
\begin{equation*}
\gamma=\frac{\pi^{2}}{2} \frac{N}{\varepsilon_{\mathrm{F}}}, \text { i.e. } C_{V}=\frac{\pi^{2}}{2} N \frac{T}{\varepsilon_{\mathrm{F}}} \ll N . \tag{3.70}
\end{equation*}
$$

\]

This important result deserves a discussion. First, note that within the range of validity of the Sommerfeld approximation ( $T \ll \varepsilon_{\mathrm{F}}$ ), the specific heat of the degenerate gas is much smaller than that of the classical gas, even without internal degrees of freedom, $C_{V}=(3 / 2) N$-see Eq. (19). The reason for such a small heat capacity is that particles deep inside the Fermi sea cannot pick up thermal excitations with available energies of the order of $T \ll \varepsilon_{\mathrm{F}}$, because all states around them are already occupied. The only particles (or rather quantum states) that may be excited with such small energies are those at the very Fermi surface, more exactly within a surface layer of thickness $\Delta \varepsilon \sim T \ll \varepsilon_{\mathrm{F}}$, and Eq. (69) presents a very vivid expression of this fact.

The second important feature of Eqs. (69)-(70) is the linear dependence of the heat capacity on temperature, which decreases with a reduction of $T$ much slower than that of crystal vibrations - see Eq. (2.99) and it discussion. This means that in metals the specific heat at temperatures $T \ll T_{\mathrm{D}}$ is dominated by the conduction electrons. Indeed, experiments confirm not only the linear dependence (70) of the specific heat, ${ }^{28}$ but also the values of the proportionality coefficient $\gamma \equiv C_{V} / T$ for cases when $\varepsilon_{\mathrm{F}}$ can be calculated independently, for example for alkali metals - see the right two columns of Table 1. More typically, Eq. (69) is used for the experimental measurement of the density of states on the Fermi surface, $g\left(\varepsilon_{\mathrm{F}}\right)$ - the factor which participates in many theoretical results, in particular in transport properties of degenerate Fermi gases (see Chapter 6 below).

### 3.4. Bose-Einstein condensation

Now let us explore what happens at cooling of an ideal gas of bosons. Figure 3a shows on a more appropriate, log-log scale, the same plot as Fig. 1b, i.e. the numerical solution of Eq. (47) with the appropriate (negative) sign in the denominator. One can see that that the chemical potential $\mu$ indeed tends to zero at some finite "critical temperature" $T_{c}$. This temperature may be found by taking $\mu=0$ in Eq. (47), which is then reduced to a table integral: ${ }^{29}$

$$
\begin{equation*}
T_{c}=T_{0}\left[\frac{1}{\sqrt{2} \pi^{2}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi}-1}\right]^{-2 / 3}=T_{0}\left[\frac{1}{\sqrt{2} \pi^{2}} \Gamma\left(\frac{3}{2}\right) \zeta\left(\frac{3}{2}\right)\right]^{-2 / 3} \approx 3.313 T_{0} \tag{3.71}
\end{equation*}
$$

the result explaining the $T_{c} / T_{0}$ ratio mentioned in Sec. 2.
Hence we must have a good look at the temperature interval $0<T<T_{c}$, which may look rather mysterious. Indeed, within this range, chemical potential $\mu$ cannot be either negative or zero, because then Eq. (41) would give a value of $N$ fewer than the number of particles we actually have. On the other hand, $\mu$ cannot be positive either, because integral (41) would diverge at $\varepsilon \rightarrow \mu$ due to the divergence of $\langle N(\varepsilon)\rangle$ - see, e.g., Fig. 2.15. The only possible resolution of the paradox, suggested by A. Einstein, is as follows: at $T<T_{c}$, the chemical potential of each particle still equals exactly zero, but a certain number

[^859]( $N_{0}$ of $N$ ) of them are in the ground state (with $\varepsilon \equiv p^{2} / 2 m=0$ ), forming the so-called Bose-Einstein condensate, very frequently referred to as BEC.

(a)


Fig. 3.3. The Bose-Einstein condensation: (a) chemical potential of the gas and (b) its pressure, as functions of temperature. The dashed line corresponds to the classical gas.

Since the condensate particles do not contribute to Eq. (41) (because of the factor $\varepsilon^{1 / 2}=0$ ), their number $N_{0}$ may be calculated by using Eq. (44), with $\mu=0$, to find the number ( $N-N_{0}$ ) of particles still remaining in the gas, i.e. having energy $\varepsilon>0$ :

$$
\begin{equation*}
N-N_{0}=\frac{g V(m T)^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi}-1} . \tag{3.72}
\end{equation*}
$$

This result is even simpler than it may look. Indeed, let us write it for case $T=T_{c}$, when $N_{0}=0: 30$

$$
\begin{equation*}
N=\frac{g V\left(m T_{c}\right)^{3 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{1 / 2} d \xi}{e^{\xi}-1} . \tag{3.73}
\end{equation*}
$$

Since the dimensionless integrals in both equations are similar, we may just divide them, getting an extremely simple and elegant result:

$$
\begin{equation*}
\frac{N-N_{0}}{N}=\left(\frac{T}{T_{c}}\right)^{3 / 2}, \quad \text { so that } \quad N_{0}=N\left[1-\left(\frac{T}{T_{c}}\right)^{3 / 2}\right], \quad \text { at } T \leq T_{c} . \tag{3.74a}
\end{equation*}
$$

Please note that this result is only valid for the particles whose motion, within volume $V$, is free in other words, for the particles trapped in a rigid-wall box of volume $V$. In typical experiments with the Bose-Einstein condensation of diluted gases of neutral (and hence weakly interacting) atoms, particles

[^860]are trapped at the bottom of a "soft" potential well, which may be well approximated by a 3D quadratic parabola: $U(\mathbf{r})=m \omega^{2} r^{2} / 2$. It is straightforward to show (and hence left for reader's exercise) that in this case the temperature dependence of $N_{0}$ is somewhat different:
\[

$$
\begin{equation*}
N_{0}=N\left[1-\left(\frac{T}{T_{c}^{*}}\right)^{3}\right], \quad \text { at } T \leq T_{c}^{*} \tag{3.74b}
\end{equation*}
$$

\]

where $T_{c}{ }^{*}$ is a critical temperature that depends on $\hbar \omega$, i.e. the confining potential's "steepness", rather than on the gas' volume (which in this case is not fixed). Figure 4 shows one of the first sets of experimental data for the Bose-Einstein condensation of dilute gases of neutral atoms. Taking into account the finite number of particles in the experiment, the agreement with the simple theory is surprisingly good.


Fig. 3.4. Total number $N$ of trapped ${ }^{87} \mathrm{Rb}$ atoms (inset) and their ground-state fraction $N_{0} / N$, as functions of the ratio $T / T_{c}$, as measured by J. Ensher et al., Phys. Rev. Lett. 77, 4984 (1996). In this experiment, $T_{c}{ }^{*}$ was as low as $0.28 \times 10^{-6} \mathrm{~K}$. The solid line shows the simple theoretical dependence $N(T)$, given by Eq. (74b), while other lines correspond to more complex theories taking into account the finite number $N$ of trapped atoms. © 1996 APS.

Now returning to the rigid-wall box model, let us explore what happens at the critical temperature and below it with other gas parameters. Equation (52) with the appropriate (lower) sign shows that approaching this point from higher temperatures, gas energy and hence its pressure do not vanish (Fig. 3b). Indeed, at $T=T_{\mathrm{c}}$ (where $\mu=0$ ), that equation yields ${ }^{31}$

$$
\begin{equation*}
E\left(T_{c}\right)=g V \frac{m^{3 / 2} T_{c}^{5 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{3 / 2} d \xi}{e^{\xi}-1}=g V \frac{m^{3 / 2} T_{c}^{5 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \Gamma\left(\frac{5}{2}\right) \zeta\left(\frac{5}{2}\right)=\frac{3}{2} \frac{\zeta(5 / 2)}{\zeta(3 / 2)} N T_{c} \approx 0.7701 N T_{c}, \tag{3.75}
\end{equation*}
$$

so that using the universal relation (48), we get a pressure value,

$$
\begin{equation*}
P\left(T_{c}\right)=\frac{2}{3} \frac{E\left(T_{c}\right)}{V}=\frac{\zeta(5 / 2)}{\zeta(3 / 2)} \frac{N}{V} T_{c} \approx 0.5134 \frac{N}{V} T_{c} \approx 1.701 P_{0}, \tag{3.76}
\end{equation*}
$$

which is somewhat lower than, but comparable to $P(0)$ for the fermions - cf. Eq. (57). Now we can use the same Eq. (52), also with $\mu=0$, to calculate the energy of the gas at $T<T_{\mathrm{c}}$,

[^861]\[

$$
\begin{equation*}
E(T)=g V \frac{m^{3 / 2} T^{5 / 2}}{\sqrt{2} \pi^{2} \hbar^{3}} \int_{0}^{\infty} \frac{\xi^{3 / 2} d \xi}{e^{\xi}-1} \tag{3.77}
\end{equation*}
$$

\]

Comparing this relation with the first form of Eq. (75), which features the same integral, we immediately get one more simple temperature dependence:

$$
\begin{equation*}
E(T)=E\left(T_{c}\right)\left(\frac{T}{T_{c}}\right)^{5 / 2}, \quad \text { at } T \leq T_{c} \tag{3.78}
\end{equation*}
$$

From the universal relation (48), we immediately see that pressure follows the same dependence:

$$
\begin{equation*}
P(T)=P\left(T_{c}\right)\left(\frac{T}{T_{c}}\right)^{5 / 2}, \quad \text { at } T \leq T_{c} \tag{3.79}
\end{equation*}
$$

This temperature dependence of pressure is shown with the blue line in Fig. 3b. The plot shows that for all temperatures (both below and above $T_{c}$ ) the pressure of bosonic gas is below that of the classical gas of the same density. Note also that since, according to Eqs. (57) and (76), $P\left(T_{c}\right) \propto P_{0} \propto V^{5 / 3}$, while, according to Eqs. (37) and (71), $T_{c} \propto T_{0} \propto V^{2 / 3}$, pressure (79) does not depend on volume at all! The physics of this result (that is valid at $T<T_{\mathrm{c}}$ only) is that as we decrease the volume at fixed total number of particles, more and more of them go to the condensate, decreasing the number $\left(N-N_{0}\right)$ of particles in the gas phase, but not changing its pressure. Such behavior is very typical for phase transitions - see, in particular, the next chapter.

The last thermodynamic variable of major interest is the heat capacity, because it may be readily measured in many systems. For temperatures $T \leq T_{c}$, it may be easily calculated from Eq. (78):

$$
\begin{equation*}
C_{V}(T) \equiv\left(\frac{\partial E}{\partial T}\right)_{N, V}=E\left(T_{c}\right) \frac{5}{2} \frac{T^{3 / 2}}{T_{c}^{5 / 2}} \tag{3.80}
\end{equation*}
$$

so that below $T_{c}$, the capacity increases, at the critical temperature reaching the value,

$$
\begin{equation*}
C_{V}\left(T_{c}\right)=\frac{5}{2} \frac{E\left(T_{c}\right)}{T_{c}} \approx 1.925 \mathrm{~N} \tag{3.81}
\end{equation*}
$$

which is approximately $28 \%$ above that ( $3 N / 2$ ) of the classical gas - in both cases ignoring the possible contributions from the internal degrees of freedom. The analysis for $T \geq T_{c}$ is a little bit more cumbersome, because differentiating $E$ over temperature - say, using Eq. (52) - one should also take into account the temperature dependence of $\mu$ that follows from Eq. (40) - see also Fig. 1b. However, the most important feature of the result may be predicted without the calculation (which is being left for reader's exercise). Since at $T \gg T_{c}$ the heat capacity has to approach the classical value, it must decrease at $T>T_{c}$, thus forming a sharp maximum (a "cusp") at the critical point $T=T_{c}-$ see Fig. 5.

Such a cusp is good indication of the Bose-Einstein condensation in virtually any experimental system, especially because inter-particle interactions (unaccounted for in our simple discussion) typically make this feature even more substantial, turning it into a weak (logarithmic) singularity. Historically, such a singularity (called the $\lambda$-point because of the characteristic shape of the $C_{V}(T)$ dependence) was the first noticed, though not immediately understood sign of the Bose-Einstein condensation, observed in 1931 by W. Keesom and K . Clusius in liquid ${ }^{4} \mathrm{He}$ at $T=T_{c} \approx 2.17 \mathrm{~K}$. Other milestones of the Bose-Einstein condensation studies include:

- the experimental discovery of superconductivity in metals, by H. Kamerlingh-Onnes in 1911;
- the development of the Bose-Einstein statistics implying the condensation, in 1924-1925;
- the discovery of superfluidity in liquid ${ }^{4} \mathrm{He}$ by P. Kapitza and (independently) by J. Allen and D. Misener in 1937, and its explanation as a result of the Bose-Einstein condensation by F. and H. Londons and L. Titza, with further elaborations by L. Landau (all in 1938);
- the explanation of superconductivity as the result of formation of Cooper pairs of electrons, with an integer total spin, with the simultaneous Bose-Einstein condensation of such effective bosons, by J. Bardeen, L. Cooper, and J. Schrieffer in 1957;
-the discovery of superfluidity of two different phases of ${ }^{3} \mathrm{He}$, due to the similar Bose-Einstein condensation of pairs of its fermion atoms, by D. Lee, D. Osheroff, and R. Richardson in 1972;
- the first observation of the Bose-Einstein condensation in dilute gases $\left({ }^{87} \mathrm{Ru}\right.$ by E. Cornell, C. Wieman et al. and ${ }^{23} \mathrm{Na}$ by W. Ketterle et al.) in 1995.


Fig. 3.5. Temperature dependences of the heat capacity of an ideal Bose-Einstein gas, calculated from Eqs. (52) and (40) for $T \geq T_{c}$, and from Eq. (80) for $T \leq T_{c}$.

The importance of the last achievement (and of the continuing intensive work in this direction ${ }^{32}$ ) stems from the fact that in contrast to other Bose-Einstein condensates, in dilute gases (with the typical density $n$ as low as $\sim 10^{14} \mathrm{~cm}^{-3}$ ) the particles interact very weakly, and hence many experimental results are very close to the simple theory described above and its straightforward elaborations - see, e.g., Fig. 4. On the other hand, the importance of prior implementations of the Bose-Einstein condensates, which involve more complex and challenging physics, should not be underestimated - as it sometimes is.

The most important feature of any Bose-Einstein condensate is that all $N_{0}$ condensed particles are in the same quantum state, and hence are described by exactly the same wavefunction. This wavefunction is substantially less "feeble" than that of a single particle - in the following sense. In the second quantization language, ${ }^{33}$ the well-known Heisenberg's uncertainty relation may be rewritten for the creation/annihilation operators; in particular, for bosons,

$$
\begin{equation*}
\left[\hat{a}, \hat{a}^{\dagger}\right]=1 \tag{3.82}
\end{equation*}
$$

[^862]Since $\hat{a}$ and $\hat{a}^{\dagger}$ are quantum-mechanical operators of the complex amplitude $a=A \exp \{i \varphi\}$ and its complex conjugate $a^{*}=A \exp \{-i \varphi\}$, where $A$ and $\varphi$ are real amplitude and phase of the wavefunction. Equation (82) yields the following approximate uncertainty relation (strict in the limit $\delta \varphi \ll 1$ ) between the number of particles $N=A A^{*}$ and phase $\varphi$

$$
\begin{equation*}
\delta N \delta \varphi \geq 1 / 2 \tag{3.83}
\end{equation*}
$$

This means that a condensate of $N \gg 1$ bosons may be in a state with both phase and amplitude of the wavefunction behaving virtually as $c$-numbers, with negligible relative uncertainties: $\delta N \ll N$, $\delta \varphi \ll 1$. Moreover, such states are much less susceptible to perturbations by experimental instruments. For example, the supercurrent $I_{S}$ carried along a superconducting wires by a coherent Bose-Einstein condensate of Cooper pairs may be as high as hundreds of amperes. As a result, the "strange" behaviors predicted by the quantum mechanics are not averaged out as in the usual particle ensembles (see, e.g., the discussion of the density matrix in Sec. 2.1), but may be directly revealed in macroscopic, measurable behaviors of the condensate.

For example, density $\mathbf{j}_{S}$ of the supercurrent may be described by the same formula as the usual probability current density of a single particle, ${ }^{34}$ multiplied by the Cooper pair density $n$ and the electric charge $q=-2 e$ of a single pair:

$$
\begin{equation*}
\mathbf{j}_{S}=q n \frac{\hbar}{m}\left(\nabla \varphi-\frac{q}{\hbar} \mathbf{A}\right), \tag{3.84}
\end{equation*}
$$

where $\mathbf{A}$ is the vector-potential of the (electro)magnetic field. If a superconducting wire is not extremely thin, current flow does not penetrate its interior, ${ }^{35}$ so that $\mathbf{j}_{S}$ may be taken for zero. As a result, the integral of Eq. (84), taken along a contour inside a closed wire loop yields

$$
\begin{equation*}
\frac{q}{\hbar} \oint_{C} \mathbf{A} \cdot d \mathbf{r}=\Delta \varphi=2 \pi m \tag{3.85}
\end{equation*}
$$

where $m$ is an integer. But, according to electrodynamics, the integral participating in this equation is nothing more than flux $\Phi$ of the magnetic field $\mathcal{B}$ piercing the wire loop area $A$. Thus we immediately arrive at the famous magnetic flux quantization effect

$$
\begin{equation*}
\Phi \equiv \int_{A} \mathcal{B}_{n} d^{2} r=m \Phi_{0}, \quad \Phi_{0} \equiv \frac{2 \pi \hbar}{|q|}=\frac{h}{2 e} \approx 2.07 \times 10^{-15} \mathrm{~Wb} \tag{3.86}
\end{equation*}
$$

which was theoretically predicted in 1950 and experimentally observed in 1961. Most fantastically, this effect holds true even in very large loops, sustained by the Bose-Einstein condensate of Cooper pairs, "coherent over miles of dirty lead wire", citing J. Bardeen's famous expression.

Other prominent examples of such macroscopic quantum effects in Bose-Einstein condensates include not only the superfluidity and superconductivity as such, but also the Josephson effect,

[^863]quantized Abrikosov vortices, etc. Some of these effects are briefly discussed in other parts of this series. ${ }^{36}$

### 3.5. Gases of weakly interacting particles

Now let us discuss the weak particle interaction effects on macroscopic properties of their gas. (Unfortunately, I will have time to do that only for a brief discussion of these effects in classical gases of indistinguishable particles. ${ }^{37}$ )

In most cases of interest, particle interaction may be described by certain potential energy $U$, so that the total energy is

$$
\begin{equation*}
E=\sum_{k=1}^{N} \frac{p_{k}^{2}}{2 m}+U\left(\mathbf{r}_{1}, . ., \mathbf{r}_{j}, \ldots, \mathbf{r}_{N}\right) \tag{3.87}
\end{equation*}
$$

where $\mathbf{r}_{k}$ is the position of $k^{\text {th }}$ particle's center. Let us see how far would the statistical physics allow us to proceed for an arbitrary potential $U$. For $N \gg 1$, at the calculation of the Gibbs statistical sum (2.59), we may perform the usual transfer from the summation over all quantum states of the system to integration over the 6 N -dimensional space, with the correct Boltzmann counting:

$$
\begin{align*}
Z & =\sum_{m} e^{-E_{m} / T} \rightarrow \frac{1}{N!} \frac{g^{N}}{(2 \pi \hbar)^{3 N}} \int \exp \left\{-\sum_{k=1}^{N} \frac{p_{j}^{2}}{2 m T}\right\} d^{3} p_{1} \ldots d^{3} p_{N} \int \exp \left\{-\frac{U\left(\mathbf{r}_{1}, \ldots \mathbf{r}_{N}\right)}{T}\right\} d^{3} r_{1} \ldots d^{3} r_{N} \\
& =\left(\frac{1}{N!} \frac{g^{N} V^{N}}{(2 \pi \hbar)^{3 N}} \int \exp \left\{-\sum_{k=1}^{N} \frac{p_{j}^{2}}{2 m T}\right\} d^{3} p_{1} \ldots d^{3} p_{N}\right) \times\left(\frac{1}{V^{N}} \int \exp \left\{-\frac{U\left(\mathbf{r}_{1}, \ldots \mathbf{r}_{N}\right)}{T}\right\} d^{3} r_{1} \ldots d^{3} r_{N}\right) \tag{3.88}
\end{align*}
$$

But according to Eq. (14), the first operand in the last product is the statistical sum of an ideal gas (with the same $g, N, V$, and $T$ ), so that we may use Eq. (2.63) to write

$$
\begin{equation*}
F=F_{\text {ideal }}-T \ln \left[\frac{1}{V^{N}} \int d^{3} r_{1} \ldots d^{3} r_{N} e^{-U / T}\right]=F_{\text {ideal }}-T \ln \left[1+\frac{1}{V^{N}} \int d^{3} r_{1} \ldots d^{3} r_{N}\left(e^{-U / T}-1\right)\right], \tag{3.89}
\end{equation*}
$$

where $F_{\text {ideal }}$ is the free energy of the ideal gas (i.e. the same gas but with $U=0$ ), given by Eq. (16).
I believe that Eq. (89) is a very convincing demonstration of the enormous power of the statistical physics. Instead of trying to solve an impossibly complex problem of classical dynamics of $N$ >> 1 (think of $N \sim 10^{23}$ ) interacting particles, and calculating appropriate ensemble averages later on, the Gibbs approach reduces finding the free energy (and then, from thermodynamic relations, all other thermodynamic variables) to the calculation of just one integral in its right-hand part of Eq. (89). Still, this integral is 3 N -dimensional and may be worked out analytically only if particle interaction is weak in some sense. Indeed, the last form of Eq. (89) makes its especially evident that if $U \rightarrow 0$ everywhere, the term in parentheses under the integral vanishes, and so does the integral itself, and hence the addition to $F_{\text {ideal }}$.

[^864]Now let us see what would this integral yield for the simplest, short-range interactions, in which potential $U$ is substantial only when the mutual distance $\mathbf{r}_{j j^{\prime}} \equiv \mathbf{r}_{j}-\mathbf{r}_{j^{\prime}}$, between particle centers is smaller than certain value $2 r_{0}$, where $r_{0}$ may be interpreted as the particle size scale. If the gas in sufficiently dilute, so that the particle radius $r_{0}$ is much smaller than the average distance $r_{\mathrm{A}}$ between the particles, the integral in Eq. (89) is of the order of $\left(2 r_{0}\right)^{3 N}$, i.e. much smaller than $r_{A}{ }^{3 N} \sim V^{N}$. Then we may expand the logarithm in Eq. (89) into the Taylor series with respect to the small second term in the square brackets, and keep just the first term of the series:

$$
\begin{equation*}
F \approx F_{\text {ideal }}-\frac{T}{V^{N}} \int d^{3} r_{1} \ldots d^{3} r_{N}\left(e^{-U / T}-1\right) \tag{3.90}
\end{equation*}
$$

Even more importantly, if the gas density is so low that the chances for 3 or more particles to come close to each other and interact (collide) are very small, pair collisions are the most important. In this case, we may recast the integral in Eq. (90) as a sum of $N(N-1) / 2 \approx N^{2} / 2$ similar terms describing such pair interactions, each of the type

$$
\begin{equation*}
V^{N-2} \int\left(e^{-U\left(\mathbf{r}_{k k^{\prime}}\right) / T}-1\right) d^{3} r_{k} d^{3} r_{k^{\prime}} \tag{3.91}
\end{equation*}
$$

It is convenient to think about $\mathbf{r}_{k k^{\prime}}$ as the radius-vector of particle $k$ in the reference frame with the origin placed at particle $k$ ' - see Fig. 6a.


Fig. 3.6. The definition of interparticle distance vectors at their (a) pair and (b) triple interactions.

Then it is clear that in Eq. (91), we may first calculate the integral over $\mathbf{r}_{k}$, while keeping the distance vector $\mathbf{r}_{k k^{\prime}}$, and hence $U\left(\mathbf{r}_{k k^{\prime}}\right)$, constant, getting one more factor $V$. Moreover, since all particle pairs are similar, in the remaining integral over $\mathbf{r}_{k k^{\prime}}$ we may drop the radius-vector index, so that Eq. (90) becomes

$$
\begin{equation*}
F=F_{\text {ideal }}-\frac{T}{V^{N}} \frac{N^{2}}{2} V^{N-1} \int\left(e^{-U(\mathbf{r}) / T}-1\right) d^{3} r=F_{\text {ideal }}+\frac{T}{V} N^{2} B(T), \tag{3.92}
\end{equation*}
$$

where $B(T)$, called the second virial coefficient, ${ }^{38}$ has an especially simple form for sphericallysymmetric interactions:

[^865]\[

$$
\begin{equation*}
B(T) \equiv \frac{1}{2} \int\left(1-e^{-U(\mathbf{r}) / T}\right) d^{3} r \rightarrow \frac{1}{2} \int_{0}^{\infty} 4 \pi r^{2} d r\left(1-e^{-U(r) / T}\right) . \tag{3.93}
\end{equation*}
$$

\]

From Eq. (92), and the second of the thermodynamic relations (1.35), we already can already tell something important about the equation of state:

$$
\begin{equation*}
P=-\left(\frac{\partial F}{\partial V}\right)_{T, N}=P_{\text {ideal }}+\frac{N^{2} T}{V^{2}} B(T)=T\left[\frac{N}{V}+B(T) \frac{N^{2}}{V^{2}}\right] \tag{3.94}
\end{equation*}
$$

We see that at a fixed gas density $n=N / V$, the pair interaction creates additional pressure, proportional to $(N / V)^{2}=n^{2}$ and a function of temperature, $B(T) T$.

Let us calculate $B(T)$ for a couple of simple models of particle interactions. Solid line in Fig. 7 shows (schematically) a typical form of the interaction potential between electrically neutral molecules with zero spontaneous electric dipole momentum.


Fig. 3.7. Pair interaction of particles. Solid line: a typical interaction potential; dashed line: its hardball model (95); dash-dotted line: the improved model (97) - schematically. The inset illustrates the idea of the hardball model.

At large distances the interaction of particles that do not their own permanent electrical dipole moment $\mathbf{p}$, is dominated by the attraction (the so-called London dispersion force) between correlated components of the spontaneously induced dipole moments, giving $U(r) \rightarrow r^{-6}$ at $r \rightarrow \infty$. ${ }^{39}$ At closer distances the potential is always repulsive $(U>0)$ and growing very fast at $r \rightarrow 0$, but its quantitative form is specific for each particular molecule. ${ }^{40}$ The crudest description of such repulsion is given by the so-called hardball model:

[^866]\[

U(r)= $$
\begin{cases}+\infty, & \text { for } 0<r<2 r_{0},  \tag{3.95}\\ 0, & \text { for } 2 r_{0}<r<\infty,\end{cases}
$$
\]

- see the dashed line and inset in Fig. 7. According to Eq. (93), in this model the second virial coefficient is temperature-independent:

$$
\begin{equation*}
B(T)=b \equiv \frac{1}{2} \int_{0}^{2 r_{0}} 4 \pi r^{2} d r=\frac{2 \pi}{3}\left(2 r_{0}\right)^{3}, \tag{3.96}
\end{equation*}
$$

(and is 4 times larger than the hardball volume $V_{0}=(4 \pi / 3) r_{0}{ }^{3}$ ), so that the equation of state (94) still gives a linear dependence of pressure on temperature.

A correction to this result may be obtained by the following approximate account of the longrange attraction (see the dash-dotted line in Fig. 7):41

$$
U(r)= \begin{cases}+\infty, & \text { for } 0<r<2 r_{0},  \tag{3.97}\\ U(r), & \text { with }|U| \ll T, \\ \text { for } 2 r_{0}<r<\infty,\end{cases}
$$

which is sometimes called the hard core model. Then Eq. (93) yields:

$$
\begin{equation*}
B(T)=b+\frac{1}{2} \int_{2 r_{0}}^{\infty} 4 \pi r^{2} d r \frac{U(r)}{T}=b-\frac{a}{T}, \quad \text { with } a \equiv 2 \pi \int_{2 r_{0}}^{\infty} r^{2} d r|U(r)| . \tag{3.98}
\end{equation*}
$$

In this model, the equation of state (94) acquires a temperature-independent term:

$$
\begin{equation*}
P=T\left[\frac{N}{V}+\left(\frac{N}{V}\right)^{2}\left(b-\frac{a}{T}\right)\right] . \tag{3.99}
\end{equation*}
$$

Still, the correction to the ideal-gas pressure is proportional to $(N / V)^{2}$, and has to be relatively small for Eq. (99) to be valid, so that the right-hand part of Eq. (99) may be considered as the sum of two leading terms in the general expansion of $P$ into the Taylor series in low density $n=N / V$ of the gas:

$$
\begin{equation*}
P=T\left[\frac{N}{V}+B(T)\left(\frac{N}{V}\right)^{2}+C(T)\left(\frac{N}{V}\right)^{3}+\ldots\right] \tag{3.100}
\end{equation*}
$$

where $C(T)$ is called the third virial coefficient. It is natural to ask how can we calculate $C(T)$ and the higher virial coefficients.

Generally, this may be done just by a careful analysis of Eq. (90), ${ }^{42}$ but I would like to use this occasion to demonstrate a different, very interesting approach, called the cluster expansion method, ${ }^{43}$

[^867]which allows to streamline such calculations. Let us apply to our system, with energy (87), the grand canonical distribution. (Just as in Sec. 2, we may argue that if the average number $\langle N\rangle$ of particles in a member of a grand canonical ensemble, with fixed $\mu$ and $T$, is much larger than 1 , the relative fluctuations of that number are small, so that all its thermodynamic properties should be similar to those when $N$ is exactly fixed - as it is assumed when applying the Gibbs distribution valid for the canonical ensemble.) For our case, the grand canonical distribution, Eq. (2.109), may be recast as
\[

$$
\begin{equation*}
\Omega=-T \ln \sum_{N=0}^{\infty} Z_{N}, \quad Z_{N} \equiv e^{\mu N / T} \sum_{m} e^{-E_{m, N} / T}, \quad E_{m, N}=\sum_{k=1}^{N} \frac{p_{k}^{2}}{2 m}+U\left(r_{1}, \ldots, r_{N}\right) \tag{3.101}
\end{equation*}
$$

\]

(Notice that here, as always in the grand canonical distribution, $N$ means a particular rather than average number of particles.) Now, let us try to forget for a second that in real systems of interest the number of particles is extremely large, and start to calculate, one by one, the first terms $Z_{N}$.

In the term with $N=0$, both contributions to $E_{m, N}$ vanish, and so does $\mu N / T$, so that $Z_{0}=1$. In the next term, with $N=1$, the interaction term vanishes, so that $E_{m, 1}$ is reduced to kinetic energy of one particle, giving

$$
\begin{equation*}
Z_{1}=e^{\mu / T} \sum_{k} \exp \left\{-\frac{p_{k}^{2}}{2 m T}\right\} \tag{3.102}
\end{equation*}
$$

Making the usual transition from summation to integration, we may write

$$
\begin{equation*}
Z_{1}=Z I_{1}, \quad \text { where } Z \equiv e^{\mu / T} \frac{g V}{(2 \pi \hbar)^{3}} \int \exp \left\{-\frac{p^{2}}{2 m T}\right\} d^{3} p, \quad \text { and } I_{1} \equiv 1 \tag{3.103}
\end{equation*}
$$

This is the same simple (Gaussian) integral as in Eq. (6), giving

$$
\begin{equation*}
Z=e^{\mu / T} \frac{g V}{(2 \pi \hbar)^{3}}(2 \pi m T)^{3 / 2}=e^{\mu / T} g V\left(\frac{m T}{2 \pi \hbar^{2}}\right)^{3 / 2} \tag{3.104}
\end{equation*}
$$

Now let us explore the next term, with $N=2$, which describes, in particular, pair interactions $U=$ $U(\mathbf{r})$, with $\mathbf{r}=\mathbf{r}-\mathbf{r}$ ". Due to the particle indistinguishability, this term needs the "correct Boltzmann counting" factor $1 / 2$ ! - cf. Eqs. (12) and (88):

$$
\begin{equation*}
Z_{2}=e^{2 \mu / T} \frac{1}{2!} \sum_{k, k^{\prime}}\left(\exp \left\{-\frac{p_{k}^{2}}{2 m T}-\frac{p_{k^{\prime}}^{2}}{2 m T}\right\} e^{-U(\mathbf{r}) / T}\right) \tag{3.105}
\end{equation*}
$$

Since $U$ is coordinate-dependent, here the transfer from summation to integration should be done more carefully than in the first term - cf. Eqs. (24) and (88):

$$
\begin{equation*}
Z_{2}=e^{2 \mu / T} \frac{1}{2!} \frac{(g V)^{2}}{(2 \pi \hbar)^{6}} \int \exp \left\{-\frac{p^{2}}{2 m T}\right\} d^{3} p \int \exp \left\{-\frac{p^{\prime 2}}{2 m T}\right\} d^{3} p^{\prime} \times \frac{1}{V} \int e^{-U(\mathbf{r}) / T} d^{3} r \tag{3.106}
\end{equation*}
$$

Comparing this expression with the definition of parameter $Z$ in Eq. (103), we get

[^868]\[

$$
\begin{equation*}
Z_{2}=\frac{Z^{2}}{2!} I_{2}, \quad \text { where } I_{2} \equiv \frac{1}{V} \int e^{-U(\mathbf{r}) / T} d^{3} r \tag{3.107}
\end{equation*}
$$

\]

Acting absolutely similarly, for the third term of the grand canonical sum we may get

$$
\begin{equation*}
Z_{3}=\frac{Z^{3}}{3!} I_{3}, \quad I_{3} \equiv \frac{1}{V^{2}} \int e^{-U\left(\mathbf{r}^{\prime}, \mathbf{r}^{\prime \prime}\right) / T} d^{3} r^{\prime} d^{3} r^{\prime \prime} \tag{3.108}
\end{equation*}
$$

where $\mathbf{r}$ ' and $\mathbf{r}$ " are the vectors characterizing the mutual positions of 3 particles - see Fig. 6b.
These result may be extended by induction to an arbitrary $N$. Plugging the expression for $Z_{N}$ into Eq. (101) and recalling that $\Omega=-P V$, we get the equation of state of the gas in the form

$$
\begin{equation*}
P=\frac{T}{V} \ln \left(1+Z I_{1}+\frac{Z^{2}}{2!} I_{2}+\frac{Z^{3}}{3!} I_{3}+\ldots\right) . \tag{3.109}
\end{equation*}
$$

As a sanity check, at $U=0$, all integrals $I_{N}$ are obviously equal to 1 , the expression under the logarithm in just the Taylor expansion of $e^{Z}$, giving $P=T Z / V$, and $\Omega=-P V=-T Z$. In this case, according to the last of Eqs. (1.62), the average number of particles of particles in the system is $\langle N\rangle=-$ $(\partial \Omega / \partial \mu)_{T, V}=Z$, because since $Z \propto \exp \{\mu / T\}, \partial Z / \partial \mu=Z / T$. Thus, we have happily recovered the equation of state of the ideal gas. ${ }^{44}$

Returning to the general case of nonvanishing interactions, let us assume that the logarithm in Eq. (109) may be also presented as a Taylor series in $Z$ :

$$
\begin{equation*}
P=\frac{T}{V} \sum_{l=1}^{\infty} \frac{J_{l}}{l!} Z^{l} \tag{3.110}
\end{equation*}
$$

(The lower limit of the sum reflects the fact that according to Eq. (109), at $Z=0, P=(T / V) \ln 1=0$.) According to Eq, (1.60), this expansion corresponds to the grand potential

$$
\begin{equation*}
\Omega=-P V=-T \sum_{l=1}^{\infty} \frac{J_{l}}{l!} Z^{l} . \tag{3.111}
\end{equation*}
$$

Again using the last of Eqs. (1.62), we get

Cluster expansion of $\langle N\rangle$

$$
\begin{equation*}
\langle N\rangle=\sum_{l=1}^{\infty} \frac{J_{l}}{(l-1)!} Z^{l} \tag{3.112}
\end{equation*}
$$

This equation, for given $\langle N\rangle$, may be used to find $Z$ and hence for the calculation of the equation of state from Eq. (110). The only remaining conceptual action item is to express coefficients $J_{l}$ via the integrals $I$ participating in expansion (109). This may be done using the well-known Taylor expansion of the logarithm function, ${ }^{45}$

[^869]\[

$$
\begin{equation*}
\ln (1+\xi)=\sum_{l=1}^{\infty}(-1)^{l+1} \frac{\xi^{l}}{n} . \tag{3.113}
\end{equation*}
$$

\]

Using it together with Eq. (109), we get a Taylor series in $Z$, starting as

$$
\begin{equation*}
P=\frac{T}{V}\left(Z+\frac{Z^{2}}{2!}\left(I_{2}-1\right)+\frac{Z^{3}}{3!}\left[\left(I_{3}-1\right)-3\left(I_{2}-1\right)\right]+\ldots\right) . \tag{3.114}
\end{equation*}
$$

Comparing this expression with Eq. (110), we see that

$$
\begin{align*}
J_{1} & =1, \\
J_{2} & =I_{2}-1=\frac{1}{V} \int\left(e^{-U(\mathbf{r}) / T}-1\right) d^{3} r  \tag{3.115}\\
J_{3} & =\left(I_{3}-1\right)-3\left(I_{2}-1\right) \\
& =\frac{1}{V^{2}} \int\left(e^{-U\left(\mathbf{r}^{\prime}, \mathbf{r}^{\prime \prime}\right) / T}-e^{-U\left(\mathbf{r}^{\prime}\right) / T}-e^{-U\left(\mathbf{r}^{\prime \prime}\right) / T}-e^{-U\left(\mathbf{r}^{\prime \prime \prime}\right) / T}+2\right) d^{3} r^{\prime} d^{3} r^{\prime \prime}
\end{align*}
$$

where $\mathbf{r}^{\prime \prime \prime} \equiv \mathbf{r}^{\prime}-\mathbf{r}^{\prime \prime}$ - see Fig. 6 b. The expression of $J_{2}$, describing the pair interactions of particles, is (within a numerical factor) equal to the second virial coefficient $B(T)$ - see Eq. (93). As a reminder, the subtraction of 1 from integral $I_{2}$ in the second of Eqs. (115) makes the contribution of each elementary 3D volume $d^{3} r$ into integral $J_{2}$ nonvanishing only if at this $\mathbf{r}$ two particles interact $(U \neq 0)$. Very similarly, in the last of Eqs. (115), the subtraction of three pair-interaction terms from ( $I_{3}-1$ ) makes the contribution from elementary 6D volume $d^{3} r^{\prime} d^{3} r$ '" into integral $J_{3}$ finite only if at that mutual location of particles all three of them interact simultaneously.

In order to illustrate the cluster expansion method at work, let us eliminate factor $Z$ from the system of equations (110) and (112), keeping (for the sake of simplicity) the terms up to $O\left(Z^{3}\right)$ only, as has been done in Eq. (114):

$$
\begin{align*}
& \frac{P V}{T}=J_{1} Z+\frac{J_{2}}{2} Z^{2}+\frac{J_{3}}{6} Z^{3}+\ldots,  \tag{3.116}\\
& \langle N\rangle=J_{1} Z+J_{2} Z^{2}+\frac{J_{3}}{2} Z^{3}+\ldots \tag{3.117}
\end{align*}
$$

Dividing these two expressions, we get a result,

$$
\begin{equation*}
\frac{P V}{\langle N\rangle T} \approx \frac{1+\left(J_{2} / 2 J_{1}\right) Z+\left(J_{3} / 6 J_{1}\right) Z^{2}}{1+\left(J_{2} / J_{1}\right) Z+\left(J_{3} / 2 J_{1}\right) Z^{2}}=1-\frac{J_{2}}{2 J_{1}} Z+\left(\frac{J_{2}^{2}}{2 J_{1}^{2}}-\frac{J_{3}}{3 J_{1}}\right) Z^{2}+\ldots . \tag{3.118}
\end{equation*}
$$

which is accurate with to terms $O\left(Z^{2}\right)$. In this approximation, we may use Eq. (117), solved for $Z$ with the same accuracy:

$$
\begin{equation*}
Z \approx\langle N\rangle-\frac{J_{2}}{J_{1}}\langle N\rangle^{2} . \tag{3.119}
\end{equation*}
$$

Plugging this expression into Eq. (118), we get expansion (100) with

$$
\begin{equation*}
B(T)=-\frac{J_{2}}{2 J_{1}} V, \quad C(T)=\left(\frac{J_{2}^{2}}{J_{1}^{2}}-\frac{J_{3}}{3 J_{1}}\right) V^{2} . \tag{3.120}
\end{equation*}
$$

The first of these relations, combined with the first two of Eqs. (115), yields, for the $2^{\text {nd }}$ virial coefficient, the same Eq. (93) that was obtained from the Gibbs distribution, while the second one allows us to calculate the $3^{\text {rd }}$ virial coefficient $C(T)$. (Let me leave the calculation of $J_{3}$ and $C(T)$, for the hardball model, for the reader's exercise.) Evidently, a more accurate expansion of Eqs. (110), (112), and (114) may be used to calculate an arbitrary virial coefficient, though starting from the $5^{\text {th }}$ coefficient, such calculations may be completed only numerically even in the simplest hardball model.

### 3.6. Exercise problems

3.1. Use the Maxwell distribution for an alternative (statistical) calculation of the mechanical work performed (per cycle) by the Maxwell-Demon heat engine discussed in Sec. 2.3.

Hint: You may assume the simplest geometry of the engine - see Fig. 2.4.
3.2.* Use the Maxwell distribution to find the damping coefficient $\eta_{P} \equiv-\partial P / \partial u$, where $P$ is pressure excerted by an ideal classical gas on a piston moving with very low velocity $u$, in the simplest geometry shown in Fig. on the right, assuming that collisions of gas
 particles with the piston are elastic.
3.3. An ideal gas of $N \gg 1$ classical particles of mass $m$ is confined in a container of volume $V$. At some moment, a very small hole, of area $A \ll V^{2 / 3}, l^{2}$ (where 1 is the mean free path of the particles) is open in its wall, allowing the particles to escape into the surrounding vacuum. Find the r.m.s. velocity of the escaped particles, assuming that the gas stays in a virtual thermal equilibrium at temperature $T$.
3.4.* For the system analyzed in the previous problem, calculate the law of reduction of the number of particles in time after opening the hole.
3.5. Derive the equation of state of the ideal classical gas from the grand canonical distribution.
3.6. ${ }^{*}$ A round cylinder of radius $R$ and length $L$, containing an ideal classical gas of $N \gg 1$ particles of mass $m$, is rotated about its symmetry axis with angular velocity $\omega$. Assuming that the gas rotates with the cylinder, and is in the thermodynamic equilibrium at temperature $T$,
(i) calculate the gas pressure distribution along its radius, and analyze it temperature dependence,
(ii) neglecting the internal degrees of freedom of the particles, calculate the total energy of the gas and its heat capacity in the high- and low-temperature limits, and
(iii) formulate the conditions of validity of your result in terms of strong inequalities between the following length scales: the quantum correlation length $r_{c} \equiv \hbar /(m T)^{1 / 2}$, the effective particle size $r_{0}$, the average distance $r_{A} \equiv\left(\pi R^{2} L / N\right)^{1 / 3}$ between the particles, and cylinder's radius $R$.

Hint: One of considerations in (iii) should be the role of particle's mean free path.
3.7. Prove that Eq. (22), derived for the change of entropy at mixing of two ideal classical gases of completely distinguishable particles (that had equal densities $N / V$ and temperatures $T$ before mixing) is also valid if particles in each of the initial volumes are identical to each other, but different from those in the counterpart sub-volume. Assume that masses of all the particles are equal.
3.8. $N$ classical, non-interacting, indistinguishable particles of mass $m$ are confined in a parabolic, spherically-symmetric 3D potential well $U(\mathbf{r})=\kappa r^{2} / 2$. Use two different approaches to calculate all major thermodynamic characteristics of the system, in thermal equilibrium at temperature $T$, including its heat capacity. What of the results should be changed if the particles are distinguishable, and how?

Hint: Suggest a reasonable replacement of the notions of volume and pressure for this system.
3.9. Calculate the basic thermodynamic characteristics, including all relevant thermodynamic potentials, specific heat, and the surface tension for an ideal, non-relativistic 2D electron gas with given areal density $n=N / A$ :
(i) at $T=0$, and
(ii) at low but nonvanishing temperatures (to the first substantial order in $T / \varepsilon_{\mathrm{F}} \ll 1$ ),
neglecting the Coulomb interaction effects.
3.10. How does the Fermi statistics of an ideal gas affect the barometric formula (28)?
3.11.* Calculate the free carrier density in a semiconductor with bandgap $\Delta \gg T$, assuming isotropic, parabolic dispersion laws of excitations in its conduction and valence bands.

Hint: In semiconductor physics, the names of conduction and valence bands are used for two adjacent allowed energy bands ${ }^{46}$ that at $T=0$, all states of the valence band are fully occupied by electrons, while the conduction band is completely empty - see Fig. on the right. Within the simple model mentioned in the assignment (which gives a good approximation for semiconductors of the $\mathrm{A}_{3} \mathrm{~B}_{5}$ group, e.g., GaAs) the energy of an electron-like excitation, with its energy in the conduction band, follows the isotropic, parabolic law (3.3), but with the origin at the band edge $\varepsilon_{C}$, and an effective mass $m_{C}$ usually smaller than the free electron mass $m_{e}$. Similarly, the parabolic dispersion law of a single "no-electron"
 excitation (called the hole) in the valence band is offset to the edge of that band, $\varepsilon_{V}$, and corresponds to a negative effective mass $\left(-m_{V}\right)$ - see Fig. on the right:

$$
\varepsilon=\left\{\begin{array}{ll}
\varepsilon_{C}+p^{2} / 2 m_{C}, & \text { for } \varepsilon \geq \varepsilon_{C}, \\
\varepsilon_{V}-p^{2} / 2 m_{V}, & \text { for } \varepsilon \leq \varepsilon_{V},
\end{array} \text { where } \varepsilon_{C}-\varepsilon_{V} \equiv \Delta\right.
$$

The excitations of both types follow the Fermi-Dirac statistics, and (within this simple model) do not interact directly.
3.12.* Using the same energy band model as in the previous problem, calculate the chemical potential and the equilibrium density of electrons and holes in an $n$-doped semiconductor, with $n_{D}$ dopants per unit volume.

[^870]Hint: $n$-doping means placing, into a semiconductor crystal, a relatively small density $n_{D}$ of different atoms, called dopants or donors, which may be easily single-ionized - in the case of donors, giving an additional electron to the semiconductor crystal, with the donor atom becoming a positive ion. As a result, the $n$-doping may be represented as a set of additional electrons with the ground state energy on an additional discrete level $\varepsilon_{D}$ slightly below the
 conduction band edge $\varepsilon_{C}-$ see Fig. on the right.
3.13. ${ }^{*}$ Generalize the solution of the previous problem to the case when the $n$-doping with dopant density $n_{D}$ is complemented with the simultaneous $p$ doping by acceptor atoms, whose energy of accepting an additional electron (and hence the negative ionization) is much less than the bandgap.

Hint: Similarly to the $n$-doping, the effect of $p$-doping may be described as an addition of a discrete electron energy level $\varepsilon_{A}$, slightly above
 the valence band edge $\varepsilon_{V}-$ see Fig. on the right.
3.14. Calculate the paramagnetic response (the Pauli paramagnetism) of a degenerate ideal gas of spin- $1 / 2$ particles to a weak external magnetic field, due to partial spin alignment with the field.
3.15.* Explore the Thomas-Fermi model ${ }^{47}$ of a heavy atom, with nuclear charge $Q=Z e \gg e$, in which the electrons are treated as a degenerate Fermi gas, interacting with each other only via their contribution to the common electrostatic potential $\phi(\mathbf{r})$. In particular, derive the ordinary differential equation obeyed by the radial distribution of the potential, and use it to estimate the effective radius of the atom.
3.16.* Use the Thomas-Fermi model, explored in the previous problem, to calculate the total binding energy of a heavy atom. Compare the result with that for the simpler model, in which the electron-electron interaction is completely ignored.
3.17. Derive the general expressions for the calculation of energy $E$ and chemical potential $\mu$ of a Fermi gas of $N$ non-interacting, indistinguishable, ultra-relativistic particles confined in volume $V .48$ Calculate $E$, and also gas pressure $P$ explicitly in the degenerate gas limit $T \rightarrow 0$. In particular, is Eq. (3.48) of the lecture notes, $P V=(2 / 3) E$, valid in this case?
3.18. Calculate the pressure of an ideal gas of ultra-relativistic, indistinguishable quantum particles, for an arbitrary temperature, as a function of the total energy $E$ of the gas, and its volume $V$. Compare the result with the corresponding relations for the electromagnetic blackbody radiation and an ideal gas of non-relativistic particles.
3.19.* Calculate the speed of sound in an ideal gas of ultra-relativistic fermions of density $n$ at negligible temperature.

[^871]3.20. Calculate the effective latent heat $\Lambda \equiv-N\left(\partial Q / \partial N_{0}\right)_{N, V}$, of the Bose-Einstein condensate evaporation, as a function of temperature $T$. Here $Q$ is the heat absorbed by the (condensate + gas) system as a whole, while $N_{0}$ is the number of particles in the condensate alone.
3.21. ${ }^{*}$ For an ideal Bose gas, calculate the law of the chemical potential disappearance at $T \rightarrow T_{c}$, and use the result to prove that the gas' specific heat $C_{V}$ is a continuous function of temperature at the critical point $T=T_{c}$.
3.22. In Chapter 1 of the lecture notes, several thermodynamic equations involving entropy have been discussed, including the first of Eqs. (1.39):
$$
S=-(\partial G / \partial T)_{P}
$$

If we combine this expression with the fundamental relation (1.56), $G=\mu N$, it looks like that for the Bose-Einstein condensate, whose chemical potential $\mu$ vanishes at temperatures below the critical value $T_{c}$, the entropy should vanish as well. On the other hand, dividing both parts of Eq. (1.19) by $d T$, and assuming that at this temperature change the volume is kept constant, we get

$$
C_{V}=T(\partial S / \partial T)_{V}
$$

If $C_{V}$ is known as a function of temperature, the last equation may be integrated to calculate $S$ :

$$
S=\int_{V=\text { const }} \frac{C_{V}(T)}{T} d T+\text { const. }
$$

For the Bose-Einstein condensate, we have calculated the specific heat to be proportional to $T^{3 / 2}$, so that the integration gives nonvanishing entropy $S \propto T^{3 / 2}$. Explain this paradox.
3.23. The standard approach to the Bose-Einstein condensation, outlined in Sec. 4, may seem to ignore the energy quantization of particles confined in volume $V$. Use the particular case of a cubic confining volume $V=a \times a \times a$ with rigid walls to analyze whether the main conclusions of the standard theory, in particular Eq. (71) for the critical temperature, are affected by such quantization.
3.24. ${ }^{*}$ An ideal 3D Bose gas of $N \gg 1$ non-interacting particles is confined at the bottom of a soft, spherically-symmetric potential well, whose potential may be approximated as $U(\mathbf{r})=m \omega^{2} r^{2} / 2$. Develop the theory of the Bose-Einstein condensation in this system; in particular, prove Eq. (3.74b) of the lecture notes, and calculate the critical temperature $T_{c}{ }^{*}$. Looking at the solution, what is the most straightforward way to detect the condensation?
3.25. Calculate the chemical potential of an ideal 2D gas of spin-0 Bose particles as a function of its areal density $n$ (the number of particles per unit area), and find out whether such a gas can condense at low temperatures.
3.26. ${ }^{*}$ Use Eqs. (115) and (120) to calculate the third virial coefficient $C(T)$ for the hardball model of particle interactions.

## Chapter 4. Phase Transitions

This chapter is a brief discussion of coexistence between different states ("phases") of collections of the same particles, and the laws of transitions between these phases. Due to the complexity of these phenomena, which involve interaction of the particles, quantitative results have been obtained only for a few very simple models, typically giving only a very approximate description of real systems.

### 4.1. First-order phase transitions

From everyday experience, say with ice, water, and water vapor, we know that one chemical substance (i.e. a set of many similar particles) may exist in several stable states - phases. A typical substance may have:
(i) a dense solid phase, in which interatomic forces keep all atoms in fixed relative positions, with just small thermal fluctuations about them;
(ii) a liquid phase, of comparable density, in which the relative distances between atoms or molecules are almost constant, but the particles are free to move about each other, and
(iii) the gas phase, typically of a much lower density, in which the molecules are virtually free to move all around the containing volume. ${ }^{1}$

Experience also tells us that at certain conditions, two phases may be in thermal and chemical equilibrium - say, ice floating on water, with temperature at the freezing point. Actually, in Sec. 3.4 we already discussed a qualitative theory of one such equilibrium, the Bose-Einstein condensate coexistence with the uncondensed "vapor" of similar particles. However, this is a rather rare case when the phase coexistence is due to the quantum nature of particles (bosons) that may not interact directly. Much more frequently, the formation of different phases, and transitions between them, is an essentially classical effect due to particle interactions.

Phase transitions are sometimes classified by their order. ${ }^{2}$ I will start my discussion with the first-order phase transitions that feature non-vanishing latent heat $\Lambda$ - the amount of heat that is necessary to give to one phase in order to turn it into another phase, even if temperature and pressure are kept constant. ${ }^{3}$ Let us discuss the most simple and popular phenomenological model of the first-order phase transition, suggested in 1873 by J. van der Waals.

In the last chapter, we have derived Eq. (3.99) for the classical gas of weakly interacting particles, which takes into account (albeit approximately) both interaction components necessary for a

[^872]realistic discussion of gas condensation - the long-range attraction of the particles and their short-range repulsion. Let us rewrite that result as follows:
\[

$$
\begin{equation*}
P+a \frac{N^{2}}{V^{2}}=\frac{N T}{V}\left(1+\frac{N b}{V}\right) \tag{4.1}
\end{equation*}
$$

\]

As we saw in Sec. 3.5, the physical meaning of constant $b$ is the effective volume of space taken by a particle pair collision. Equation (1) is quantitatively valid only if the second term in the parentheses is small, $N b \ll V$, i.e. if the total volume excluded from particles' free motion because of their collisions is much smaller than the whole volume $V$ of the system. In order to describe the condensed phase (which I will call "liquid"), ${ }^{4}$ we need to generalize this relation to the case $N b \sim V$. Since the effective volume left for particles' motion is $V-N b$, it is very natural to make the following replacement: $V \rightarrow V-N b$, in the ideal gas' equation of state. If we still keep the term $a N^{2} / V^{2}$, which describes the long-range attraction of particles, we get the van der Waals equation

$$
\begin{equation*}
P+a \frac{N^{2}}{V^{2}}=\frac{N T}{V-N b} \tag{4.2}
\end{equation*}
$$

Van der Waals equation

The advantage of this simple model is that in the rare gas limit, $N b \ll V$, it reduces back to Eq. (1). (To check this, it is sufficient to Taylor-expand the right-hand part of Eq. (2) in small parameter $N b / V \ll 1$, and retain only two leading terms corresponding to two first virial coefficients.) Let us explore properties of this model.

It is frequently convenient to discuss any equation of state in terms of its isotherms, i.e. $P(V)$ curves plotted at constant $T$. As Eq. (2) shows, in the van der Waals model such a plot depends on 4 parameters ( $a, b, N$, and $T$.) However, for its analysis it is convenient to introduce dimensionless variables: pressure $p \equiv P / P_{c}$, volume $v \equiv V / V_{c}$, and temperature $t \equiv T / T_{c}$, normalized to their so-called critical values,

$$
\begin{equation*}
P_{c} \equiv \frac{1}{27} \frac{a}{b^{2}}, \quad V_{c} \equiv 3 N b, \quad T_{c} \equiv \frac{8}{27} \frac{a}{b} . \tag{4.3}
\end{equation*}
$$

In these notations, Eq. (2) acquires the following form,

$$
\begin{equation*}
\left(p+\frac{3}{v^{2}}\right)=\frac{8 t}{(3 v-1)} \tag{4.4}
\end{equation*}
$$

so that the normalized isotherms $p(v)$ depend on only one parameter, the normalized temperature $t-$ see Fig. 1. The most important property of these plots is that the isotherms have qualitatively different shapes in two temperature regions. ${ }^{5}$ At $t>1$, i.e. $T>T_{c}$, pressure increases monotonically at gas compression (just like in an ideal gas, to which this system tends at $T \gg T_{c}$ ), i.e. $(\partial P / \partial V)_{T}<0$ at all points of the isotherm. However, below the critical temperature $T_{c}$, all isotherms feature segments with $(\partial P / \partial V)_{T}>0$. It is easy to understand that, as least in a constant pressure experiment (see, for example,

[^873]Fig. 1.5), ${ }^{6}$ these segments describe a mechanically unstable equilibrium. Indeed, if due to a random fluctuation, the volume deviated upward from the equilibrium value, the pressure would also increase, forcing the environment (say, the heavy piston in Fig. 1.5) to allow a further expansion of the system, leading to even higher pressure, etc. A similar deviation of volume downward would lead to a similar avalanche-like decrease of the volume. Such avalanche instability would develop further and further until the system has reached one of the stable branches with a negative slope $(\partial P / \partial V)_{T}$. In the range where the single-phase equilibrium state is unstable, the system as a whole may be stable only if it consists of the two phases (one with a smaller, and another with a higher density $n=N / V$ ) that are described by the two stable branches.


Fig. 4.1. The van der Waals equation plotted on the $[p, v]$ plane for several values of reduced temperature $t \equiv T / T_{c}$. Shading shows the single-phase instability range in which $(\partial P / \partial V)_{T}>0$. (The reader is invited to contemplate the physical sense and possibility of experimental observation of the negative values of pressure, predicted by the model.)

In order to understand the basic properties of this two-phase system, let us recall the general conditions of equilibrium of two thermodynamic systems, which have been discussed in Chapter 1:

$$
\begin{gather*}
T_{1}=T_{2} \text { (thermal equilibrium) },  \tag{4.5}\\
\mu_{1}=\mu_{2} \text { ("chemical" equilibrium) } \tag{4.6}
\end{gather*}
$$

the latter condition meaning that the average energy of a single ("probe") particle in both systems is the same. To those, we should add the evident condition of mechanical equilibrium,

$$
\begin{equation*}
P_{1}=P_{2}(\text { mechanical equilibrium }) \tag{4.7}
\end{equation*}
$$

that immediately follows from the balance of normal forces exerted on an inter-phase boundary.
If we discuss isotherms, Eq. (5) is fulfilled automatically, while Eq. (7) means that the effective isotherm $P(V)$ describing a two-phase system should be a horizontal line (Fig. 2): ${ }^{7}$

$$
\begin{equation*}
P=P_{0}(T) . \tag{4.8}
\end{equation*}
$$

[^874]

Fig. 4.2. Phase equilibrium at $T<T_{\mathrm{c}}$ (schematically).

Along this line, internal properties of each phase do not change; only the particle distribution is: it evolves gradually from all particles being in the liquid phase at point 1 to all particles being in the gas phase at point $2 .{ }^{8}$ In particular, according to Eq. (6), the chemical potentials $\mu$ of the phases should be equal at each point of the horizontal line (8). This fact enables us to find the line's position: it has to connect points 1 and 2 in which the chemical potentials of the phases are equal to each other.

Let us recast this condition as

$$
\begin{equation*}
\int_{1}^{2} d \mu=0, \quad \text { i.e. } \int_{1}^{2} d G=0 \tag{4.9}
\end{equation*}
$$

where the integral may be taken along the single-phase isotherm. (For this mathematical calculation, the mechanical instability of some states on this curve is not important.) Along that curve, $N=$ const and $T$ $=$ const, so that according to Eq. (1.53c), $d G=-S d T+V d P+\mu d N$, for a slow (reversible) change, $d G=$ $V d P$. Hence Eq. (9) yields

$$
\begin{equation*}
\int_{1}^{2} V d P=0 \tag{4.10}
\end{equation*}
$$

From Fig. 2, it is easy to see that geometrically this equality means that the shaded areas $A_{d}$ and $A_{u}$ should be equal, and hence Eq. (10) may be rewritten in the form of the so-called Maxwell's rule

$$
\begin{equation*}
\int_{1}^{2}\left[P-P_{0}(T)\right] d V=0 \tag{4.11}
\end{equation*}
$$

[^875]This relation is more convenient for calculations than Eq. (10) if the equation of state may be explicitly solved for $P$ - as it is the case for the van der Waals equation (2). Such calculation (left for

[^876]reader's exercise) shows that for that model, the temperature dependence of the saturated gas pressure at low $T$ is exponential,
\[

$$
\begin{equation*}
P_{0}(T)=27 P_{c} \exp \left\{-\frac{U_{0}}{T}\right\}, \quad \text { with } U_{0} \equiv \frac{a}{b}=\frac{27}{8} T_{c}, \quad \text { for } T \ll T_{c}, \tag{4.12}
\end{equation*}
$$

\]

corresponding very well to the physical picture of the rate of particle activation from the potential well of depth $U_{0 .}{ }^{9}$

The signature parameter of the first-order phase transition, the latent heat of evaporation

$$
\begin{equation*}
\Lambda \equiv \int_{1}^{2} d Q \tag{4.13}
\end{equation*}
$$

may be found by a similar integration along the single-phase isotherm. Indeed, using Eq. (1.19), $d Q=$ $T d S$, we get

$$
\begin{equation*}
\Lambda \equiv \int_{1}^{2} T d S=T\left(S_{2}-S_{1}\right) \tag{4.14}
\end{equation*}
$$

Instead of calculating entropy from the equation of state (as was done for the ideal gas in Sec. 1.4), it is easier to express the right-hand side of Eq. (14) directly via that equation. For that, let us take the full derivative of Eq. (6) over temperature, considering each value of $G=N \mu$ as a function of $P$ and $T$, and taking into account that according to Eq. (7), $P_{1}=P_{2}=P_{0}(T)$ :

$$
\begin{equation*}
\left(\frac{\partial G_{1}}{\partial T}\right)_{P}+\left(\frac{\partial G_{1}}{\partial P}\right)_{T} \frac{d P_{0}}{d T}=\left(\frac{\partial G_{2}}{\partial T}\right)_{P}+\left(\frac{\partial G_{2}}{\partial P}\right)_{T} \frac{d P_{0}}{d T} \tag{4.15}
\end{equation*}
$$

According to the first of Eqs. (1.39), the partial derivative $(\partial G / \partial T)_{P}$ is just minus entropy, while according to the second of those equations, $(\partial G / \partial P)_{T}$ is the volume. Thus Eq. (15) becomes

$$
\begin{equation*}
-S_{1}+V_{1} \frac{d P_{0}}{d T}=-S_{2}+V_{2} \frac{d P_{0}}{d T} \tag{4.16}
\end{equation*}
$$

Solving this equation for $\left(S_{2}-S_{1}\right)$, and plugging the result into Eq. (14), we get the Clapeyron-Clausius formula

ClapeyronClausius formula

$$
\begin{equation*}
\Lambda=T\left(V_{2}-V_{1}\right) \frac{d P_{0}}{d T} \tag{4.17}
\end{equation*}
$$

For the van der Waals model, this formula may be readily used for the analytical calculation of $\Lambda$ may in two limits: $T \ll T_{c}$ and $\left(T_{c}-T\right) \ll T_{c}-$ the exercise left for the reader. In the latter limit, $\Lambda \propto\left(T_{c}-\right.$ $T)^{1 / 2}$, naturally vanishing at the critical temperature.

Finally, some important properties of the van der Waals' model may be revealed more easily by looking at the set of its isochores $P=P(T)$ for $V=$ const, rather than at the isotherms. Indeed, as Eq. (2) shows, all single-phase isochores are straight lines. However, if we interrupt these lines at the points when the single phase becomes metastable, and complement them with the (very nonlinear!) dependence $P_{0}(T)$, we get the pattern (called the phase diagram) shown schematically in Fig. 3a.

[^877]

Fig. 4.3. (a) The van der Waals model's isochores, the saturated gas pressure diagram and the critical point, and (b) the phase diagram of a typical 3-phase system (schematically).

At this plot, one more meaning of the critical point $\left\{P_{c}, T_{c}\right\}$ becomes very clear. At fixed pressure $P<P_{c}$, the liquid and gaseous phases are clearly separated by the transition line $P_{0}(T)$, so if we achieve the transition just by changing temperature, and hence volume (shown with the red line in Fig. 3), we will pass through the phase coexistence stage. However, if we perform the same final transition by changing both the pressure and temperature, going around above the critical point (the blue line in Fig. 3), no definite point of transition may be observed: the substance stays in a single phase, and it is a subjective judgment of the observer in which region that phase should be called the liquid, and which region the gas. For water, the critical point corresponds to $647 \mathrm{~K}\left(374^{\circ} \mathrm{C}\right)$ and $P_{c} \approx 22.1 \mathrm{MPa}$ (i.e. $\sim 200$ bars), so that a lecture demonstration of its critical behavior would require substantial safety precautions. This is why such demonstrations are typically carried out with other fluids such as the diethyl ether, ${ }^{10}$ with much lower $T_{c}\left(194{ }^{\circ} \mathrm{C}\right)$ and $P_{c}(3.6 \mathrm{MPa})$. Though the ether is colorless and clear in both gas and liquid phases, their separation (due to gravity) is visible (due to a difference in an optical refraction coefficient) at $P<P_{c}$, but not above $P_{C} .{ }^{11}$

Thus, in the van der Waals model, two phases may coexist, though only at certain conditions ( $P$ $<P_{c}$ ). Now the natural question is whether the coexistence of more than two phases of the same substance is possible. For example, can the water ice, liquid water, and water vapor (steam) be in thermodynamic equilibrium? The answer is essentially given by Eq. (6). From thermodynamics, we know that for a uniform system (with $G=\mu N$ ), pressure and temperature completely define the chemical potential. Hence, dealing with two phases, we have to satisfy just one chemical equilibrium condition (6) for two common parameters $P$ and $T$. Evidently, this leaves us with one extra degree of freedom, so that the two-phase equilibrium is possible within a certain range of $P$ at fixed $T$ (or vice versa) - see Fig.

[^878]3a. Now, if we want three phases to be in equilibrium, we need to satisfy two equations for these variables:

$$
\begin{equation*}
\mu_{1}(P, T)=\mu_{2}(P, T)=\mu_{3}(P, T) . \tag{4.18}
\end{equation*}
$$

Typically, functions $\mu(P, T)$ are monotonic, so that Eqs. (18) have just one solution, the so-called triple point $\left\{P_{t}, T_{t}\right\}$. Of course, the triple point $\left\{P_{t}, T_{t}\right\}$ of equilibrium between three phases should not to be confused with the critical points $\left\{P_{c}, T_{c}\right\}$ of transitions between two phase pairs. Fig. 3b shows, very schematically, their relation for a typical three-phase system solid-liquid-gas. For example, water, ice, and water vapor are at equilibrium at a triple point corresponding to 0.612 KPa and (by definition, exactly) $273.16 \mathrm{~K} .{ }^{12}$ The particular importance of this particular temperature point is that by an international agreement it has been accepted for the Celsius scale definition, as $0.01^{\circ} \mathrm{C}$, so that the absolute temperature zero corresponds to exactly $-273.15^{\circ} \mathrm{C}$. More generally, triple points of pure substances (such as $\mathrm{H}_{2}, \mathrm{~N}_{2}, \mathrm{O}_{2}, \mathrm{Ar}, \mathrm{Hg}$, and $\mathrm{H}_{2} \mathrm{O}$ ) are broadly used for thermometer calibration, defining the so-called international temperature scales including the currently accepted scale ITS-90.

This result may be readily generalized to multi-component systems consisting of particles of several (say, $L$ ) sorts. ${ }^{13}$ If such a system is in a single phase, i.e. macroscopically uniform, its chemical potential may be defined by the natural generalization of Eq. (1.53c):

$$
\begin{equation*}
d G=-S d T+V d P+\sum_{l=1}^{L} \mu^{(l)} d N^{(l)} . \tag{4.19}
\end{equation*}
$$

Typically, a single phase is not a pure substance, but has certain concentrations of other components, so that $\mu^{(l)}$ may depend not only on $P$ and $T$, but also on concentrations $c^{(l)} \equiv N^{(l)} / N$ of particles of each sort. If the total number $N$ of particles is fixed, the number of independent concentrations is $(L-1)$. For the chemical equilibrium of $R$ phases, all $R$ values of $\mu_{r}^{(l)}(r=1,2, \ldots, R)$ have to be equal for particles of each sort: $\mu_{1}{ }^{(l)}=\mu_{2}{ }^{(l)}=\ldots=\mu_{R}{ }^{(l)}$, with each $\mu_{r}{ }^{(l)}$ depending on $(L-1)$ concentrations $c_{r}{ }^{(l)}$, and also on $P$ and $T$. This requirement gives $L(R-1)$ equations for $(L-1) R$ concentrations $c_{r}{ }^{(l)}$, plus two common arguments $P$ and $T$, i.e. for $[(L-1) R+2]$ independent variables. This means that the number of phases has to satisfy the limitation

Gibbs phase rule

$$
\begin{equation*}
L(R-1) \leq(L-1) R+2, \quad \text { i.e. } R \leq L+2 \tag{4.20}
\end{equation*}
$$

where the equality sign may be reached in just one point in the whole parameter space. This is the Gibbs phase rule. As a sanity check, for a single-component system, $L=1$, the rule yields $R \leq 3$ - exactly the result we have already discussed.

### 4.2. Continuous phase transitions

As Fig. 2 shows, if we fix pressure $P$ in a system with a first-order phase transition, and start changing its temperature, crossing the transition point, defined by equation $P_{0}(T)=P$, requires the insertion (or extraction) a non-vanishing latent heat $\Lambda$. Relations (14) and (17) show that the latent heat

[^879]is directly related to the a non-vanishing difference between entropies and volumes of the two phases (at the same pressure). As we know from Chapter 1, both $S$ and $V$ may be presented as first derivatives of appropriate thermodynamic potentials. This is why such transitions, involving a jump of potentials' first derivatives, are called first-order phase transitions.

On the other hand, there are phase transitions that have zero latent heat $(\Lambda=0)$ and no first derivative jumps at the transition temperature $T_{c}$, so that the temperature point is clearly marked, for example, by a jump of a second derivative of a thermodynamic potential - for example, the derivative $\partial C / \partial T$ which, according to Eq. (1.24), equals to $\partial^{2} E / \partial T^{2}$. In the initial classification by P. Ehrenfest, this was an example of a second-order phase transition. However, most features of such phase transitions are also pertinent to some systems in which the second derivatives of potentials are continuous as well. Due to this reason, I will use a more recent terminology (suggested by M. Fisher), in which all phase transitions with $\Lambda=0$ are called continuous.

Most continuous phase transitions result from particle interactions. Here are some examples:
(i) At temperatures above $\sim 120^{\circ} \mathrm{C}$, the crystal lattice of barium titanate $\left(\mathrm{BaTiO}_{3}\right)$ is cubic, with a Ba ion in the center of each Ti-cornered cube (or vice versa) - see Fig. 4a. However, as temperature is being lowered below that critical value, the sublattice of Ba ions starts moving along one of 6 sides of the $\mathrm{TiO}_{3}$ sublattice, leading to a small deformation of both lattices - which become tetragonal. This is a typical example of a structural transition, in this particular case combined with a ferroelectric transition, because (due to the positive electric charge of Ba ions) below the critical temperature the $\mathrm{BaTiO}_{3}$ crystal acquires a spontaneous electric polarization.


Fig. 4.4. Cubic lattices of
(a) $\mathrm{BaTiO}_{3}$ and (b) CuZn .
(ii) A different kind of phase transition happens, for example, in $\mathrm{Cu}_{x} \mathrm{Zn}_{1-x}$ alloys (brasses). Their crystal lattice is always cubic, but above certain critical temperature $T_{c}$ (which depends on $x$ ) any of its nodes is occupied by either a copper or a zinc atom, at random. At $T<T_{c}$, a trend towards atom alternation arises, and at low temperatures, the atoms are fully ordered, as shown in Fig. 4b for the stoichiometric case $x=0.5$. This is a good example of an order-disorder transition.
(iii) At ferromagnetic transitions (happening, e.g., in Fe at $1,388 \mathrm{~K}$ ) and antiferromagnetic transitions (e.g., in MnO at 116 K ), lowering of temperature below the critical value ${ }^{14}$ does not change atom positions substantially, but results in a partial ordering of atomic spins, eventually leading to their full ordering (Fig. 5).

[^880](iv) Finally, the Bose-Einstein condensation of atoms in liquid helium and electrons in superconducting metals and metal oxides may be also considered as continuous phase transitions. At the first glance, this contradicts to the nonvanishing latent heat given by the BEC theory outlined in Sec. 3.4. However, that theory shows that $\Lambda \rightarrow 0$ at $T \rightarrow 0$ and hence $P(T) \rightarrow 0-$ see Eq. (3.79). Hence, at zero pressure the Bose Einstein condensation of an ideal gas could may be considered a continuous phase transition. For a gas, this is just not a very interesting limit, because of the vanishing gas density. On the contrary, the Bose-Einstein condensation of strongly interacting particles in liquids or solids is not affected by pressure - at least on the ambient pressure scale, and taking $P=0$ is quite a legitimate assumption. ${ }^{15}$


Fig. 4.5. Classical images of completely ordered phases: (a) a ferromagnet, and (b) an antiferromagnet.

Besides these standard examples, some other threshold phenomena, such as formation of a coherent optical field in a laser, and even the self-excitation of oscillators with negative damping (see, e.g., CM Sec. 4.4), may be treated, at certain conditions, as continuous phase transitions. ${ }^{16}$

The general feature of all these transitions is the gradual formation, at $T<T_{\mathrm{c}}$, of certain ordering, which may be characterized by some order parameter $\eta \neq 0$. The simplest example of such order parameter is the magnetization at the ferromagnetic transitions, and this is why the continuous phase transitions are usually discussed on certain models of ferromagnetism. (I will follow this tradition, while mentioning in passing other important cases that require a substantial modification of theory.) Most of such models are defined on an infinite 3D cubic lattice (see, e.g., Fig. 5), with evident generalizations to lower dimensions. For example, the Heisenberg model of a ferromagnet is defined by the following Hamiltonian:

$$
\begin{equation*}
\hat{H}=-J \sum_{\left\{j, j^{\prime}\right\}} \hat{\boldsymbol{\sigma}}_{j} \cdot \hat{\boldsymbol{\sigma}}_{j^{\prime}}-\sum_{j} \mathbf{h} \cdot \hat{\boldsymbol{\sigma}}_{j}, \quad \text { with } \mathbf{h} \equiv \mu_{\mathrm{B}} \boldsymbol{B}, \tag{4.21}
\end{equation*}
$$

[^881]where $\hat{\boldsymbol{\sigma}}_{j}$ is the Pauli matrix operator ${ }^{17}$ acting on $j$-th spin, $\mathbf{n}_{\mathcal{B}}$ is the direction of magnetic field $\mathcal{B}$, and constant $\mu_{\mathrm{B}}$ is the Bohr magneton
\[

$$
\begin{equation*}
\mu_{\mathrm{B}}=\frac{e \hbar}{2 m_{e}} \approx 0.927 \times 10^{-23} \mathrm{~J} / \mathrm{T} \tag{4.22}
\end{equation*}
$$

\]

with ( $-e$ ) and $m_{e}$ being electron's charge and mass. The figure brackets $\{j, j ’\}$ in Eq. (21) denote the summation over the pairs of adjacent sites, so that the magnitude of constant $J$ may be interpreted as the maximum coupling energy per "bond" between two adjacent particles. At $J>0$, the coupling tries to keep spins aligned (thus minimizing the coupling energy), i.e. to implement the ferromagnetic ordering. ${ }^{18}$ The second term in Eq. (21) describes the effect of external magnetic field $\mathcal{B}$, which tries to turn all spins, with their magnetic moments, along its direction.

However, even the Heisenberg model, while being approximate, is still too complex for analysis. This is why most theoretical results have been obtained for its classical twin, the Ising model: ${ }^{19}$

$$
\begin{equation*}
E_{m}=-J \sum_{\left\{j, j^{\prime}\right\}} s_{j} s_{j^{\prime}}-h \sum_{j} s_{j} . \tag{4.23}
\end{equation*}
$$

Here $E_{m}$ are eigenvalues of energy in the magnetic field, constant $h$ mimics an external magnetic field, and $s_{j}$ are classical scalar variables that may take only two values, $s_{j}= \pm 1$. (Despite its classical character, variable $s_{j}$ modeling the real spin of an electron, is usually called "spin" for brevity, and I will follow this tradition.) Index $m$ numbers all possible combinations of variables $s_{j}$ - there are $2^{N}$ of them in a system of $N$ Ising "spins". Somewhat shockingly, even for this toy model, no analytical 3D solutions have been found, and the solution of its 2D version by L. Onsager in 1944 (see Sec. 5 below) is still considered one of the top intellectual achievements of the statistical physics. Still, Eq. (23) is very useful for the introduction of basic notions of continuous phase transitions, and methods of their analysis, and I will focus my brief discussion on this model. ${ }^{20}$

Evidently, if $T=0$ and $h=0$, the lowest value of internal energy,

$$
\begin{equation*}
E_{\min }=-J N d, \tag{4.24}
\end{equation*}
$$

where $d$ is the lattice dimensionality, is achieved in the "ferromagnetic" phase in which all spins $s_{j}$ are equal to either +1 or -1 simultaneously, so that the lattice average $\left\langle s_{j}\right\rangle= \pm 1$. On the other hand, at $J=0$ and $h=0$, the spins are independent, and in the absence of external field their signs are completely random, with the $50 \%$ probability to have either of values $\pm 1$, so that $\left\langle s_{j}\right\rangle=0$. Hence in the case of arbitrary parameters we may use the average

[^882]Ising
model's
order parameter

$$
\begin{equation*}
\eta \equiv\left\langle s_{j}\right\rangle \tag{4.25}
\end{equation*}
$$

as a good measure of spin ordering, i.e. as the order parameter. Since in a real ferromagnet, each spin carries a magnetic moment, the order parameter $\eta$ corresponds to the substance magnetization, at $\eta h>$ 0 , directed along the applied magnetic field. ${ }^{21}$

Due to the difficulty of calculating the order parameter for arbitrary temperatures, most theoretical discussions of continuous phase transitions are focused on its temperature dependence just below $T_{c}$. Both experiment and theory show that (in the absence of external field) this dependence is close to a certain power,

$$
\begin{equation*}
\eta \propto \tau^{\beta}, \text { for } \tau>0 \tag{4.26}
\end{equation*}
$$

of the small deviation from the critical temperature, which is conveniently normalized as

$$
\begin{equation*}
\tau \equiv \frac{T_{c}-T}{T_{c}} . \tag{4.27}
\end{equation*}
$$

Remarkably, most other key variables follow a similar temperature behavior, with the same critical exponent for both signs of $\tau$. In particular, the heat capacity at fixed magnetic field behaves as ${ }^{22}$

$$
\begin{equation*}
C_{h} \propto \frac{1}{|\tau|^{\alpha}} . \tag{4.28}
\end{equation*}
$$

Similarly, the (normalized) low-field susceptibility ${ }^{23}$

$$
\begin{equation*}
\left.\chi \equiv \frac{\partial \eta}{\partial h}\right|_{h=0} \propto \frac{1}{|\tau|^{\gamma}} . \tag{4.29}
\end{equation*}
$$

Two more important critical exponents, $\zeta$ and $v$, describe temperature behavior of the correlation function $\left\langle s_{j} s_{j}\right\rangle$, whose dependence on distance $r_{j j}$, between two spins may be well fitted by the following law,

$$
\begin{equation*}
\left\langle s_{j} s_{j^{\prime}}\right\rangle \propto \frac{1}{r_{i j j^{\prime}} d-2+\zeta} \exp \left\{-\frac{r_{j j^{\prime}}}{r_{c}}\right\}, \tag{4.30}
\end{equation*}
$$

with the correlation radius

$$
\begin{equation*}
r_{c} \propto \frac{1}{|\tau|^{v}} \tag{4.31}
\end{equation*}
$$

Finally, three more critical exponents, usually denoted $\varepsilon, \delta$, and $\mu$, describe the external field dependences of, respectively, $c, \eta$ and $r_{c}$ at $\tau=0$. For example, $\delta$ is defined as

[^883]\[

$$
\begin{equation*}
\eta \propto h^{1 / \delta} . \tag{4.32}
\end{equation*}
$$

\]

(Other field exponents are used less frequently, and for their discussion I have to refer the interested reader to the special literature listed above.)

The second column of Table 1 shows experimental values of the critical exponents for various 3D physical systems featuring continuous phase transitions. One can see that their values vary from system to system, leaving no hope for a universal theory that would describe them all. However, certain combination of the exponents are much more reproducible - see the bottom lines of the table.

Table 4.1. Major critical exponents of continuous phase transitions

| Exponents and <br> combinations | Experimental <br> range (3D) ${ }^{(\mathrm{a})}$ | Mean-field <br> theory | 2D Ising <br> model | 3D Ising <br> model | 3D Heisenberg <br> Model $^{(\mathrm{d})}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\alpha$ | $0-0.14$ | $0^{(\mathrm{b})}$ | (c) | 0.12 | -0.14 |
| $\beta$ | $0.32-0.39$ | $1 / 2$ | $1 / 8$ | 0.31 | 0.3 |
| $\gamma$ | $1.3-1.4$ | 1 | $7 / 4$ | 1.25 | 1.4 |
| $\delta$ | $4-5$ | 3 | 15 | 5 | - |
| $\nu$ | $0.6-0.7$ | $1 / 2$ | 1 | 0.64 | 0.7 |
| $\zeta$ | 0.05 | 0 | $1 / 4$ | 0.05 | 0.04 |
| $(\alpha+2 \beta+\gamma) / 2$ | $1.00 \pm 0.005$ | 1 | 1 | 1 | 1 |
| $\delta-\gamma / \beta$ | $0.93 \pm 0.08$ | 1 | 1 | 1 | $?$ |
| $(2-\zeta) v / \gamma$ | $1.02 \pm 0.05$ | 1 | 1 | 1 | 1 |
| $(2-\alpha) / v d$ | (e) | $4 / d$ | 1 | 1 | 1 |

${ }^{(a)}$ Experimental data are from the monograph by A. Patashinskii and V. Pokrovskii, cited above.
${ }^{(b)}$ Discontinuity at $\tau=0-$ see below.
${ }^{(c)}$ Instead of following Eq. (28), in this case $C_{h}$ diverges as $\ln |\tau|$.
${ }^{(d)}$ With the order parameter $\eta$ defined as $\left\langle\boldsymbol{\sigma}_{j} \cdot \mathbf{n}_{\mathcal{B}}\right\rangle$.
${ }^{(e)}$ I could not find any data on this.

Historically the first (and perhaps the most fundamental) of these universal relations was derived in 1963 by J. Essam and M. Fisher:

$$
\begin{equation*}
\alpha+2 \beta+\gamma=2 \tag{4.33}
\end{equation*}
$$

It may be proved, for example, by finding the temperature dependence such magnetic field value, $h_{\tau}$, which changes the order parameter by the amount similar to that already existing at $h=0$, due to a finite temperature deviation $\tau>0$. First, we may compare Eqs. (26) and (29), to get

$$
\begin{equation*}
h_{\tau} \propto \tau^{\beta+\gamma} . \tag{4.34}
\end{equation*}
$$

By the physical sense of $h_{\tau}$ we may expect that such field has to affect system's free energy ${ }^{24} F(T, h)$ by the amount comparable to the effect of a bare temperature change $\tau$. Ensemble-averaging the last term of Eq. (23) and using the definition (25) of the order parameter $\eta$, we see that the change of $F$ (per particle) due to the field equals $-h_{\tau} \eta$ and, according to Eq. (26), scales as $h_{\tau} \tau^{\beta} \propto \tau^{(2 \beta+\gamma)}$.

In order to estimate the thermal effect on $F$, let us first derive one more useful general thermodynamic formula. ${ }^{25}$ Dividing Eq. (1.19) by $d T$, we may present heat capacity of a system as

$$
\begin{equation*}
C_{X}=T\left(\frac{\partial S}{\partial T}\right)_{X} \tag{4.35}
\end{equation*}
$$

where $X$ is the variable maintained constant at the temperature variation. For example, in the standard " $P-V$ " thermodynamics, we may use the first of Eqs. (1.35) to recast Eq. (35) for $X=V$ as

$$
\begin{equation*}
C_{V}=T\left(\frac{\partial S}{\partial T}\right)_{V}=-T\left(\frac{\partial^{2} F}{\partial T^{2}}\right)_{V} \tag{4.36}
\end{equation*}
$$

while for $\mathrm{X}=\mathrm{P}$ it may be combined with Eq. (1.39) to get

$$
\begin{equation*}
C_{P}=T\left(\frac{\partial S}{\partial T}\right)_{P}=-T\left(\frac{\partial^{2} G}{\partial T^{2}}\right)_{P} \tag{4.37}
\end{equation*}
$$

As was just discussed, in the Ising model the role of pressure $P$ is played by the external magnetic field $h$, and of $G$ by $F$, so that the last form of Eq. (37) means that the thermal part of $F$ may be found by double integration of $\left(-C_{h} / T\right)$ over temperature. In the context of our current discussion, this means that near $T_{\mathrm{c}}$, the free energy scales as the double integral of $C_{h} \propto \tau^{-\alpha}$ over $\tau$. In the limit $\tau \ll 1$, factor $T$ may be treated as a constant; as a result, the change of $F$ due to $\tau>0$ alone scales as $\tau^{(2-\alpha)}$. Requiring this change to be proportional to the same power of $\tau$ as the field-induced part of energy, we get the Essam-Fisher relation (33).

Using similar reasoning, it is straightforward to derive a few other universal relations of critical exponents, including the Widom relation,

[^884]\[

$$
\begin{equation*}
\delta-\frac{\gamma}{\beta}=1, \tag{4.38}
\end{equation*}
$$

\]

very similar relations for other high-field exponents $\varepsilon$ and $\mu$ (which I do not have time to discuss), and the Fisher relation

$$
\begin{equation*}
v(2-\zeta)=\gamma . \tag{4.39}
\end{equation*}
$$

A slightly more complex reasoning, involving the so-called scaling hypothesis, yields the dimensionality-dependent Josephson relation

$$
\begin{equation*}
v d=2-\alpha . \tag{4.40}
\end{equation*}
$$

Table 1 shows that at least three of these relations are in a very reasonable agreement with experiment, so that we will use them as a testbed for various theoretical approaches to continuous phase transitions.

### 4.3. Landau's mean-field theory

The most general approach to analysis of the continuous phase transitions, formally not based on any particular model (though in fact implying the Ising model (23) or one of it siblings), is the meanfield theory developed in 1937 by L. Landau, on the basis of prior ideas by P.-E. Weiss - to be discussed in the next section. The main approximation of this phenomenological approach is to present the free energy change $\Delta F$ at the phase transition as an explicit function of the order parameter $\eta(25)$. Generally this function may be complicated and model-specific, but near $T_{c}, \eta$ has to tend to zero, so that the change of the relevant thermodynamic potential, the free energy,

$$
\begin{equation*}
\Delta F \equiv F(T)-F\left(T_{c}\right), \tag{4.41}
\end{equation*}
$$

may be expanded into the Taylor series in $\eta$, and only a few, most important first terms of that expansion retained. In order to keep the symmetry between two possible signs of the order parameter in the absence of external field, at $h=0$ this expansion should not include odd powers of $\eta$ :

$$
\begin{equation*}
\left.\frac{\Delta F}{V}\right|_{h=0}=A(T) \eta^{2}+\frac{1}{2} B(T) \eta^{4}+\ldots \tag{4.42}
\end{equation*}
$$

As we will see imminently, these two terms are sufficient to describe finite (non-vanishing but limited) stationary values of the order parameter; this is why Landau's theory ignores the higher terms of the Taylor expansion - which are much smaller at $\eta \rightarrow 0$.

Now let us discuss temperature dependences of coefficients $A$ and $B$. The equilibrium of the system should correspond to minimum of $F$. Equation (42) shows that, first of all, coefficient $B(T)$ has to be positive for any sign of $\tau$, to ensure the equilibrium at a finite value of $\eta^{2}$. Thus, it is reasonable to ignore the temperature dependence of $B$ near the critical temperature altogether and use approximation

$$
\begin{equation*}
B(T)=b>0 . \tag{4.43}
\end{equation*}
$$

On the other hand, as Fig. 6 shows, coefficient $A(T)$ has to change sign at $T=T_{c}$, being positive at $T>$ $T_{c}$ and negative at $T<T_{c}$, to ensure the transition from $\eta=0$ at $T>T_{c}$ to a certain non-vanishing value at $T<T_{\mathrm{c}}$. Since $A$ should be a smooth function of temperature, we may approximate it by the leading term in its Taylor expansion in $\tau$ :

$$
\begin{equation*}
A(T)=-a \tau, \quad \text { with } a>0, \tag{4.44}
\end{equation*}
$$

so that Eq. (42) becomes

$$
\begin{equation*}
\left.\frac{\Delta F}{V}\right|_{h=0}=-a \tau \eta^{2}+\frac{1}{2} b \eta^{4} . \tag{4.45}
\end{equation*}
$$



Fig. 4.6. Free energy (42) as a function of (a) $\eta$ and (b) $\eta^{2}$ in Landau's mean-field theory, for two different signs of coefficient $A(\tau)$.

The main strength of Landau's theory is the possibility of its straightforward extension to the effects of the external field and of spatial variations of the order parameter. First, averaging of the field term of Eq. (23) over all sites of the system, with the account of Eq. (25), gives an energy addition of $h \eta$ per particle, i.e. - $n h \eta$ per unit volume, where $n$ is the particle density. Second, since (according to Eq. (23) with $v>0$, see Table 1) the correlation radius diverges at $\tau \rightarrow 0$, spatial variations of the order parameter should be slow, $|\nabla \eta| \rightarrow 0$. Hence, the effects of the gradient on $\Delta F$ may be approximated by the first nonvanishing term of its expansion into the Taylor series in $(\nabla \eta)^{2}$. As a result, Eq. (45) may be generalized as

$$
\begin{equation*}
\Delta F=\int \Delta f d^{3} r, \quad \text { with } \quad \Delta f=-a \tau \eta^{2}+\frac{1}{2} b \eta^{4}-n h \eta+c(\nabla \eta)^{2} \tag{4.46}
\end{equation*}
$$

where $c$ is a factor independent of $\eta$. In order to avoid the unphysical effect of spontaneous formation of spatial variations of the order parameter, that factor has to be positive at all temperatures, and hence may be taken for constant in a small vicinity of $T_{c}$ - the only region where Eq. (46) may be expected to provide quantitatively correct results.

Relation (46) is the full version of the free energy in Landau's theory. ${ }^{26}$ Now let us find out what critical exponents are predicted by this phenomenological approach. First of all, we may find equilibrium values of the order parameter from the condition of $F$ having a minimum, $\partial F / \partial \eta=0$. At $h=$ 0 , it is easier to use the equivalent equation $\partial F / \partial\left(\eta^{2}\right)=0$, where $F$ is given by Eq. (45) - see Fig. 6b. This immediately yields

$$
\eta= \begin{cases}(a \tau / b)^{1 / 2}, & \text { for } \tau>0  \tag{4.47}\\ 0, & \text { for } \tau<0\end{cases}
$$

[^885]Comparing this result with Eq. (26), we see that in the Landau theory, $\beta=1 / 2$. Next, plugging result (47) back into Eq. (45), for the equilibrium (minimal) value of the free energy, we get

$$
\Delta f= \begin{cases}-a^{2} \tau^{2} / 2 b, & \text { for } \tau>0  \tag{4.48}\\ 0, & \text { for } \tau<0\end{cases}
$$

From here and Eq. (36), the specific heat,

$$
\frac{C_{h}}{V}= \begin{cases}a^{2} / b T_{c}, & \text { for } \tau>0  \tag{4.49}\\ 0, & \text { for } \tau<0\end{cases}
$$

has, at the critical point, a discontinuity rather than a singularity, i.e. the critical exponent $\alpha=0$.
In the presence of a uniform field, the equilibrium order parameter should be found from the condition $\partial f / \partial \eta=0$ applied to Eq. (46) with $\nabla \eta=0$, giving

$$
\begin{equation*}
\frac{\partial f}{\partial \eta} \equiv-2 a \tau \eta+2 b \eta^{3}-n h=0 . \tag{4.50}
\end{equation*}
$$

In the limit of small order parameter, $\eta \rightarrow 0$, term with $\eta^{3}$ is negligible, and Eq. (50) gives

$$
\begin{equation*}
\eta=-\frac{n h}{2 a \tau}, \tag{4.51}
\end{equation*}
$$

so that according to Eq. (29), $\gamma=1$. On the other hand, at $\tau=0$ (or at relatively high fields at other temperatures), the cubic term in Eq. (50) is much larger than the linear one, and this equation yields

$$
\begin{equation*}
\eta=\left(\frac{n h}{2 b}\right)^{1 / 3} \tag{4.52}
\end{equation*}
$$

so that comparison with Eq. (32) yields $\delta=3$.
Finally, according to Eq. (30), the last term in Eq. (46) scales as $c \eta^{2} / r_{c}{ }^{2}$. (If $r_{c} \neq \infty$, the effects of the pre-exponential factor in that equation are negligible.) As a result, the gradient term contribution is comparable ${ }^{27}$ with the two leading terms in $\Delta f$ (which, according to Eq. (47), are of the same order), if

$$
\begin{equation*}
r_{c} \approx\left(\frac{c}{a|\tau|}\right)^{1 / 2} \tag{4.53}
\end{equation*}
$$

so that according to definition (31) of the critical exponent $v$, it is equal to $1 / 2$.
The third column in Table 1 summarizes the critical exponents and their combinations in Landau's theory. It shows that these values are somewhat out of the experimental ranges, and while some of their universal relations are correct, some are not; for example, the Josephson relation would be only correct at $d=4$ (not the most realistic spatial dimensionality :-) The main reason for this

[^886]disappointing result is that describing the spin interaction with the field, the Landau mean-field theory neglects spin randomness, i.e. fluctuations. Though a quantitative theory of thermodynamic fluctuations will not be discussed until the next chapter, we can readily perform their crude estimate. Looking at Eq. (46), we see that its first term is a quadratic function of the effective "half-degree of freedom", $\eta$. Hence in accordance with the equipartition theorem (2.28) we may expect that the average square of its thermal fluctuations, within a $d$-dimensional volume with linear size $\sim r_{c}$, should be of the order of $T / 2$ (close to the critical temperature, $T_{c} / 2$ is a good approximation):
\[

$$
\begin{equation*}
a|\tau|\left\langle\widetilde{\eta}^{2}\right\rangle r_{c}^{d} \sim \frac{T_{c}}{2} . \tag{4.54}
\end{equation*}
$$

\]

In order to be negligible, the variance has to be negligible in comparison with the average $\eta^{2} \sim a \tau / b$. Plugging in the $\tau$-dependences of the operands of this relation, and values of the critical exponents in the Landau theory, for $\tau>0$ we get the so-called Levanyuk-Ginzburg criterion of its validity:

$$
\begin{equation*}
\frac{T_{c}}{2 a \tau}\left(\frac{a \tau}{c}\right)^{\frac{d}{2}} \ll \frac{a}{b} \tau \tag{4.55}
\end{equation*}
$$

We see that for any realistic dimensionality, $d<4$, at $\tau \rightarrow 0$ the order parameter fluctuations grow faster than the its average value, and hence the theory becomes invalid.

Thus the Landau mean-field theory is not a perfect approach to finding critical indices at continuous phase transitions in Ising-type systems with their next-neighbor interactions between the particles. Despite of that fact, this theory is very much valued because of the following reason. Any long-range interactions between particles increase the correlation radius $r_{c}$, and hence suppress the order parameter fluctuations. For an example, at laser self-excitation, the emerging coherent optical field couples all photon-emitting particles in the electromagnetic "cavity" (resonator). As another example, in superconductors the role of the correlation radius is played by the Cooper-pair size $\xi_{0}$, which is typically of the order of $10^{-6} \mathrm{~m}$, i.e. much larger than the average distance between the pairs ( $\sim 10^{-8} \mathrm{~m}$ ). As a result, the mean-field theory remains valid at all temperatures besides an extremely small temperature interval near $T_{c}$ - for bulk superconductors, of the order of $10^{-6} \mathrm{~K}$.

Another strength of Landau's classical mean-field theory is that it may be readily generalized for description of Bose-Einstein condensates, i.e. quantum fluids. Of those generalizations, the most famous is the Ginzburg-Landau theory of superconductivity developed in 1950, i.e. even before the "microscopic" explanation of this phenomenon by Bardeen, Cooper and Schrieffer in the 1956-57. In the Ginzburg-Landau theory, the real order parameter $\eta$ is replaced with the modulus of a complex function $\psi$, physically the wavefunction of the coherent Bose-Einstein condensate of Cooper pairs. Since each pair carry electric charge $q=-2 e,{ }^{28}$ and has zero spin, it interacts with magnetic field in a way different from that described by the Heisenberg or Ising models. Namely, as was already discussed in Sec. 3.4, the del operator $\nabla$ in Eq. (46) has to be complemented by term $-i(q / \hbar) \mathbf{A}$, where $\mathbf{A}$ is the vector-potential of the total magnetic field $\mathcal{B}=\nabla \times \mathbf{A}$, including not only the external magnetic field $\mathcal{H}$,

[^887]but also the field induced by the supercurrent itself. With the account for the well-known formula for the magnetic field energy in the external field, ${ }^{29}$ Eq. (46) is now replaced with
\[

$$
\begin{equation*}
\Delta f=-a \tau|\psi|^{2}+\frac{1}{2} b|\psi|^{4}-\frac{\hbar^{2}}{2 m}\left|\left(\nabla-i \frac{q}{\hbar} \mathbf{A}\right) \psi\right|^{2}+\frac{B^{2}}{2 \mu_{0}}-\boldsymbol{\mathcal { H }} \cdot \boldsymbol{B}, \tag{4.56}
\end{equation*}
$$

\]

where $m$ is a phenomenological coefficient rather than the actual particle mass. The variational minimization of the resulting $\Delta F$ over variables $\psi$ and $\mathbf{B}$ (which is suggested for reader's exercise ${ }^{30}$ ) yields two differential equations:

$$
\begin{align*}
& \frac{\nabla \times \boldsymbol{B}}{\mu_{0}}=q \frac{i \hbar}{2 m}\left[\psi\left(\nabla-i \frac{q}{\hbar} \mathbf{A}\right) \psi^{*}-\text { c.c. }\right],  \tag{4.57}\\
& a \tau \psi=b|\psi|^{2} \psi-\frac{\hbar^{2}}{2 m}\left(\nabla-i \frac{q}{\hbar} \mathbf{A}\right)^{2} \psi . \tag{4.58}
\end{align*}
$$

The first of these Ginzburg-Landau equations should be no big surprise for the reader, because according to the Maxwell equations, in magnetostatics the left-hand part of Eq. (57) has to be equal to the electric current density, while the right-hand part is the usual quantum-mechanical probability current density multiplied by $q$, i.e. the electric current (or rather supercurrent) density $\mathbf{j}_{s}$ of the Cooper pair condensate. (Indeed, after plugging $\psi=n^{1 / 2} \exp \{i \varphi\}$ into that expression, we come back to Eq. (3.84) which, as we already know, explains such macroscopic quantum phenomena as magnetic flux quantization and Meissner-Ochsenfeld effect.)

However, Eq. (58) is new - for this course. Since last term in its right-hand part is the standard wave-mechanics expression for the kinetic energy of a particle in the presence of magnetic field, ${ }^{31}$ if this term dominates that part of the equation, Eq. (58) is reduced to the stationary Schrödinger equation, $E \psi=\hat{H} \psi$, for the ground state of confinement-free Cooper pairs, with energy $E=a \tau$. However, in contrast to the usual (single-particle) Schrödinger equation, in which $|\psi|$ is determined by the normalization condition, the Cooper pair condensate density $n=|\psi|^{2}$ is determined by the thermodynamic balance of the condensate with the ensemble of "normal" (unpaired) electrons that play the role of the uncondensed part of Bose gas, discussed in Sec. 3.4. In Eq. (58), such balance is enforced by the first term $b|\psi|^{2} \psi$ of the right-hand part. ${ }^{32}$ As we have already seen, in the absence of magnetic field and spatial gradients, such term yields $|\psi| \propto\left(T_{c}-T\right)^{1 / 2}-$ see Eq. (47).

[^888]It is easy to see that as either the external magnetic field or the current density in a superconductor are increased, so is the last term in Eq. (58). This increase has to be matched by a corresponding decrease of $|\psi|^{2}$, i.e. of the condensate density $n$, until it is completely suppressed. This explains the well documented effect of superconductivity suppression by magnetic field and supercurrent. Moreover, together with the flux quantization discussed in Sec. 3.4, it explains the existence of the so-called Abrikosov vortices - thin tubes of magnetic field, each carrying one quantum $\Phi_{0}$ of magnetic flux - see Eq. (3.86). At the core part of the vortex, $|\psi|^{2}$ is suppressed (down to zero at its central line) by the persistent supercurrent, which circulates around the core and screens the rest of superconductor from the magnetic field carried by the vortex. The penetration of such vortices into the so-called type-II superconductors ${ }^{33}$ enables them to sustain vanishing electric resistance up to very high magnetic fields of the order of 20 T , and to be used in very compact magnets - including those used for beam bending in particle accelerators.

Moreover, generalizing Eq. (58) to the time-dependent case, just as it is done with the usual Schrödinger equation ( $E \rightarrow i \hbar \partial / \partial t$ ), one can describe other fascinating quantum macroscopic phenomena such as the Josephson effects, including the generation of oscillations with frequency $\omega_{\mathrm{J}}=(q / \hbar) \mathscr{V}$ by tunnel junctions between two superconductors, biased by dc voltage $V$. Unfortunately, time/space restrictions do not allow me to discuss these effects in any detail here, and I have to refer the reader to special literature. ${ }^{34}$ Let me only note that at $T \approx T_{c}$, and not extremely pure superconductors (in which the so-called non-local transport phenomena may be important), the Ginzburg-Landau equations are exact, and may be derived (and their parameters $T_{c}, a, b, q$, and $m$ determined) from the "microscopic" theory of superconductivity based on the initial work by Bardeen, Cooper and Schrieffer. ${ }^{35}$ Most importantly, such derivation proves that $q=-2 e$ - the electric charge of a singe Cooper pair.

### 4.4. Ising model: The Weiss' molecular-field theory

The Landau mean-field theory is phenomenological in the sense that even within the range of its validity, it tells us nothing about the value of the critical temperature $T_{c}$ and other parameters (in Eq. (46), $a, b$, and $c$ ), so that they have to be found from a particular "microscopic" model of the system under analysis. In this course, we would have time to discuss only the Ising model (23) for various dimensionalities $d$.

The most simplistic way to map the model on a mean-field theory is to assume that all spins are exactly equal, $s_{j}=\eta$, with an additional condition $\eta^{2} \leq 1$, forgetting for a minute that in the genuine Ising model, $s_{j}$ may equal only +1 or -1 . Plugging this relation into Eq. (23), we get ${ }^{36}$

[^889]\[

$$
\begin{equation*}
F=-(N J d) \eta^{2}-N h \eta \tag{4.59}
\end{equation*}
$$

\]

This energy is plotted in Fig. 7a as a function of $\eta$, for several values of $h$. The plots show that at $h=0$, the system may be in either of two stable states, with $\eta= \pm 1$, corresponding to two different directions of spins (magnetization), with equal energy. ${ }^{37}$ (Formally, the state with $\eta=0$ is also stationary, because at this point $\partial F / \partial \eta=0$, but it is unstable, because for the ferromagnetic interaction, $J$ $>0$, the second derivative $\partial^{2} F / \partial \eta^{2}$ is negative.)


Fig. 4.7. Field dependence of (a) the free energy profile and (b) order parameter (i.e. magnetization) in the crudest mean-field approach to the Ising model.

As the external field is increased, it tilts the potential profile, and finally at a critical field,

$$
\begin{equation*}
h_{c} \equiv 2 J d, \tag{4.60}
\end{equation*}
$$

the state with $\eta=-1$ becomes unstable, leading to system's jump into the only remaining state with opposite magnetization, $\eta=+1$. Application of the similar external field of the opposite polarity leads to the similar switching back to $\eta=-1$, so that the full field dependence of $\eta$ follows the hysteretic pattern shown in Fig. 7b. Such a pattern is the most visible experimental feature of actual ferromagnetic materials, with the coercive magnetic field $\mathbb{Z}_{c}$ (modeled with $h_{c}$ ) of the order of $10^{3} \mathrm{~A} / \mathrm{m}$, and the saturated magnetization (modeled with $\eta= \pm 1$ ) corresponding to much higher fields $B$ - of the order of a few tesla. The most important property of these materials, also called permanent magnets, is their stability, i.e. the ability to retain the history-determined direction of magnetization in the absence of external field, for a very long time. In particular, this property is the basis of all magnetic systems for data recording, including the ubiquitous hard disk drives with their incredible information density currently approaching 1 Terabit per square inch. ${ }^{38}$

So, this simplest mean-field theory gives a crude description of the ferromagnetic ordering, but grossly overestimates the stability of these states with respect to thermal fluctuations. Indeed, in this

[^890]theory, there is no thermally-induced randomness at all, until $T$ becomes comparable with the height of the energy barrier separating two stable states,
\[

$$
\begin{equation*}
\Delta F \equiv F(\eta=0)-F(\eta= \pm 1)=N J d \tag{4.61}
\end{equation*}
$$

\]

which is proportional to the number of particles. At $N \rightarrow \infty$, this value diverges, and in this sense the critical temperature is infinite, while numerical experiments and more refined theories of the Ising model show that actually the ferromagnetic phase is suppressed at $T_{c} \sim J d-$ see below. ${ }^{39}$

The mean-field approach may be dramatically improved by even an approximate account for thermally-induced randomness. In this approach, suggested in 1908 by P.-E. Weiss under the name of molecular-field theory, ${ }^{40}$ random deviations of individual spin values from the lattice average,

$$
\begin{equation*}
\widetilde{s}_{j} \equiv s_{j}-\eta, \quad \eta \equiv\left\langle s_{j}\right\rangle, \tag{4.62}
\end{equation*}
$$

are allowed, but considered small, $\left|\widetilde{s}_{j}\right| \ll \eta$. This assumption allows us, after plugging expression $s_{j}=\eta+\widetilde{s}_{j}$ into the first term of the right-hand part of Eq. (23),

$$
\begin{equation*}
E_{m}=-J \sum_{\left\{j, j^{\prime}\right\}}\left(\eta+\widetilde{s}_{j}\right)\left(\eta+\widetilde{s}_{j^{\prime}}\right)-h \sum_{j} s_{j}, \tag{4.63}
\end{equation*}
$$

ignore the term proportional to $\widetilde{s}_{j} \widetilde{s}_{j^{\prime}}$. Making replacement (62) in the terms proportional to $\widetilde{s}_{j}$, we get

$$
\begin{equation*}
E_{m} \rightarrow E_{m}^{\prime} \equiv(N J d) \eta^{2}-h_{\mathrm{ef}} \sum_{j} s_{j} \tag{4.64}
\end{equation*}
$$

where $h_{\text {ef }}$ is defined as the sum

$$
\begin{equation*}
h_{\mathrm{ef}} \equiv h+(2 J d) \eta . \tag{4.65}
\end{equation*}
$$

The physical interpretation of $h_{\text {ef }}$ is the effective external field, which (besides the real external field $h$ ) takes into account the effect that would be exerted on spin $s_{j}$ by its $2 d$ next neighbors, if they all had unperturbed (but possibly fractional) spins $s_{j^{\prime}}=\eta$. Such an addition to external field,

$$
\begin{equation*}
h_{\mathrm{mol}} \equiv h_{\mathrm{ef}}-h=(2 J d) \eta, \tag{4.66}
\end{equation*}
$$

is called the molecular field - giving its name to the theory.
From the point of view of statistical physics, at fixed parameters of the system (including the order parameter $\eta$ ), the first term in the right-hand part of Eq. (64) is merely a constant energy offset, and $h_{\text {ef }}$ is just another constant, so that

$$
E_{m}^{\prime}=\text { const }+\sum_{j} E_{j}, \quad E_{j}=-h_{\mathrm{ef}} s_{j}= \begin{cases}-h_{\mathrm{ef}}, & \text { for } s_{j}=+1,  \tag{4.67}\\ +h_{\mathrm{ef}}, & \text { for } s_{j}=-1 .\end{cases}
$$

[^891]Such separability of energies means that in the Weiss approximation the spin fluctuations are independent, and their statistics may be examined individually, using energy spectrum $E_{j}$. But this is exactly the two-level system which was the subject of three exercise problems in Chapter 2. Actually, its statistics is so simple that it is easier to redo this fundamental problem starting from scratch, rather than to use the results of those exercises (which would require changing notation). Indeed, according to the Gibbs distribution (2.58)-(2.59), the equilibrium probabilities of states $s_{j}= \pm 1$ may be found as

$$
\begin{equation*}
W_{ \pm}=\frac{1}{Z} e^{ \pm h_{\mathrm{ef}} / T}, \quad Z=\exp \left\{+\frac{h_{\mathrm{ef}}}{T}\right\}+\exp \left\{-\frac{h_{\mathrm{ef}}}{T}\right\}=2 \cosh \frac{h_{\mathrm{ef}}}{T} . \tag{4.68}
\end{equation*}
$$

From here, we may readily calculate $F=-T \ln Z$ and other thermodynamic variables, but let us immediately use Eq. (68) to calculate the statistical average of $s_{j}$, i.e. the order parameter:

$$
\begin{equation*}
\eta \equiv\left\langle s_{j}\right\rangle=(+1) W_{+}+(-1) W_{-}=\frac{e^{+h_{\mathrm{ef}} / T}-e^{-h_{\mathrm{ef}} / T}}{2 \cosh \left(h_{\mathrm{ef}} / T\right)}=\tanh \frac{h_{\mathrm{ef}}}{T} \tag{4.69}
\end{equation*}
$$

Now comes the main trick of the Weiss' approach: plugging this result back into Eq. (65), we may write the condition of self-consistency of the molecular field theory:

$$
\begin{equation*}
h_{\mathrm{ef}}-h=2 J d \tanh \frac{h_{\mathrm{ef}}}{T} . \tag{4.70}
\end{equation*}
$$

This is a transcendental equation that evades an explicit analytical solution, but its properties may be readily understood by plotting its both parts as functions of their argument, so that the stationary state(s) of the system corresponds to the intersection point(s) of these plots.

First of all, let us explore the field-free case $(h=0)$, when $h_{\text {ef }}=h_{\text {mol }} \equiv 2 d J \eta$, so that Eq. (70) is reduced to

$$
\begin{equation*}
\eta=\tanh \left(\frac{2 J d}{T} \eta\right) \tag{4.71}
\end{equation*}
$$

giving one of the patterns sketched in Fig. 8, depending on the dimensionless parameter 2Jd/T.


Fig. 4.8. Ferromagnetic phase transition in Weiss' molecular-field theory: two sides of Eq. (71) plotted as functions of $\eta$ for 3 temperatures: above $T_{c}$ (red), below $T_{c}$ (blue) and equal to $T_{c}$ (green).

If this parameter is small, the right-hand part of Eq. (71) grows slowly with $\eta$ (red line in Fig. 8), and there is only one intersection point with the left-hand part plot, at $\eta=0$. This means that the spin system features no spontaneous magnetization - the so-called paramagnetic phase. However, if parameter $2 J d / T$ exceeds 1 , i.e. $T$ is decreased below the following critical value,

$$
\begin{equation*}
T_{c}=2 J d \tag{4.72}
\end{equation*}
$$

the right-hand part grows, at small $\eta$, faster than the left-hand part, so that their plots intersect it in 3 points: $\eta=0$ and $\eta= \pm \eta_{0}$. It is almost evident that the former stationary point is unstable while two latter points are stable. ${ }^{41}$ Thus, below $T_{c}$ the system is in the ferromagnetic phase, with one of two possible directions of spontaneous magnetization, so that the critical (Curie) temperature, given by Eq. (72), marks the transition between the paramagnetic and ferromagnetic phases. (Since the stable minimum value of energy $G$ is a continuous function of temperature at $T=T_{c}$, this is the continuous phase transition.)

Now let us repeat the same graphics to examine how each of these phases responds to external magnetic field $h \neq 0$. According to Eq. (70), the effect of $h$ is just a shift of the straight line plot of its left-hand part - see Fig. 9.


(b)

Fig. 4.9 External field effect on:
(a) a paramagnet ( $T>T_{\mathrm{c}}$ ), and
(b) a ferromagnet ( $T<T_{\mathrm{c}}$ ).

In the paramagnetic case (Fig. 9a) the resulting dependence $h_{\text {ef }}(h)$ is evidently continuous, but the coupling effect $(J>0)$ makes it more steep than it would be without spin interaction. This effect may be characterized by the low-field susceptibility defined by Eq. (29). To calculate it, let us notice that for small $h$, and hence $h_{\text {ef }}$, function tanh in Eq. (70) is approximately equal to argument, so that Eq. (70) becomes

$$
\begin{equation*}
h_{\mathrm{ef}}-h=\frac{2 J d}{T} h_{\mathrm{ef}} . \tag{4.73}
\end{equation*}
$$

Solving this equation for $h_{\text {ef }}$, and then using Eq. (72), we get

$$
\begin{equation*}
h_{\mathrm{ef}}=\frac{h}{1-2 J d / T}=\frac{h}{1-T_{c} / T} . \tag{4.74}
\end{equation*}
$$

Recalling Eq. (66), we can rewrite this result for the order parameter,

$$
\begin{equation*}
\eta=\frac{h_{\mathrm{ef}}-h}{T_{c}}=\frac{h}{T-T_{c}}, \tag{4.75}
\end{equation*}
$$

meaning that the low-field susceptibility

[^892]\[

$$
\begin{equation*}
\left.\chi \equiv \frac{\partial \eta}{\partial h}\right|_{h=0}=\frac{1}{T-T_{c}}, \quad \text { for } T>T_{c} \tag{4.76}
\end{equation*}
$$

\]

## Curie- <br> Weiss <br> law

This is the famous Curie-Weiss law, which shows that the susceptibility diverges at the approach to the Curie temperature $T_{c}$.

In the ferromagnetic case, the graphic solution (Fig. 9b) of Eq. (70) gives a qualitatively different result. A field increase leads, depending on the spontaneous magnetization, either the further saturation of $h_{\text {mol }}$ (with the order parameter $\eta$ gradually approaching 1 ), or, if the initial $\eta$ was negative, a jump to positive $\eta$ at some critical (coercive) field $h_{c}$. In contrast with the crude mean-field approximation (59), at $T>0$ the coercive field is smaller than that given by Eq. (60), and the magnetization saturation is gradual, in a good (semi-qualitative) accordance with experiment.

To summarize, the Weiss' molecular-field theory gives a more realistic description of the ferromagnetic and paramagnetic phases in the Ising model, and a very simple prediction (72) of the temperature of the phase transition between them, for an arbitrary dimensionality $d$ of the cubic lattice. It also allows finding all other parameters of the mean-field theory for that model - an easy exercise left for the reader.

### 4.5. Ising model: Exact and numerical results

In order to evaluate the main prediction (72) of the Weiss theory, let us now discuss the exact (analytical) and quasi-exact (numerical) results obtained for the Ising model, going from the lowest dimensionality $d=0$ to its higher values.

Zero dimensionality means that a spin has no nearest neighbors at all, so that the first term of Eq. (23) vanishes. Hence Eq. (64), with $h_{\text {ef }}=h$, is exact, and so is its solution (69). Now we can repeat the calculations that have led us to Eq. (76), with $J=0$, i.e. $T_{c}=0$, and reduce this result to the so-called Curie law:

$$
\begin{equation*}
\chi=\frac{1}{T} . \tag{4.77}
\end{equation*}
$$

It shows that $T_{\mathrm{c}}=0$, i.e. the system is paramagnetic at any temperature. One may say that for this case the Weiss molecular-field theory is exact - or in some sense trivial, because it provides an exact, fully quantum-mechanical treatment of spin- $1 / 2$ particles at negligible interaction. Experimentally, the Curie law is approximately valid for many so-called paramagnetic materials, i.e. 3D systems with a weak interaction between particle spins.

The case $d=1$ is more complex, but has an exact analytical solution. Probably the simplest way to obtain it is to use the so-called transfer matrix approach. ${ }^{42}$ For this, first of all, we may argue that properties of a 1D system of $N \gg 1$ spins (say, put at equal distances on a straight line) should not change noticeably if we bend that line gently into a closed loop (Fig. 10), i.e. assume that spins $s_{1}$ and $s_{N}$ form one more pair of next neighbors, giving one more contribution, $-J s_{1} s_{\mathrm{N}}$, to energy (23):

$$
\begin{equation*}
E_{m}=-\left(J s_{1} s_{2}+J s_{2} s_{3}+\ldots+J s_{N} s_{1}\right)-\left(h s_{1}+h s_{2}+\ldots+h s_{N}\right) . \tag{4.78}
\end{equation*}
$$

[^893]Let us regroup terms of this sum in the following way:

$$
\begin{equation*}
E_{m}=-\left[\left(\frac{h}{2} s_{1}+J s_{1} s_{2}+\frac{h}{2} s_{2}\right)+\left(\frac{h}{2} s_{2}+J s_{2} s_{3}+\frac{h}{2} s_{3}\right)+\ldots+\left(\frac{h}{2} s_{N}+J s_{N} s_{1}+\frac{h}{2} s_{1}\right)\right], \tag{4.79}
\end{equation*}
$$

so that the group in each parentheses depends only on the state of two adjacent spins. The corresponding statistical sum,

$$
\begin{equation*}
Z=\sum_{\substack{s_{j}= \pm 1 \\ j=1,2 \ldots N}} \exp \left\{h \frac{s_{1}}{2 T}+J \frac{s_{1} s_{2}}{T}+h \frac{s_{2}}{2 T}\right\} \exp \left\{h \frac{s_{2}}{2 T}+J \frac{s_{2} s_{3}}{T}+h \frac{s_{3}}{2 T}\right\} \ldots \exp \left\{h \frac{s_{N}}{2 T}+J \frac{s_{N} s_{1}}{T}+h \frac{s_{1}}{2 T}\right\}, \tag{4.80}
\end{equation*}
$$

has $2^{N}$ terms, each corresponding to a certain combination of signs of $N$ spins. Each operand of the product under the sum may take 4 values for 4 different combinations of its two arguments:

$$
\exp \left\{h \frac{s_{j}}{2 T}+J \frac{s_{j} s_{j+1}}{T}+h \frac{s_{j+1}}{2 T}\right\}=\left\{\begin{align*}
\exp \{(J+h) / T\}, & \text { for } s_{j}=s_{j+1}=+1  \tag{4.81}\\
\exp \{(J-h) / T\}, & \text { for } s_{j}=s_{j+1}=-1 \\
\exp \{-J / T\}, & \text { for } s_{j}=-s_{j+1}
\end{align*}\right.
$$



Fig. 4.10. 1D Ising system on a circular loop.

These values do not depend on index $j,{ }^{43}$ and may be presented as elements of the so-called transfer matrix

$$
M=\left(\begin{array}{cc}
\exp \{(J+h) / T\} & \exp \{-J / T\}  \tag{4.82}\\
\exp \{-J / T\} & \exp \{(J-h) / T\}
\end{array}\right),
$$

and the whole statistical sum may be recast as a product:

$$
\begin{equation*}
Z=\sum_{\substack{s_{j} \pm \pm 1 \\ j=1, \ldots, \ldots N}} M_{S_{1} s_{2}} M_{S_{2} s_{3}} \ldots M_{S_{N} s_{1}} . \tag{4.83}
\end{equation*}
$$

According to the basic rule of matrix multiplication, this sum is just

[^894]\[

$$
\begin{equation*}
\mathrm{Z}=\operatorname{Tr}\left(\mathrm{M}^{N}\right) \tag{4.84}
\end{equation*}
$$

\]

Matrix algebra tells us that this trace may be presented just as

$$
\begin{equation*}
Z=\lambda_{+}^{N}+\lambda_{-}^{N} \tag{4.85}
\end{equation*}
$$

where $\lambda_{ \pm}$are the eigenvalues of the transfer matrix M , i.e. the roots of its characteristic equation,

$$
\left|\begin{array}{cc}
\exp \{(J+h) / T\}-\lambda & \exp \{-J / T\}  \tag{4.86}\\
\exp \{-J / T\} & \exp \{(J-h) / T\}-\lambda
\end{array}\right|=0 .
$$

A straightforward calculation yields

$$
\begin{equation*}
\lambda_{ \pm}=\exp \left\{\frac{J}{T}\right\}\left[\cosh \frac{h}{T} \pm\left(\sinh ^{2} \frac{h}{T}+\exp \left\{-\frac{4 J}{T}\right\}\right)^{1 / 2}\right] \tag{4.87}
\end{equation*}
$$

Now the last simplification comes from condition $N \gg 1$ - which we needed anyway, to make the loop model equivalent to an in infinite 1D system. In this limit, even a small difference of exponents, $\lambda_{+}>\lambda_{\text {-, makes the second term in Eq. (85) negligible, so that we finally get }}$

$$
\begin{equation*}
Z=\lambda_{+}^{N}=\exp \left\{\frac{N J}{T}\right\}\left[\cosh \frac{h}{T}+\left(\sinh ^{2} \frac{h}{T}+\exp \left\{-\frac{4 J}{T}\right\}\right)^{1 / 2}\right]^{N} . \tag{4.88}
\end{equation*}
$$

From here, we can find the free energy per particle

$$
\begin{equation*}
\frac{F}{N}=\frac{T}{N} \ln \frac{1}{Z}=-J-T \ln \left[\cosh \frac{h}{T}+\left(\sinh ^{2} \frac{h}{T}+\exp \left\{-\frac{4 J}{T}\right\}\right)^{1 / 2}\right] \tag{4.89}
\end{equation*}
$$

and hence can calculate all variables of interest from thermodynamic relations. In particular, the equilibrium value of the order parameter may be found from the last of Eqs. (1.39), with the replacements discussed above: $G \rightarrow F, P \rightarrow-h$, and hence $V=(\partial G / \partial P)_{T} \rightarrow-(\partial F / \partial h)_{T}=N \eta$. For low fields ( $h \ll T$ ), this formula yields

$$
\begin{equation*}
\eta=\frac{h}{T} \exp \left\{\frac{2 J}{T}\right\} \tag{4.90}
\end{equation*}
$$

This result describes linear magnetization with the following low-field susceptibility,

$$
\begin{equation*}
\left.\chi \equiv \frac{\partial \eta}{\partial h}\right|_{h=0}=\frac{1}{T} \exp \left\{\frac{2 J}{T}\right\} \tag{4.91}
\end{equation*}
$$

and means that the 1D Ising model does not exhibit a phase transition, i.e., $T_{c}=0$. However, its susceptibility grows, at $T \rightarrow 0$, much faster than the Curie law (77). This gives us a hint that at low temperatures the system is "virtually ferromagnetic", with has the ferromagnetic order with some rare violations. (In physics, such violations are called low-temperature excitations.) This perception may be confirmed by the following approximate calculation.

It is almost evident that the lowest-energy excitation of a 1 D ferromagnet at $h=0$ is the reversal of signs of all spins in one of its parts (Fig. 11). Indeed, since such excitation (called the Bloch wall)
involves the change of sign of just one product $s_{j} s_{j}$, according to Eq. (23), its energy $E_{W}$ (defined as the difference between values of $E_{m}$ with and without the excitation) equals $2 J$, regardless of the wall position. Since in a ferromagnet, parameter $J$ is positive, $E_{W}>0$. If the system tried to minimize its potential energy, having any wall in the system would be energy-disadvantageous. However, thermodynamics tells us that at finite $T$, system's equilibrium corresponds to the minimum of free energy rather than just energy. ${ }^{44}$ Hence, we have to calculate Bloch wall's contribution $F_{W}$ to the free energy. Since in a linear chain of $N \gg 1$ spins, the wall can take $(N-1) \approx N$ positions with the same energy $E_{W}$, we may claim that the entropy $S_{W}$ associated with an excitation of this type is $\ln N$, and its according to definition (1.33) of the free energy,

$$
\begin{equation*}
F_{W}=E_{W}-T S_{W} \approx 2 J-T \ln N . \tag{4.92}
\end{equation*}
$$



Fig. 4.11. A Bloch wall in a 1D Ising system.

This result tells us that in the limit $N \rightarrow \infty$, and at $T \neq 0$, walls are always free-energy-beneficial, thus explaining the absence of the perfect ferromagnetic order in the 1D Ising system. Note, however, that since the logarithm grows extremely slowly at large values of its argument, one may argue that a large but finite 1D system would still feature a quasi-critical temperature

$$
\begin{equation*}
" T_{c} "=\frac{2 J}{\ln N}, \tag{4.93}
\end{equation*}
$$

below which it would feature a virtually complete ferromagnetic order. (The exponentially large susceptibility (91) is a manifestation of this fact.)

Now let us apply a similar approach to estimate $T_{c}$ of a 2D Ising model. Here the Bloch wall is a line of certain length $L$ - see Fig. 12. (For this example, counting from the left to the right, $L=2+1+4$ $+2+3=12$ lattice periods.)


Fig. 4.12. A Bloch wall in a 2D Ising system.

Evidently, the additional energy associated with such wall is $E_{\mathrm{W}}=2 J L$, while wall's entropy may be estimated approximately using the following reasoning. Let the wall be formed by the path of a "Manhattan pedestrian" traveling through the lattice between its nodes. At each junction, the pedestrian

[^895]may select 3 choices of 4 directions (except the one that leads backward), so that there are approximately $3^{(L-1)}$ options for a walk starting from a certain point, i.e. approximately $M \sim 2(N-$ 1) ${ }^{1 / 2} \times 3^{L} \approx 2 N^{1 / 2} 3^{L}$ different walks starting from two sides of a square-shaped lattice (of linear size $N^{1 / 2}$ ). Again calculating $S_{W}$ as $\ln M$, we get
\[

$$
\begin{equation*}
F_{W}=E_{W}-T S_{W} \approx 2 J L-T \ln \left(2 N^{1 / 2} \times 3^{L}\right)=L(2 J-T \ln 3)-T \ln \left(2 N^{1 / 2}\right) . \tag{4.94}
\end{equation*}
$$

\]

Since $L$ scales as $N^{1 / 2}$ or higher, at $N \rightarrow \infty$ the last term is negligible, and we see that sign of $\partial F_{W} / \partial L$ depends on whether the temperature is higher or lower than the following critical value

$$
\begin{equation*}
T_{c}=\frac{2}{\ln 3} J \approx 1.82 \mathrm{~J} . \tag{4.95}
\end{equation*}
$$

At $T<T_{c}$, the Free energy minimum corresponds to $L \rightarrow 0$, i.e. Bloch walls are free-energy-beneficial, and the system is in the ferromagnetic phase.

So, for $d=2$ the estimates predict a finite critical temperature of the same order as the Weiss' theory $\left(T_{\mathrm{c}}=4 J\right)$. The major approximation in the calculation leading to Eq. (95) is disregarding possible self-crossing of the "Manhattan walk". An accurate counting of such self-crossings is rather difficult. It had been carried out in 1944 by L. Onsager; since then his calculations have been redone in several easier ways, but even they are rather cumbersome, and I will not have time to discuss then in detail. ${ }^{45}$ The final result, however, is surprisingly simple:

$$
\begin{equation*}
\tanh \frac{J}{T_{c}}=\sqrt{2}-1, \quad \text { giving } T_{c} \approx 2.269 \mathrm{~J} \tag{4.96}
\end{equation*}
$$

Onsager's result
i.e. showing that the simple estimate (95) is only $\sim 20 \%$ off the mark.

The Onsager solution, as well as all alternative solutions of the problem that were found later, are so "artificial" (2D-specific) that they do not give a clear clue to their generalization to other (higher) dimensions. As a result, the 3D Ising problem is still unsolved analytically. Nevertheless, we do know $T_{c}$ for that case with an extremely high precision - at least to the $6^{\text {th }}$ decimal place. This has been achieved by numerical methods; they deserve a thorough discussion, are applicable to other problems as well. Conceptually, this task is rather simple: just compute, to the desired precision, the statistical sum of system (23):

$$
\begin{equation*}
Z=\sum_{\substack{s_{j}= \pm 1 \\ j=1,2, \ldots, N}} \exp \left\{\frac{J}{T} \sum_{\left\{j, j^{\prime}\right\}} s_{j} s_{j^{\prime}}+\frac{h}{T} \sum_{j} s_{j}\right\} . \tag{4.97}
\end{equation*}
$$

As soon as this has been done for a sufficient number of values of dimensionless parameters $J / T$ and $h / T$, everything else is easy; in particular, we can compute the dimensionless function

$$
\begin{equation*}
F / T=-\ln Z \tag{4.98}
\end{equation*}
$$

and then find the ratio $J / T_{c}$ as the smallest value of parameter $J / T$, at that $F / T$ (as a function of ratio $h / T$ ) has a minimum at zero field. However, for any system of a reasonable size $N$, the "exact" computation of the statistical sum (97) is impossible, because it contains to many terms for any supercomputer to

[^896]handle. For example, let us take a relatively small 3D lattice with $N=10 \times 10 \times 10=10^{3}$ spins, which still feature substantial boundary effects even using the periodic boundary conditions (similar to the BornKarman conditions in the wave theory), so that its phase transition is smeared about $T_{c}$ by $\sim 1 \%$. Still, even for that crude model, $Z$ would include $2^{1,000}=\left(2^{10}\right)^{100} \approx\left(10^{3}\right)^{100}=10^{300}$ terms. Let us suppose we are using a prospective exaflops-scale computer performing $10^{18}$ floating-point operations per second, i.e. $\sim 10^{26}$ such operations per year. With those resources, the computation of just one statistical sum would require $\sim 10^{(300-26)}=10^{274}$ years. To call such number "astronomic" would be a strong understatement. (As a reminder, the age of our Universe is believed to be close to $1.3 \times 10^{10}$ years -a very humble number in comparison.)

This situation may be improved dramatically by noticing that any statistical sum,

$$
\begin{equation*}
Z=\sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\} \tag{4.99}
\end{equation*}
$$

is dominated by terms with lower values of $E_{m}$. In order to find those lowest-energy states, we may use the following powerful approach (belonging to a broad class of Monte-Carlo techniques), which essentially mimics one (randomly selected) path of system's evolution in time. One could argue that for that we would need to know the exact laws of evolution of statistical systems, ${ }^{46}$ that may differ from one system to another, even if their energy spectra $E_{m}$ are the same. This is true, but since the equilibrium value of $Z$ should be independent of these details, it may be evaluated using any kinetic model, provided that it satisfies certain general rules. In order to reveal these rules, let us start from a system with just two states, $E_{m}$ and $E_{m}=E_{m}+\Delta$ - see Fig. 13.


Fig. 4.13. Deriving the detailed balance equation.

In the absence of quantum coherence between the states (see Sec. 2.1), equations for time evolution of the corresponding probabilities $W_{m}$ and $W_{m}$, should depend only on the probabilities (plus certain constant coefficients). Moreover, since equations of quantum mechanics are linear, the equations of probability evolution should be also linear. Hence, it is natural to expect them to have the following form,

$$
\begin{equation*}
\frac{d W_{m}}{d t}=W_{m^{\prime}} \Gamma_{\downarrow}-W_{m} \Gamma_{\uparrow}, \quad \frac{d W_{m^{\prime}}}{d t}=W_{m} \Gamma_{\uparrow}-W_{m^{\prime}} \Gamma_{\downarrow} \tag{4.100}
\end{equation*}
$$

where constant coefficients $\Gamma \uparrow$ and $\Gamma \downarrow$ have the physical sense of rates of the corresponding transitions see Fig. 13. According to the master equations (100) the rates have simple meaning: for example, $\Gamma \uparrow d t$ is the probability of the system's transition into state $m^{\prime}$ during an infinitesimal time interval $d t$, provided that in the beginning of that interval it was in state $m$ with full certainty: $W_{m}=1, W_{m^{\prime}}=0 .{ }^{47}$

[^897]Since for the system with just two energy levels, the time derivatives of the probabilities are equal and opposite, Eqs. (100) describe an (irreversible) redistribution of the probabilities while keeping their sum $W=W_{m}+W_{m}$, constant. At $t \rightarrow \infty, d / d t \rightarrow 0$, and the probabilities settle to their stationary values related as

$$
\begin{equation*}
\frac{W_{m^{\prime}}}{W_{m}}=\frac{\Gamma_{\uparrow}}{\Gamma_{\downarrow}} . \tag{4.101}
\end{equation*}
$$

Now let us require that these stationary values obey the Gibbs distribution (2.58); then

$$
\begin{equation*}
\frac{W_{m^{\prime}}}{W_{m}}=\exp \left\{\frac{E_{m}-E_{m^{\prime}}}{T}\right\}=\exp \left\{-\frac{\Delta}{T}\right\}<1 . \tag{4.102}
\end{equation*}
$$

Comparing these two expressions, we see that the rates have to satisfy the following detailed balance relation

$$
\begin{equation*}
\frac{\Gamma_{\uparrow}}{\Gamma_{\downarrow}}=\exp \left\{-\frac{\Delta}{T}\right\} . \tag{4.103}
\end{equation*}
$$

By the way, this relation may serve as an important sanity check: the rates calculated using any reasonable model of a quantum system have to satisfy it. ${ }^{48}$

Now comes the final argument: since the rates of transition between two particular states should not depend on other states and their occupation, Eq. (103) has to be valid for each pair of states of any multi-state system. The detailed balance yields only one equation for two rates $\Gamma_{\uparrow}$ and $\Gamma_{\downarrow}$; if our only goal is the calculation of $Z$, the choice of the other equation is not too important. Perhaps the simplest choice is

$$
\Gamma(\Delta) \propto \gamma(\Delta) \equiv\left\{\begin{array}{lc}
1, & \text { if } \Delta<0  \tag{4.104}\\
\exp \{-\Delta / T\}, & \text { otherwise }
\end{array}\right.
$$

where $\Delta$ is the energy change resulting from the transition. This model, which evidently satisfies the detailed balance relation (103), is the most popular for its simplicity, despite the uphysical cusp this function has at $\Delta=0$. The simplicity of Eq. (104) enables the following Metropolis algorithm (Fig. 14). The calculation starts from setting a certain initial state of the system. At relatively high temperatures, the state may be generated randomly; for example, for the Ising system, the initial state of each spin $s_{j}$ may be selected independently, with the $50 \%$ probability. At low temperatures, starting the calculations from the lowest-energy state (in particular, for the Ising model, from the ferromagnetic state $s_{j}=\operatorname{sgn}(h)$ $=$ const) may give the fastest convergence of the sum (97).

Now one spin is flipped at random, and the corresponding change of energy $(\Delta)$ is calculated, ${ }^{49}$ and plugged into Eq. (104) to calculate $\gamma(\Delta)$. Next, a pseudo-random number generator is used to generate a random number $\xi$, with the probability density uniformly distributed on segment $[0,1]$. (Such

[^898]functions, typically called RND, are available in virtually any numerical library.) If the resulting $\xi$ is less than $\gamma(\Delta)$, the transition is accepted, while if $\xi>\gamma(\Delta)$, it is rejected. In the view of Eq. (104), this means that any transition down the energy spectrum $(\Delta<0)$ are always accepted, while those up the energy profile $(\Delta>0)$ are accepted with the probability proportional to $\exp \{-\Delta / T\}$. The latter feature is necessary to avoid system trapping in local minima of its multidimensional energy profile $E_{m}\left(s_{1}, s_{2}, \ldots, s_{N}\right)$. Now the statistical sum may be calculated approximately as a partial sum over the states passed by the system. (It is better to discard the contributions from a few first steps to avoid an error due to the initial state choice.)


Fig. 4.14. Crude scheme of the Monte Carlo algorithm for the Ising model simulation.

This algorithm is extremely efficient. Even with modest computers available in the 1980s, it has allowed to simulate a 3D Ising system of $(128)^{3}$ spins to get the following result: $J / T_{c} \approx 0.221650 \pm$ 0.000005 . For all practical purposes, this result is exact (so that perhaps the largest benefit of the possible analytical solution for the infinite 3D Ising system would be a virtually certain Nobel Prize for the author :-). Table 2 summarizes values of $T_{c}$ for the Ising model. Very visible is the fast improvement of prediction accuracy of the molecular-field theory - which is asymptotically correct at $d \rightarrow \infty$.

Table 2. Critical temperature $T_{c}$ (in the units of $J$ ) of the Ising model of a ferromagnet $(J>0)$ for several values of dimensionality $d$

| $d$ | Molecular-field theory - Eq. (72) | Exact value | Exact value's source |
| :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | Gibbs distribution |
| 1 | 2 | 0 | Transfer matrix theory |
| 2 | 4 | $2.269 \ldots$ | Onsager's solution |
| 3 | 6 | $4.513 \ldots$ | Numerical simulation |

Finally, I need to mention the renormalization-group ("RG") approach, ${ }^{50}$ despite its low efficiency for the Ising problem. The basic idea of this approach stems from the scaling law (30)-(31): at $T=T_{c}$ the correlation radius $r_{c}$ diverges. Hence, the critical temperature may be found from the requirement for the system to be spatially self-similar. Namely, let us form larger and larger groups ("blocks") of adjacent spins, and require that all properties of the resulting system of the blocks approach those of the initial system, as $T$ approaches $T_{c}$.

Let us see how does this idea work for the simplest nontrivial (1D) case, which is described by statistical sum (80). Assuming $N$ to be even (which does not matter at $N \rightarrow \infty$ ), and adding an inconsequential constant $C$ to each exponent (for the purpose that will be clear later on), we may rewrite this expression as

$$
\begin{equation*}
Z=\sum_{s_{j}= \pm 1} \prod_{j=1,2, \ldots N} \exp \left\{\frac{h}{2 T} s_{j}+\frac{J}{T} s_{j} s_{j+1}+\frac{h}{2 T} s_{j+1}+C\right\} \tag{4.105}
\end{equation*}
$$

Let us group each two adjacent exponents to recast this expression as a product over only even numbers j,

$$
\begin{equation*}
Z=\sum_{s_{j}= \pm 1} \prod_{j=2,4, \ldots N} \exp \left\{\frac{h}{2 T} s_{j-1}+s_{j}\left[\frac{J}{T}\left(s_{j-1}+s_{j+1}\right)+\frac{h}{T}\right]+\frac{h}{2 T} s_{j+1}+2 C\right\} \tag{4.106}
\end{equation*}
$$

and carry out the summation over two possible states of the internal spins $s_{j}$ explicitly:

$$
\begin{align*}
Z & =\sum_{\substack{\left.s_{j}= \pm 1 \\
\text { (for odd } j\right)}} \prod_{j=2,4, \ldots N}\left[\begin{array}{l}
\exp \left\{\frac{h}{2 T} s_{j-1}+\frac{J}{T}\left(s_{j-1}+s_{j+1}\right)+\frac{h}{T}+\frac{h}{2 T} s_{j+1}+2 C\right\} \\
+\exp \left\{\frac{h}{2 T} s_{j-1}-\frac{J}{T}\left(s_{j-1}+s_{j+1}\right)-\frac{h}{T}+\frac{h}{2 T} s_{j+1}+2 C\right\}
\end{array}\right]  \tag{4.107}\\
& =\sum_{\substack{\left.s_{j} \pm 11 \\
\text { (for odd } j\right)}} \prod_{j=2,4, \ldots N} 2 \cosh \left\{\frac{J}{T}\left(s_{j-1}+s_{j+1}\right)+\frac{h}{T}\right\} \exp \left\{\frac{h}{2 T}\left(s_{j-1}+s_{j+1}\right)+2 C\right\} .
\end{align*}
$$

Now let us require this statistical sum (and hence all statistical properties of the system of 2-spin blocks) to be identical to that of the Ising system of $N / 2$ spins, numbered by odd $j$ :

$$
\begin{equation*}
Z^{\prime}=\sum_{\substack{s_{j}= \pm 1 \\\left(\text { for odd } s_{j}\right)}} \prod_{j=2,4, \ldots, N} \exp \left\{\frac{J^{\prime}}{T} s_{j-1} s_{j+1}+\frac{h^{\prime}}{T} s_{j+1}+C^{\prime}\right\} \tag{4.108}
\end{equation*}
$$

with some different parameters $h^{\prime}, J^{\prime}$, and $C^{\prime}$, for all 4 possible values of $s_{j-1}= \pm 1$ and $s_{j+1}= \pm 1$. Since the right-hand part of Eq. (107) depends only on the sum $\left(s_{j-1}+s_{j+1}\right)$, this requirement yields only 3 (rather than 4) independent equations for finding $h^{\prime}, J^{\prime}$, and $C^{\prime}$. Of them, equations for $h$ ' and $J^{\prime}$ depend only on $h$ and $J$ (but not on $C$ ), ${ }^{51}$ and may be presented in an especially simple form,

[^899]equations for 1D Ising model
\[

$$
\begin{equation*}
x^{\prime}=\frac{x(1+y)^{2}}{(x+y)(1+x y)}, \quad y^{\prime}=\frac{y(x+y)}{1+x y} \tag{4.109}
\end{equation*}
$$

\]

using notation

$$
\begin{equation*}
x \equiv \exp \left\{-4 \frac{J}{T}\right\}, \quad y \equiv \exp \left\{-2 \frac{h}{T}\right\} . \tag{4.110}
\end{equation*}
$$

Now the grouping procedure may be repeated, with the same result (109)-(110). Hence these equations may be considered as recurrence relations describing repeated doubling of the spin block size. Figure 15 shows (schematically) the trajectories of this dynamic system on the phase plane $[x, y]$. (A trajectory is defined by the following property: for each of its points $\{x, y\}$, the point $\left\{x^{\prime}, y^{\prime}\right\}$ defined by the "mapping" Eq. (109) is also on the same trajectory.) For ferromagnetic coupling ( $J>0$ ) and $h>0$, we may limit the analysis to the unit square $0 \leq x, y \leq 1$. If this flow diagram had a stable fixed point with $x^{\prime}=x=x_{\infty} \neq 0$ (i.e. $T / J<\infty$ ) and $y^{\prime}=y=1$ (i.e. $h=0$ ), then the first of Eqs. (110) would immediately give us the critical temperature of the phase transition in the field-free system:

$$
\begin{equation*}
T_{c}=\frac{4 J}{\ln \left(1 / x_{\infty}\right)} . \tag{4.111}
\end{equation*}
$$

However, Fig. 15 shows that the only fixed point of the 1 D system is $x=y=0$, which (at finite coupling $J)$ should be interpreted as $T_{c}=0$. This is of course in agreement with the exact result of the transfermatrix analysis, but does not give any additional information.

$$
y=\exp \left\{-\frac{2 h}{T}\right\} \uparrow \text { Coment }
$$

Fig. 4.15. The RG flow diagram of the 1D Ising system (schematically).

Unfortunately, for higher dimensionalities the renormalization-group approach rapidly becomes rather cumbersome, and requires certain approximations, whose accuracy cannot be easily controlled. For 2D Ising system, such approximations lead to the prediction $T_{\mathrm{c}} / J \approx 2.55$, i.e. to a substantial difference from the exact (Onsager's) result.

### 4.6. Exercise problems

4.1. Compare the third virial coefficient $C(T)$ for the hardball model of particle interactions, that follows from the van der Waals equation, with the exact result (whose calculation was the subject of Problem 3.18).
4.2. Calculate the entropy and the internal energy of the van der Waals gas, and discuss the results.
4.3. Use two different approaches to calculate $(\partial E / \partial V)_{T}$ for the van der Waals gas, and the change of temperature of such a gas, with temperature-independent $C_{V}$, at its fast expansion into free space.
4.4.* Derive as many analytical results as you can for temperature dependence of the phaseequilibrium pressure $P_{0}(T)$ and the latent heat $\Lambda(T)$ within the van der Waals model. In particular, explore the low-temperature limit $\left(T \ll T_{C}\right)$, and the close vicinity of the critical point $T_{C}$.
4.5.* Calculate the critical values $P_{c}, V_{c}$, and $T_{c}$ for the so-called Redlich-Kwong model of the real gas, with the following phenomenological equation of state: ${ }^{52}$

$$
P+\frac{a}{V(V+N b) T^{1 / 2}}=\frac{N T}{V-N b} .
$$

Hint: Be prepared to solve a cubic equation with particular (numerical) coefficients.
4.6. Use the Clapeyron-Clausius formula (4.17) to calculate the latent heat $\Lambda$ of the BoseEinstein condensate, and compare the result with that obtained in Problem 3.18.
4.7. In the simplest model of the liquid-gas equilibrium, ${ }^{53}$ temperature and pressure do not affect molecule's condensation energy $\Delta$. Calculate the concentration and pressure of the gas over liquid's surface, assuming that its molecules are classical, non-interacting particles.
4.8. Assuming the hardball model, with volume $V_{0}$ per molecule, for the liquid phase, but still treating the gaseous phase an ideal gas, describe how do the results of the previous problem change if the liquid phase is in the form of spherical drops of radius $R \gg V_{0}{ }^{1 / 3}$. Briefly discuss the implications of the result for water cloud formation.
4.9. A classical ideal gas of $N \gg 1$ particles is placed into a container of volume $V$ and wall surface area $A$. The particles may condense on container walls, loosing potential energy $\Delta$ per particle, and forming an ideal 2D gas. Calculate the equilibrium number of condensed particles and gas pressure, and discuss their temperature dependences.
4.10. The inner surfaces of the walls of a closed container of volume $V$, filled with $N \gg 1$ indistinguishable particles, have $N_{S} \gg 1$ similar traps (small potential wells). Each trap can hold only one particle, at energy $-\Delta<0$. Assuming that the gas is ideal and classical, derive the equation for the chemical potential $\mu$ of the system in equilibrium, and use it to calculate the potential and the gas pressure in the limits of small and large values of the ratio $N / N_{S}$.

[^900]4.11. Superconductivity may be suppressed by a sufficiently strong magnetic field. In the simplest case of a bulk, long cylindrical sample of the type-I superconductor, placed into an external magnetic field $\mathcal{B}_{\text {ext }}$ parallel to its surface, this suppression takes a form of a simultaneous transition of the whole sample from the superconducting to the "normal" (non-superconducting) state at certain critical magnitude $B_{c}(T)$. The critical field gradually decreases with temperature from the maximum value $B_{c}(0)$ at $T \rightarrow 0$ to zero at the critical temperature $T_{c}$. Assuming that the function $B_{c}(T)$ is known, calculate the latent heat of transition as a function of temperature, and find its values at $T \rightarrow 0$ and $T=$ $T_{c}$.

Hint: In this context, "bulk" means a sample much larger than the intrinsic length scales of the superconductor (such as the London penetration depth $\delta_{\mathrm{L}}$ and the coherence length $\xi$ ). ${ }^{54}$ For such bulk samples, magnetic properties of the superconducting state may be well described just as a perfect diamagnetism, with zero magnetic permeability $\mu$.
4.12. In some textbooks, the discussion of thermodynamics of superconductivity is started with displaying, as self-evident, the following formula:

$$
F_{n}(T)-F_{s}(T)=\frac{B_{c}^{2}(T)}{2 \mu_{0}} V,
$$

where $F_{s}$ and $F_{n}$ are the free energy values in the superconducting and non-superconducting ("normal") phases, and $B_{c}(T)$ is the critical value of field. Is this formula correct, and if not, what modification is necessary to make it valid? Assume that all conditions of the simultaneous field-induced phase transition in the whole sample, spelled out in the previous problem, are satisfied.
4.13. In Sec. 4, we have discussed Weiss' molecular-field approach to the Ising model, in which the lattice average $\left\langle s_{j}\right\rangle$ plays the role of the order parameter $\eta$. Use the results of that analysis to find coefficients $a$ and $b$ in the corresponding Landau expansion (46) of the free energy. List the values of critical exponents $\alpha$ and $\beta$, defined by Eqs. (26) and (28), within this approach.
4.14. Calculate the average order parameter and the low-field susceptibility $\chi$ of a ring of three Ising-type "spins" $\left(s_{j}= \pm 1\right)$, with similar ferromagnetic coupling $J$ between all sites, in thermal equilibrium. From the result, can you predict the low-temperature behavior of $\chi$ in an $N$-spin ring?
4.15. Use Eq. (88) to calculate the average energy, free energy, entropy and heat capacity (all per lattice site), as functions of temperature $T$ and field $h$, for the 1D Ising model. Sketch the temperature dependence of the heat capacity for various values of ratio $h / J$, and give a physical interpretation of the result.
4.16. Use the molecular-field theory to calculate the critical temperature and low-field susceptibility of a d-dimensional cubic lattice of spins described by the so-called classical Heisenberg model: 55

[^901]$$
E_{m}=-J \sum_{\left.\left\{, j^{\prime}\right)^{\prime}\right\}} \mathbf{s}_{j} \cdot \mathbf{s}_{j^{\prime}}-\sum_{j} \mathbf{h} \cdot \mathbf{s}_{j} .
$$

Here, in contrast to the (otherwise, very similar) Ising model (23), the spin of each site is modeled by a classical 3D vector $\mathbf{s}_{j}=\left\{s_{x j}, s_{y j}, s_{z j}\right\}$ of unit length: $s_{j}^{2}=1$.

## Chapter 5. Fluctuations

This chapter discusses fluctuations of statistical variables, mostly at thermodynamic equilibrium. In particular, I will describe the intimate connection between fluctuations and dissipation (damping) in a dynamic system weakly coupled to a multi-particle environment, which culminates in the Einstein relation between the diffusion coefficient and mobility, the Nyquist formula, and their quantummechanical generalization - the fluctuation-dissipation theorem. An alternative approach to the same problem, based on the Smoluchowski and Fokker-Planck equations, is also discussed in brief.

### 5.1. Characterization of fluctuations

In the beginning of Chapter 2, we have discussed the notion of averaging, $\langle f\rangle$, of a variable $f$ over a statistical ensemble - see Eqs. (2.7) and (2.10). Now, the variable's fluctuation may be defined simply as its deviation from the average:

$$
\begin{equation*}
\widetilde{f} \equiv f-\langle f\rangle \tag{5.1}
\end{equation*}
$$

this deviation is, evidently, also a random variable. The most important property of any fluctuation is that its average (over the same statistical ensemble) equals zero:

$$
\begin{equation*}
\langle\tilde{f}\rangle=\langle f-\langle f\rangle\rangle=\langle f\rangle-\langle\langle f\rangle\rangle=\langle f\rangle-\langle f\rangle=0 \tag{5.2}
\end{equation*}
$$

As a result, such average cannot characterize fluctuations' intensity, whose simplest characteristic is the variance (also called "dispersion"):

Variance: definition

Th

$$
\begin{equation*}
\left\langle\widetilde{f}^{2}\right\rangle=\left\langle(f-\langle f\rangle)^{2}\right\rangle \tag{5.3}
\end{equation*}
$$

The following simple property of the variance is frequently convenient for its calculation:

$$
\begin{equation*}
\left\langle\widetilde{f}^{2}\right\rangle=\left\langle(f-\langle f\rangle)^{2}\right\rangle=\left\langle f^{2}-2 f\langle f\rangle+\langle f\rangle^{2}\right\rangle=\left\langle f^{2}\right\rangle-2\langle f\rangle^{2}+\langle f\rangle^{2} \tag{5.4a}
\end{equation*}
$$

so that, finally:
Variance via

As the simplest example of its application, consider a variable which can take only two values, $\pm 1$, with equal probabilities $W_{j}=1 / 2$. For such a variable,

$$
\begin{gather*}
\langle f\rangle=\sum_{j} W_{j} f_{j}=\frac{1}{2}(+1)+\frac{1}{2}(-1)=0, \quad \text { but }\left\langle f^{2}\right\rangle=\sum_{j} W_{j} f_{j}^{2}=\frac{1}{2}(+1)^{2}+\frac{1}{2}(-1)^{2}=1,  \tag{5.5}\\
\text { so that }\left\langle\tilde{f}^{2}\right\rangle=\left\langle f^{2}\right\rangle-\langle f\rangle^{2}=1 .
\end{gather*}
$$

The square root of variance,
R.m.s. fluctuation

$$
\begin{equation*}
\delta f \equiv\left\langle\widetilde{f}^{2}\right\rangle^{1 / 2} \tag{5.6}
\end{equation*}
$$

is called the root-mean-square (r.m.s.) fluctuation. An advantage of this measure is that it has the same dimensionality as the variable itself, so that ratio $\delta f /\langle f\rangle$ is dimensionless, and may be used to characterize the relative intensity of fluctuations. In particular, as has been mentioned in Chapter 1, all results of thermodynamics are valid only if the fluctuations of thermodynamic variables (internal energy $E$, entropy $S$, etc.) are relatively small. ${ }^{1}$ Let us make the simplest estimate of the relative intensity of fluctuations by considering a system of $N$ independent, similar particles, and an extensive variable

$$
\begin{equation*}
7 \equiv \sum_{j=1}^{N} f_{j} \tag{5.7}
\end{equation*}
$$

where $f_{j}$ depends on the state of just one $\left(j^{\text {th }}\right)$ particle. The statistical average of $\neq$ is evidently

$$
\begin{equation*}
\langle\boldsymbol{\chi}\rangle=\sum_{j=1}^{N}\langle f\rangle=N\langle f\rangle, \tag{5.8}
\end{equation*}
$$

while the variance is

$$
\begin{equation*}
\left\langle\widetilde{\boldsymbol{f}}^{2}\right\rangle=\left\langle\sum_{j=1}^{N} \widetilde{f}_{j} \sum_{j^{\prime}=1}^{N} \widetilde{f}_{j^{\prime}}\right\rangle=\left\langle\sum_{j, j^{\prime}=1}^{N} \widetilde{f}_{j} \widetilde{f}_{j^{\prime}}\right\rangle=\sum_{j, j^{\prime}=1}^{N}\left\langle\widetilde{f}_{j} \widetilde{f}_{j^{\prime}}\right\rangle . \tag{5.9}
\end{equation*}
$$

Now we may use the fact that for two independent variables

$$
\begin{equation*}
\left\langle\widetilde{f}_{j} \widetilde{f}_{j^{\prime}}\right\rangle=0 ; \tag{5.10}
\end{equation*}
$$

actually, this equation may be considered as the mathematical definition of the independence. Hence, in the sum (9), only the terms with $j^{\prime}=j$ survive, and

$$
\begin{equation*}
\left\langle\widetilde{f}^{2}\right\rangle=\sum_{j, j^{\prime}=1}^{N}\left\langle\widetilde{f}_{j}^{2}\right\rangle \delta_{j, j^{\prime}}=N\left\langle\widetilde{f}^{2}\right\rangle . \tag{5.11}
\end{equation*}
$$

Comparing Eqs. (8) and (11), we see that the relative intensity of fluctuations of variable $\mathcal{\neq}$,

$$
\begin{equation*}
\frac{\delta 7}{\langle 7\rangle}=\frac{1}{N^{1 / 2}} \frac{\delta f}{\langle f\rangle} \tag{5.12}
\end{equation*}
$$

Relative fluctuation estimate
tends to zero as the system size grows $(N \rightarrow \infty)$. It is this fact that justifies the thermodynamic approach to typical physical systems, with the number $N$ of particles of the order of the Avogadro number $N_{\mathrm{A}} \approx$ $10^{24}$. Nevertheless, in many situations even small fluctuations of thermodynamic variables are important, and in this chapter we will calculate their basic properties, starting from the variance.

It will be pleasant for the reader to notice that for some simple (but important) cases, such calculation has already been done in our course. For example, for any generalized coordinate $q_{j}$ and generalized momentum $p_{j}$ that give quadratic contributions to system's Hamiltonian (2.46), we have derived the equipartition theorem (2.48), valid in the classical limit. Since the average values of these

[^902]variables, in the thermodynamic equilibrium, equal zero, Eq. (6) immediately yields their r.m.s. fluctuations:
\[

$$
\begin{equation*}
\delta p_{j}=(m T)^{1 / 2}, \quad \delta q_{j}=\left(\frac{T}{m \omega^{2}}\right)^{1 / 2} . \tag{5.13}
\end{equation*}
$$

\]

The generalization of these classical relations to the quantum-mechanical case $(T \sim \hbar \omega)$ for a 1D harmonic oscillator is provided by Eqs. (2.78) and (2.81):

$$
\begin{equation*}
\delta p_{j}=\left[\frac{\hbar m \omega}{2} \operatorname{coth} \frac{\hbar \omega}{2 T}\right]^{1 / 2}, \quad \delta q_{j}=\left[\frac{\hbar}{2 m \omega} \operatorname{coth} \frac{\hbar \omega}{2 T}\right]^{1 / 2} . \tag{5.14}
\end{equation*}
$$

However, the intensity of fluctuations in other systems requires special calculations. Moreover, only a few cases allow for general, model-independent results. Let us review some of them.

### 5.2. Energy and the number of particles

First of all, note that fluctuations of macroscopic variables depend on particular conditions. ${ }^{2}$ For example, in a mechanically- and thermally-insulated system, e.g., a member of a microcanonical ensemble, there are no fluctuations of internal energy: $\delta E=0$.

However, if a system is in a thermal contact with environment, for example is a member of a canonical ensemble (Fig. 2.6), the Gibbs distribution (2.58)-(2.59) is valid. We already know that application of this distribution to energy itself,

$$
\begin{equation*}
\langle E\rangle=\sum_{m} W_{m} E_{m}, \quad W_{m}=\frac{1}{Z} \exp \left\{-\frac{E_{m}}{T}\right\}, \quad Z=\sum_{m} \exp \left\{-\frac{E_{m}}{T}\right\}, \tag{5.15}
\end{equation*}
$$

yields Eq. (2.61b), which may be rewritten in the form

$$
\begin{equation*}
\langle E\rangle=\frac{1}{Z} \frac{\partial Z}{\partial(-\beta)}, \quad \text { with } \beta \equiv \frac{1}{T}, \tag{5.16}
\end{equation*}
$$

more convenient for our current purposes. Now let us carry out a similar calculation for variable $E^{2}$ :

$$
\begin{equation*}
\left\langle E^{2}\right\rangle=\sum_{m} W_{m} E_{m}^{2}=\frac{1}{Z} \sum_{m} E_{m}^{2} \exp \left\{-\beta E_{m}\right\} . \tag{5.17}
\end{equation*}
$$

It is straightforward to check, by double differentiation, that this expression may be rewritten as

$$
\begin{equation*}
\left\langle E^{2}\right\rangle=\frac{1}{Z} \frac{\partial^{2}}{\partial(-\beta)^{2}} \sum_{m} \exp \left\{-\beta E_{m}\right\}=\frac{1}{Z} \frac{\partial^{2} Z}{\partial(-\beta)^{2}} . \tag{5.18}
\end{equation*}
$$

Now it is straightforward to use Eq. (4) to calculate the energy fluctuation variance:

$$
\begin{equation*}
\left\langle\widetilde{E}^{2}\right\rangle=\left\langle E^{2}\right\rangle-\langle E\rangle^{2}=\frac{1}{Z} \frac{\partial^{2} Z}{\partial(-\beta)^{2}}-\frac{1}{Z^{2}}\left(\frac{\partial Z}{\partial(-\beta)}\right)^{2}=\frac{\partial}{\partial(-\beta)}\left(\frac{1}{Z} \frac{\partial Z}{\partial(-\beta)}\right)=\frac{\partial\langle E\rangle}{\partial(-\beta)} . \tag{5.19}
\end{equation*}
$$

[^903]Since Eq. (15) is valid only if system's volume $V$ is fixed, it is customary to rewrite this extremely simple and important result as follows:

$$
\begin{equation*}
\left\langle\widetilde{E}^{2}\right\rangle=\frac{\partial\langle E\rangle}{\partial(-1 / T)}=T^{2}\left(\frac{\partial\langle E\rangle}{\partial T}\right)_{V}=C_{V} T^{2} \tag{5.20}
\end{equation*}
$$

This is a remarkably simple, fundamental result. As a sanity check, for a system of $N$ similar, independent particles, $\langle E\rangle$ and hence $C_{V}$ and are proportional to $N$, so that $\delta E \propto N^{1 / 2}$ and $\delta E /\langle E\rangle \propto N^{1 / 2}$, in agreement with Eq. (12). Let me emphasize that the classically-looking Eq. (20) is based on the general Gibbs distribution, and hence is valid for any system - either classical or quantum.

We will discuss the corollaries of this result in the next section, and now let me carry out a very similar calculation for a system whose number $N$ of particles in a system is not fixed, because they may go to, and come from the environment at will. If the chemical potential $\mu$ of the environment and its temperature $T$ are fixed, we are dealing with the grand canonical ensemble (Fig. 2.13), and may use the grand canonical distribution (2.106)-(2.107):

$$
\begin{equation*}
W_{m, N}=\frac{1}{Z_{G}} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\}, \quad Z_{G}=\sum_{N, m} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\} . \tag{5.21}
\end{equation*}
$$

Acting exactly as we did above for energy, we get

$$
\begin{align*}
\langle N\rangle & =\frac{1}{Z_{G}} \sum_{m, N} N \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\}=\frac{T}{Z_{G}} \frac{\partial Z_{G}}{\partial \mu},  \tag{5.22}\\
\left\langle N^{2}\right\rangle & =\frac{1}{Z_{G}} \sum_{m, N} N^{2} \exp \left\{\frac{\mu N-E_{m, N}}{T}\right\}=\frac{T^{2}}{Z_{G}} \frac{\partial^{2} Z_{G}}{\partial \mu^{2}}, \tag{5.23}
\end{align*}
$$

so that the particle number variance is

$$
\begin{equation*}
\left\langle\tilde{N}^{2}\right\rangle=\left\langle N^{2}\right\rangle-\langle N\rangle^{2}=\frac{T^{2}}{Z_{G}} \frac{\partial Z_{G}}{\partial \mu}-\frac{T^{2}}{Z_{G}^{2}}\left(\frac{\partial Z_{G}}{\partial \mu}\right)^{2}=T \frac{\partial}{\partial \mu}\left(\frac{T}{Z_{G}} \frac{\partial Z_{G}}{\partial \mu}\right)=T \frac{\partial\langle N\rangle}{\partial \mu}, \tag{5.24}
\end{equation*}
$$

Fluctuations of $E$
we get from Eq. (24) a surprisingly simple result:

Fluctuations of $N$ in classical gas

$$
\begin{equation*}
\left\langle\widetilde{N}^{2}\right\rangle=\langle N\rangle, \quad \text { i.e. } \delta N=\langle N\rangle^{1 / 2} \tag{5.27}
\end{equation*}
$$

This relation is so simple and important that I will now show how it may be derived in a different way, in order to prove that this result is valid for systems with an arbitrary (say, small) $N$, and also get more detailed information about the statistics of fluctuations of that number. Let us consider an ideal classical gas of $N_{0}$ particles in a volume $V_{0}$, and calculate the probability $W_{N}$ to have exactly $N \leq N_{0}$ of these particles in a part $V \leq V_{0}$ of this volume - see Fig. 1.


Fig. 5.1. Deriving the binomial and Poissonian distributions.

For one particle such probability is of course $W=V / V_{0} \leq 1$, while the probability of one particle being in the remaining part of the volume is $W^{\prime}=1-W=1-V / V_{0}$. If all particles were distinguishable, the probability of having $N \leq N_{0}$ specific particles in volume $V$, and $\left(N-N_{0}\right)$ specific particles in volume ( $V-V_{0}$ ), would be $W^{N} W^{,\left(N_{0}-N\right)}$. However, if we do not distinguish the particles, we should multiply the probability by the number of possible particle combinations keeping numbers $N$ and $N_{0}$ constant, i.e. by the binomial coefficient $N_{0}!/ N!\left(N_{0}-N\right)!.^{3}$ As the result, the required probability is

$$
\begin{equation*}
W_{N}=W^{N} W^{\left(N_{0}-N\right)} \frac{N_{0}!}{N!\left(N_{0}-N\right)!}=\left(\frac{\langle N\rangle}{N_{0}}\right)^{N}\left(1-\frac{\langle N\rangle}{N_{0}}\right)^{N_{0}-N} \frac{N_{0}!}{N!\left(N_{0}-N\right)!} \tag{5.28}
\end{equation*}
$$

where in the second instance I have used the evident expression $\langle N\rangle=W N_{0}=\left(V / V_{0}\right) N_{0}$ for the average number of particles in volume $V$. Relation (28) is the so-called binomial probability distribution, valid for any $\langle N\rangle$ and $N_{0}$.

If we are interested in keeping $\langle N\rangle$ arbitrary, but do not care how large the additional volume ( $V_{0}$ $-V$ ) is, we can simplify the binomial distribution by assuming that the external part, and hence $N_{0}$, are very large:

$$
\begin{equation*}
N_{0} \gg N, \tag{5.29}
\end{equation*}
$$

where $N$ means all values of interest, including $\langle N\rangle$. In this limit we can neglect $N$ in comparison with $N_{0}$ in the second exponent of Eq. (28), and also approximate the fraction $N_{0}!/\left(N_{0}-N\right)$ !, i.e. the product of $N$ terms, $\left(N_{0}-N+1\right)\left(N_{0}-N+2\right) \ldots\left(N_{0}-1\right) N_{0}$, as just $N_{0}{ }^{N}$. As a result, we get

$$
\begin{equation*}
W_{N} \approx\left(\frac{\langle N\rangle}{N_{0}}\right)^{N}\left(1-\frac{\langle N\rangle}{N_{0}}\right)^{N_{0}} \frac{N_{0}^{N}}{N!}=\frac{\langle N\rangle^{N}}{N!}\left(1-\frac{\langle N\rangle}{N_{0}}\right)^{N_{0}}=\frac{\langle N\rangle^{N}}{N!}\left[(1-W)^{\frac{1}{W}}\right]^{\langle N\rangle} . \tag{5.30}
\end{equation*}
$$

[^904]In the limit (29), $W \rightarrow 0$, and factor inside the square brackets tends to $1 / e$, the reciprocal of the natural logarithm base. ${ }^{4}$ Thus, we finally get an expression independent of $N_{0}$ :

$$
\begin{equation*}
W_{N}=\frac{\langle N\rangle^{N}}{N!} e^{-\langle N\rangle} \tag{5.31}
\end{equation*}
$$

Poisson distribution

This is the much celebrated Poisson distribution, which describes a very broad family of random phenomena. Figure 2 shows this distribution for several values of $\langle N\rangle$ - which, in contrast to $N$, are not necessarily integer.


Fig. 5.2. The Poisson distribution for several values of $\langle N\rangle$. In contrast to that average, argument $N$ may take only integer values, so that lines are only guides for the eye.

At very small $\langle N\rangle$, function $W_{N}(N)$ distribution is close to an exponential one, $W_{N} \approx W^{N} \propto\langle N\rangle^{N}$, while in the opposite limit, $\langle N\rangle \gg 1$, it rapidly approaches the Gaussian (alternatively called "normal") distribution

$$
\begin{equation*}
W_{N}=\frac{1}{(2 \pi)^{1 / 2} \delta N} \exp \left\{-\frac{(N-\langle N\rangle)^{2}}{2(\delta N)^{2}}\right\}, \quad \text { with } \delta N=\langle N\rangle^{1 / 2} \tag{5.32}
\end{equation*}
$$

Gaussian distribution
(Note that the Gaussian distribution is also valid if both $N$ and $N_{0}$ are large, regardless of relation (29) between them - see Fig. 3.)


Fig. 5.3. Hierarchy of three major probability distributions.

[^905]The key property of the Poisson (and hence of the Gaussian) distribution is that it has the same variance as given by Eq. (27):

$$
\begin{equation*}
\left\langle\widetilde{N}^{2}\right\rangle \equiv\left\langle(N-\langle N\rangle)^{2}\right\rangle=\langle N\rangle . \tag{5.33}
\end{equation*}
$$

(This is not true for the general binomial distribution.) For our current purposes, this means that for the ideal classical gas, Eq. (27) is valid for any number of particles.

### 5.3. Volume and temperature

What are the r.m.s. fluctuations of other thermodynamic variables - like $V, T$, etc.? Again, the answer depends on conditions. For example, if the volume $V$ occupied by a gas is externally fixed (say, by rigid walls), it evidently does not fluctuate at all: $\delta V=0$. On the other hand, the volume may fluctuate in the situation when average pressure is fixed - see, e.g., Fig. 1.5. A formal calculation of these fluctuations, using the approach applied in the last section, is hampered by the fact that it is physically impracticable to fix its conjugate variable, $P$, i.e. suppress its fluctuations. For example, the force $\mathcal{F}(t)$ exerted by an ideal classical gas on vessel's wall (whose measure the pressure is) is the result of individual, independent hits of the wall by particles (Fig. 4), with time scale $\tau_{c} \sim r_{\mathrm{B}} /(T / m)^{1 / 2} \sim 10^{-16} \mathrm{~s}$, so that its frequency spectrum extends to very high frequencies, virtually impossible to control.


Fig. 5.4. Force exerted by gas particles on container's wall, as a function of time (schematically).

However, we can use the following trick, very typical for the theory of fluctuations. It is almost evident that r.m.s. fluctuations of volume are independent of the shape of the container. Let us consider the particular situation similar to that shown in Fig. 1.5, with the container of a cylindrical shape, with the base area $A .{ }^{5}$ Then the coordinate of the piston is just $q=V / A$, while the average force exerted by the gas on the cylinder is $\nexists=P A$ - see Fig. 5. Now if the piston is sufficiently massive, its free oscillation frequency $\omega$ near the equilibrium position is small enough to satisfy the following three conditions.

First, besides balancing the average force $\langle\mathcal{\not}\rangle$, and thus sustaining average pressure $\langle P\rangle=\langle\mathcal{F}\rangle / A$ of the gas, the interaction between the heavy piston and light molecules of the gas is weak because of a relatively short duration of the wall hits (Fig. 4). Because of that, the full energy of the system may be presented as a sum of those of the gas and the piston, with a quadratic contribution to piston's potential energy from small deviations of equilibrium:

$$
\begin{equation*}
U_{P}=\frac{\kappa}{2} \widetilde{q}^{2}, \quad \widetilde{q} \equiv q-\langle q\rangle=\frac{\widetilde{V}}{A}, \tag{5.34}
\end{equation*}
$$

[^906]where $\kappa$ is the effective spring constant arising from gas' compressibility.


Fig. 5.5. Deriving Eq. (37).

Second, at $\omega \rightarrow 0$, that spring constant may be calculated just as for constant variations of volume, with the gas remaining in quasi-equilibrium at all times:

$$
\begin{equation*}
\kappa=-\frac{\partial\langle\nmid\rangle}{\partial q}=A^{2}\left(-\frac{\partial\langle P\rangle}{\partial\langle V\rangle}\right) . \tag{5.35}
\end{equation*}
$$

This partial derivative ${ }^{6}$ should be taken at whatever the given thermal conditions are, e.g., with $S=$ const for adiabatic conditions (i.e., thermally insulated gas), or with $T=$ const for isothermic conditions (gas in a good thermal contact with a heat bath), etc. With that constant denoted as $X$, Eqs. (34)-(35) give

$$
\begin{equation*}
U_{P}=\frac{1}{2}\left(-A^{2} \frac{\partial\langle P\rangle}{\partial\langle V\rangle}\right)_{X}\left(\frac{\widetilde{V}}{A}\right)^{2}=\frac{1}{2}\left(-\frac{\partial\langle P\rangle}{\partial\langle V\rangle}\right)_{X} \widetilde{V}^{2} . \tag{5.36}
\end{equation*}
$$

Finally, making $\omega$ sufficiently small (namely, $\hbar \omega \ll T$ ) by a sufficiently large piston mass, we can apply, to the piston's fluctuations, the classical equipartition theorem: $\left\langle U_{P}\right\rangle=T / 2$, giving

$$
\begin{equation*}
\left\langle\widetilde{V}^{2}\right\rangle_{X}=T\left(-\frac{\partial\langle V\rangle}{\partial\langle P\rangle}\right)_{X} \tag{5.37a}
\end{equation*}
$$

Fluctuations of volume

Since this result is valid for any $A$ and $\omega$, it should not depend on system's geometry and piston mass, provided that it is large in comparison with the effective mass of a single system component (say, a gas molecule) - the condition that is naturally fulfilled in most experiments. ${ }^{7}$ For the particular case of fluctuations at constant temperature ( $X=T$ ), we may use the second of Eqs. (1.39) to rewrite Eq. (37a) as

[^907]\[

$$
\begin{equation*}
\left\langle\widetilde{V}^{2}\right\rangle_{T}=-T\left(\frac{\partial^{2} G}{\partial\langle P\rangle^{2}}\right)_{T} \tag{5.37b}
\end{equation*}
$$

\]

In the specific case of an ideal classical gas of $N$ particles, with the equation of state $\langle V\rangle=N T /\langle P\rangle$, it is easier to use directly Eq. (37a), with $X=T$, to get

$$
\begin{equation*}
\left\langle\widetilde{V}^{2}\right\rangle_{T}=-T\left(-\frac{N T}{\langle P\rangle^{2}}\right) \equiv \frac{\langle V\rangle^{2}}{N}, \quad \text { i.e. } \frac{\delta V_{T}}{\langle V\rangle}=\frac{1}{N^{1 / 2}}, \tag{5.38}
\end{equation*}
$$

in agreement with the trend given by Eq. (12).
Now let us proceed to fluctuations of temperature, for simplicity focusing on the case $V=$ const. Let us again assume that the system we are considering is weakly coupled to a heat bath of temperature $T_{0}$, in the sense that the time $\tau$ of temperature equilibration between the two is much larger than the internal temperature relaxation (thermalization) time. Then we may assume that $T$ changes in the whole system virtually simultaneously, and consider it a function of time alone:

$$
\begin{equation*}
T=\langle T\rangle+\widetilde{T}(t) \tag{5.39}
\end{equation*}
$$

Moreover, due to the (relatively) large $\tau$, we may use the stationary relation between small fluctuations of temperature and the internal energy of the system:

$$
\begin{equation*}
\widetilde{T}(t)=\frac{\widetilde{E}(t)}{C_{V}}, \quad \text { so that } \delta T=\frac{\delta E}{C_{V}} \tag{5.40}
\end{equation*}
$$

With those assumptions, Eq. (20) immediately yields the famous expression for the so-called thermodynamic fluctuations of temperature:

$$
\begin{equation*}
\delta T=\frac{\delta E}{C_{V}}=\frac{\langle T\rangle}{C_{V}^{1 / 2}} \tag{5.41}
\end{equation*}
$$

The most straightforward application of this result is to analysis of so-called bolometers broadband detectors of electromagnetic radiation in microwave and infrared frequency bands. In such a detector (Fig. 6), the incoming radiation it focused on a small sensor (e.g., either a small piece of a Ge crystal, or a superconductor thin film at temperature $T \approx T_{c}$, etc.) that is well isolated thermally from the environment.


Fig. 5.6. Conceptual scheme of a bolometer.
to electronics
As a result, the absorption of even small radiation power $\mathcal{P}$ leads to a noticeable change $\Delta T$ of sensor's average temperature $\langle T\rangle$ and hence of its electric resistance $R$, which is probed up by low-noise
external electronics. ${ }^{8}$ If power does not change in time too fast, $\Delta T$ is a certain function of $\mathcal{P}$, turning into 0 at $\mathcal{P}=0$. Hence, if $\Delta T$ is much lower than the environment temperature $T_{0}$, we may keep only the main, linear term in it Taylor expansion in $P$.

$$
\begin{equation*}
\Delta T \equiv\langle T\rangle-T_{0}=\frac{P}{g}, \tag{5.42}
\end{equation*}
$$

where coefficient $g \equiv \partial \nexists \partial T$ is called the thermal conductance of the unavoidable thermal coupling between the sensor and the heat bath - see Fig. 6. The power may be detected if the electric signal from the sensor, which results from change $\Delta T$, is not drowned in spontaneous fluctuations. In practical systems, these fluctuations are is contributed by several sources including electronic amplifiers, sensor, etc. However, in modern systems these "technical" contributions to noise are successfully suppressed, and the dominating noise source are the fundamental fluctuations of sensor temperature, described by Eq. (41). In this case the so-called noise-equivalent power ("NEP"), defined as the level of $\mathcal{P}$ that produces signal equal to r.m.s. value of noise, may be calculated by equating Eqs. (41) (with $\langle T\rangle \approx T_{0}$ ) and (42):

$$
\begin{equation*}
\mathrm{NEP}=\frac{T_{0} g}{C_{V}^{1 / 2}} . \tag{5.43}
\end{equation*}
$$

This expression shows that in order to decrease $N E P$, i.e. improve the device sensitivity, both the environment temperature $T_{0}$ and thermal conductance $g$ should be reduced. In modern receivers of radiation, their typical values (in SI units) are of the order of 0.1 K and $10^{-10} \mathrm{~W} / \mathrm{K}$, respectively.

On the other hand, Eq. (43) implies that in order to increase bolometer sensitivity, i.e. reduce NEP, the $C_{V}$ of the sensor, and hence its mass, should be increased. This conclusion is valid only to a certain extent, because due to technical reasons (parameter drift and the so-called $1 / f$ noise of the sensor and external electronics), incoming power has to be modulated with as high frequency $\omega$ as possible (in most cases, the cyclic frequency $v=\omega / 2 \pi$ of the modulation is between 10 to $1,000 \mathrm{~Hz}$ ), so that the electrical signal may be picked up from the sensor at that frequency. As a result, $C_{V}$ may be increased only until the thermal constant of the sensor,

$$
\begin{equation*}
\tau=\frac{C_{V}}{g}, \tag{5.44}
\end{equation*}
$$

becomes close to $1 / \omega$, because at $\omega \tau \gg 1$ the useful signal drops faster than noise. As a result, the lowest (i.e. the best) value of NEP,

$$
\begin{equation*}
\frac{(\mathrm{NEP})_{\min }}{v^{1 / 2}}=\alpha T_{0} g^{1 / 2}, \quad \alpha \sim 1 \tag{5.45}
\end{equation*}
$$

is reached at $v \tau \approx 1$. (The exact values of the optimal product $\omega \tau$, and the numerical constant $\alpha \sim 1$ in Eq. (45), depend on the exact law of power modulation in time, and the output signal processing procedure.) With the parameters cited above, this estimate yields (NEP) $\min / v^{1 / 2} \sim 3 \times 10^{-17} \mathrm{~W} / \mathrm{Hz}^{1 / 2}-\mathrm{a}$ very low power indeed.

[^908]However, surprisingly enough, the power modulation allows bolometric (and other broadband) receivers to register radiation with power much lower than this NEP! Indeed, picking up the sensor signal at the modulation frequency $\omega$, we can use the following electronics stages to filter out all the noise besides its components within a very narrow band, of width $\Delta v \ll v$, around the modulation frequency (Fig. 7). This is the idea of a microwave radiometer, ${ }^{9}$ currently used in all sensitive broadband receivers.


Fig. 5.7. Basic idea of the Dicke radiometer.

In order to analyze this opportunity, we need to develop theoretical tools for a quantitative description of the spectral distribution of fluctuations. Another motivation for that description is the need in analysis of variables dominated by fast (high-frequency) components, such as pressure - please have one more look at Fig. 4. Finally, during the analysis, we will run into the fundamental relation between fluctuations and dissipation, which is one of the main results of statistical physics as a whole.

### 5.4. Fluctuations as functions of time

There are two mathematically-equivalent approaches to time-dependent functions of time, called time-domain and frequency-domain pictures, with their relative convenience depending on the particular problem to be solved.

In the time domain, we cannot characterize a random fluctuation $\tilde{f}(t)$ of a classical variable by its statistical average, because it equals zero - see Eq. (2). Of course, variance (3) does not vanish, but if fluctuations are stationary, it does not depend on time either. Because of that, let us consider the following average: ${ }^{10}$

$$
\begin{equation*}
\left\langle\tilde{f}(t) \widetilde{f}\left(t^{\prime}\right)\right\rangle \tag{5.46}
\end{equation*}
$$

Generally, this is a function of two arguments. Moreover, in the systems that are stationary (whose macroscopic parameters and hence the variable expectation values do not change with time), averages like (46) may depend only on the difference,

$$
\begin{equation*}
\tau \equiv t^{\prime}-t \tag{5.47}
\end{equation*}
$$

[^909]between the two observation times. In this case, average (46) is called the correlation function of variable $f$ :
\[

$$
\begin{equation*}
K_{f}(\tau) \equiv\langle\widetilde{f}(t) \widetilde{f}(t+\tau)\rangle \tag{5.48}
\end{equation*}
$$

\]

Correlation function

This name ${ }^{11}$ catches the idea of this notion very well: $K_{\mathcal{f}}(\tau)$ tells us about the average mutual relation between the fluctuations at two times separated by interval $\tau$. Let us list the basic properties of this function.

First of all, $K_{f}(\tau)$ has to be an even function of the time delay $\tau$. Indeed, we may write

$$
\begin{equation*}
K_{f}(-\tau)=\langle\widetilde{f}(t) \widetilde{f}(t-\tau)\rangle=\langle\widetilde{f}(t-\tau) \widetilde{f}(t)\rangle=\left\langle\tilde{f}\left(t^{\prime}\right) \widetilde{f}\left(t^{\prime}+\tau\right)\right\rangle, \tag{5.49}
\end{equation*}
$$

with $t^{\prime} \equiv t-\tau$. For stationary processes, this average cannot depend on the common shift $t^{\prime}$ of the two observation times, so that averages (48) and (49) have to be equal:

$$
\begin{equation*}
K_{f}(-\tau)=K_{f}(\tau) \tag{5.50}
\end{equation*}
$$

Second, at $\tau \rightarrow 0$ the correlation function tends to the variance:

$$
\begin{equation*}
K_{f}(0)=\langle\widetilde{f}(t) \widetilde{f}(t)\rangle=\left\langle\widetilde{f}^{2}\right\rangle \tag{5.51}
\end{equation*}
$$

In the opposite limit, when $\tau$ is much larger than some characteristic correlation time $\tau_{c}$ of the system, ${ }^{12}$ the correlation function tends to zero, because fluctuations separated by such large time interval are virtually independent (uncorrelated). As a result, the correlation function typically looks like one of the plots sketched in Fig. 8. Note that on a time scale much longer than $\tau_{c}$, any physically-realistic correlation function may be well approximated with a delta-function of $\tau .{ }^{13}$


Fig. 5.8. Correlation function of fluctuations: two typical examples.

In the reciprocal, frequency domain, process $\tilde{f}(t)$ is presented as a Fourier integral,

$$
\begin{equation*}
\tilde{f}(t)=\int_{-\infty}^{+\infty} f_{\omega} e^{-i \omega t} d \omega \tag{5.52}
\end{equation*}
$$

with the reciprocal transform being
${ }^{11}$ Another term, the autocorrelation function, is sometimes used for average (48) to distinguish it from the mutual correlation function, $\langle f(t) g(t+\tau)\rangle$, of two stationary processes.
${ }^{12}$ Correlation time $\tau_{c}$ is the direct temporal analog of the correlation radius $r_{c}$ which was discussed in Sec. 4.2.
${ }^{13}$ For example, for a process which is a sum of independent very short pulses, e.g., the gas pressure force exerted on the container wall (Fig. 4), such approximation is legitimate on time scales longer than the single pulse duration, e.g., the time of particle's impact on the wall.

$$
\begin{equation*}
f_{\omega}=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \widetilde{f}(t) e^{i \omega t} d t \tag{5.53}
\end{equation*}
$$

If the initial function $\tilde{f}(t)$ is random (as it is in the case of fluctuations), with zero average, its Fourier transform $f_{\omega}$ is a random function (now of frequency) as well, also with a vanishing statistical average:

$$
\begin{equation*}
\left\langle f_{\omega}\right\rangle=\left\langle\frac{1}{2 \pi} \int_{-\infty}^{+\infty} \widetilde{f}(t) e^{i \omega t} d t\right\rangle=\frac{1}{2 \pi} \int_{-\infty}^{+\infty}\langle\widetilde{f}(t)\rangle e^{i \omega t} d t=0 \tag{5.54}
\end{equation*}
$$

The simplest nonvanishing average may be formed similarly to Eq. (46), but with due respect to the complex-variable character of the Fourier images:

$$
\begin{equation*}
\left\langle f_{\omega} f_{\omega^{\prime}}^{*}\right\rangle=\frac{1}{(2 \pi)^{2}} \int_{-\infty}^{+\infty} d t^{\prime} \int_{-\infty}^{+\infty} d t\left\langle\tilde{f}(t) \tilde{f}\left(t^{\prime}\right)\right\rangle e^{i\left(\omega^{\prime} t^{\prime}-\omega t\right)} \tag{5.55}
\end{equation*}
$$

It turns out that for a stationary process, averages (46) and (55) are directly related. Indeed, since the integration over $t^{\prime}$ in Eq. (55) is in infinite limits, we may replace it with integration over $\tau \equiv t^{\prime}-t$ (at fixed $t$ ), also in infinite limits. Replacing $t^{\prime}$ by $t+\tau$ in expressions under the integral, we see that the average is just the correlation function $K_{\mathcal{A}}(\tau)$, while the time exponent is equal to $\exp \left\{i\left(\omega^{\prime}-\right.\right.$ $\omega) t\} \exp \left\{i \omega^{\prime} \tau\right\}$. As a result, changing the order of integration, we get

$$
\begin{equation*}
\left\langle f_{\omega} f_{\omega^{\prime}}^{*}\right\rangle=\frac{1}{(2 \pi)^{2}} \int_{-\infty}^{+\infty} d t \int_{-\infty}^{+\infty} d \tau K_{f}(\tau) e^{i\left(\omega-\omega^{\prime}\right) t} e^{i \omega^{\prime} \tau}=\frac{1}{(2 \pi)^{2}} \int_{-\infty}^{+\infty} K_{f}(\tau) e^{i \omega^{\prime} \tau} d \tau \int_{-\infty}^{+\infty} e^{i\left(\omega-\omega^{\prime}\right) t} d t \tag{5.56}
\end{equation*}
$$

But the last integral is just $2 \pi \delta\left(\omega-\omega^{\prime}\right),{ }^{14}$ so that we finally get

Spectral density of fluctuations

$$
\begin{equation*}
\left\langle f_{\omega} f_{\omega^{\prime}}^{*}\right\rangle=S_{f}(\omega) \delta\left(\omega-\omega^{\prime}\right) \tag{5.57}
\end{equation*}
$$

where the real function of frequency,

$$
\begin{equation*}
S_{f}(\omega) \equiv \frac{1}{2 \pi} \int_{-\infty}^{+\infty} K_{f}(\tau) e^{i \omega \tau} d \tau=\frac{1}{\pi} \int_{0}^{\infty} K_{f}(\tau) \cos \omega \tau d \tau \tag{5.58}
\end{equation*}
$$

WienerKhinchin theorem
is called the spectral density of fluctuations at frequency $\omega$. According to Eq. (58), the spectral density is a Fourier image of the correlation function, and hence the reciprocal Fourier transform is: ${ }^{15,16}$

$$
\begin{equation*}
K_{f}(\tau)=\int_{-\infty}^{+\infty} S_{f}(\omega) e^{-i \omega \tau} d \omega=2 \int_{0}^{\infty} S_{f}(\omega) \cos \omega \tau d \omega \tag{5.59}
\end{equation*}
$$

In particular, for the variance, Eq. (59) yields

[^910]\[

$$
\begin{equation*}
\left\langle\tilde{f}^{2}\right\rangle=K_{f}(0)=\int_{-\infty}^{+\infty} S_{f}(\omega) d \omega=2 \int_{0}^{\infty} S_{f}(\omega) d \omega \tag{5.60}
\end{equation*}
$$

\]

This relation shows that term "spectral density" describes the physical sense of function $S_{f}(\omega)$ very well. Indeed, if a random signal $f(t)$ had been passed through a frequency filter with a small bandwidth $\Delta v \ll v$ of positive cyclic frequencies, the integral in Eq. (60) had to be limited to interval $\Delta \omega=2 \pi \Delta v$, i.e. that the variance of the output signal would become ${ }^{17}$

$$
\begin{equation*}
\left\langle\tilde{f}^{2}\right\rangle_{\Delta v}=2 S_{f}(\omega) \Delta \omega=4 \pi S_{f}(\omega) \Delta v \tag{5.61}
\end{equation*}
$$

To complete this introductory section, let me note an important particular case. If the spectral density of some process, is nearly constant within the frequency range of interest, $S_{f}(\omega)=$ const $=S_{f}(0),{ }^{18}$ Eq. (59) shows that its correlation function may be well approximated by a delta-function:

$$
\begin{equation*}
K_{f}(\tau)=S_{f}(0) \int_{-\infty}^{+\infty} e^{-i \omega \tau} d \omega=2 \pi S_{f}(0) \delta(\tau) \tag{5.62}
\end{equation*}
$$

From this relation stems another popular name of the white noise, the delta-correlated process. We have already seen that this is a very reasonable approximation, for example, for the gas pressure force fluctuations (Fig. 4). Of course, for spectral density of a realistic, limited physical variable the approximation of constant spectral density cannot be true for all frequencies (otherwise, for example, integral (60) would diverge, giving an unphysical, infinite value of variance), and is valid only at frequencies much lower than $1 / \tau_{c}$.

### 5.5. Fluctuations and dissipation

Now we are mathematically equipped to address one of the most important topics of statistical physics, the relation between fluctuations and dissipation This relation is especially simple for the following hierarchical situation: a relatively "heavy", slowly moving system interacting with an environment consisting of rapidly moving, "light" components. A popular theoretical term for such a system is the Brownian particle, named after botanist R. Brown who first noticed in 1827 the random motion of pollen grains, caused by their random hits by fluid molecules, under a microscope. However, the family of such systems is much broader than that of mechanical particles. ${ }^{19}$

One more important assumption of this theory is that the system's motion does not violate the thermal equilibrium of the environment - well fulfilled in many cases. (Think, for example, about a usual mechanical pendulum whose motion does not overheat the air around it.) In this case, the statistical averaging over the thermally-equilibrium environment may be performed for any (slow)

[^911]motion of the system of interest, considering the motion fixed. ${ }^{20}$ I will denote such a "primary" averaging by angular brackets $\langle\ldots\rangle$. At a later stage we may carry out another, "secondary" averaging, over an ensemble of many similar systems of interest, coupled to similar environments. If we do, it will be denoted by double angle brackets $\langle\langle\ldots\rangle\rangle$.

Let me start from a simple classical system, a 1D harmonic oscillator whose equation of evolution may be presented as

$$
\begin{equation*}
m \ddot{q}+\kappa q=\mathcal{7}_{\mathrm{det}}(t)+\gamma_{\mathrm{env}}(t)=\mathcal{\gamma}_{\mathrm{det}}(t)+\langle\boldsymbol{7}\rangle+\tilde{7}(t) \tag{5.63}
\end{equation*}
$$

where $q$ is the (generalized) coordinate of the oscillator, $\not_{\text {det }}(t)$ is the deterministic (generalized) external force, while both components of the random force $\mathcal{Z}(t)$ present the impact of the environment on oscillator's motion. Again, from the point of view of the fast-moving environmental components, the oscillator's motion is slow. The average of the force exerted by environment on such a slowly moving object may have a part depending on not only $q$, but on the velocity $\dot{q}$ as well. For most systems, the Taylor expansion of the force in small velocity would have a finite leading, linear term, so that we may take

$$
\begin{equation*}
\langle\boldsymbol{\eta}\rangle=-\eta \dot{q} \tag{5.64}
\end{equation*}
$$

so that Eq. (63) may be rewritten as

$$
\begin{equation*}
m \ddot{q}+\eta \dot{q}+\kappa q={\neq \mathrm{det}^{2}}(t)+\tilde{\gamma}(t) \tag{5.65}
\end{equation*}
$$

This way of describing the effects of environment on an otherwise Hamiltonian system is called the Langevin equation. ${ }^{21}$ Due to the linearity of the differential equation (65), its general solution may be presented as a sum of two parts: the deterministic motion of the linear oscillator due to the external force $7_{\mathrm{det}}(t)$, and random fluctuations due to the random force exerted by the environment. The former effects are well known from classical dynamics, ${ }^{22}$ so let us focus on the latter part by taking $\chi_{\operatorname{det}}(t)=0$. The remaining term in the right-hand part describes the fluctuating part of the environmental force; in contrast to the average component (64), its intensity (read: its spectral density at relevant frequencies $\omega$ $\sim \omega_{0} \equiv(\kappa / m)^{1 / 2}$ ) does not vanish at $q(t)=0$, and hence may be evaluated ignoring system's motion.

Plugging into Eq. (65) the presentation of both variables in the form similar to Eq. (52), for their Fourier images we get the following relation:

$$
\begin{equation*}
-m \omega^{2} q_{\omega}-i \omega \eta q_{\omega}+\kappa q_{\omega}=7_{\omega} \tag{5.66}
\end{equation*}
$$

which immediately gives us $q_{\omega}$ :

[^912]\[

$$
\begin{equation*}
q_{\omega}=\frac{7_{\omega}}{\left(\kappa-m \omega^{2}\right)-i \eta \omega} . \tag{5.67}
\end{equation*}
$$

\]

Now multiplying Eq. (67) by its complex conjugate, averaging both parts of the resulting equation, and using for each of them Eq. (57), ${ }^{23}$ we get the following relation between spectral densities of the oscillations and force:

$$
\begin{equation*}
S_{q}(\omega)=\frac{1}{\left(\kappa-m \omega^{2}\right)^{2}+(\eta \omega)^{2}} S_{\neq}(\omega) \tag{5.68}
\end{equation*}
$$

As the reader should know well from classical dynamics, at small damping ( $\eta \ll m \omega_{0}$ ) the first factor in the right-hand part of Eq. (68) describes the resonance, i.e. has a sharp peak near oscillator's eigenfrequency $\omega_{0}$, and may be presented in that vicinity as

$$
\begin{equation*}
\frac{1}{\left(\kappa-m \omega^{2}\right)^{2}+(\eta \omega)^{2}} \approx \frac{1}{4 m \kappa\left(\xi^{2}+\delta^{2}\right)}, \quad \text { at }|\xi| \ll \omega_{0} \quad \text { with } \xi \equiv \omega-\omega_{0}, \quad \delta \equiv \eta / 2 m \tag{5.69}
\end{equation*}
$$

In contrast, spectral density $S_{\neq}(\omega)$ of fluctuations of a typical environment is changing slowly near that frequency, so that for the purpose of integration over frequencies near $\omega_{0}$ we may replace $S_{\neq}(\omega)$ with $S_{\neq}$ $\left(\omega_{0}\right)$. As a result, the variance of the environment-imposed random oscillations may be calculated as

$$
\begin{equation*}
\left\langle\left\langle\widetilde{q}^{2}\right\rangle\right\rangle=2 \int_{0}^{\infty} S_{q}(\omega) d \omega \approx 2 \int_{\omega \approx \omega_{0}} S_{q}(\omega) d \omega \approx 2 S_{\neq}\left(\omega_{0}\right) \frac{1}{4 m \kappa} \int_{-\infty}^{+\infty} \frac{d \xi}{\xi^{2}+\delta^{2}} . \tag{5.70}
\end{equation*}
$$

The last expression includes a well-known table integral, ${ }^{24}$ equal to $\pi / \delta=2 \pi m / \eta$, so that finally

$$
\begin{equation*}
\left\langle\left\langle\widetilde{q}^{2}\right\rangle\right\rangle=2 S_{\neq}\left(\omega_{0}\right) \frac{1}{4 m \kappa} \frac{2 \pi m}{\eta}=\frac{\pi}{\kappa \eta} S_{\neq}\left(\omega_{0}\right) . \tag{5.71}
\end{equation*}
$$

But on the other hand, the weak interaction with environment should keep the oscillator in thermodynamic equilibrium at the same temperature $T$. Since our analysis has been based on the classical Langevin equation (65), we may only use it in the classical limit $\hbar \omega_{0} \ll T$, in which we may use the equipartition theorem (2.48). In our current notation, it yields

$$
\begin{equation*}
\frac{\kappa}{2}\left\langle\left\langle\widetilde{q}^{2}\right\rangle\right\rangle=\frac{T}{2} . \tag{5.72}
\end{equation*}
$$

Comparing Eqs. (71) and (72), we see that the spectral density of the random force exerted by environment is fundamentally related to the damping it provides:

$$
\begin{equation*}
S_{\neq}\left(\omega_{0}\right)=\frac{\eta}{\pi} T . \tag{5.73a}
\end{equation*}
$$

Now we may argue (rather convincingly :-) that since this relation does not depend on oscillator's parameters $m$ and $\kappa$, and hence its eigenfrequency $\omega_{0}=(\kappa / m)^{1 / 2}$, it should be valid at any (but

[^913]sufficiently low, $\omega \tau_{c} \ll 1$ ) frequency. Using Eq. (58) with $\omega \rightarrow 0$, it may be rewritten as a formula for the effective low-frequency drag (friction) coefficient:
\[

$$
\begin{equation*}
\eta=\frac{1}{T} \int_{0}^{\infty} K_{\not{\not}}(\tau) d \tau \equiv \frac{1}{T} \int_{0}^{\infty}\langle\tilde{\mathcal{F}}(0) \widetilde{\mathcal{F}}(\tau)\rangle d \tau \tag{5.73b}
\end{equation*}
$$

\]

Relation (73) reveals an intimate, fundamental connection between fluctuations and dissipation provided by a thermally-equilibrium environment. Verbally, "there is no dissipation without fluctuations" - and vice versa. ${ }^{25}$ Historically, this fact was first recognized in 1905 by A. Einstein, ${ }^{26}$ in the following form. Let us apply our result (73) to the particular case of a free 1D Brownian particle, by taking $\kappa=0$. In this case both equations (71) and (72) give infinities. In order to understand the reason for that divergence, let us go back to the Langevin equation (65) with not only $\kappa=0$, but also, just for the sake of simplicity, $m \rightarrow 0$ as well. (The latter approximation, frequently called the overdamping limit, is quite appropriate for the motion of a small particle in a viscous fluid, when $m \ll \eta \Delta t$ even for smallest time intervals $\Delta t$ between the successive observations of particle's positions.) In this approximation, Eq. (65) is reduced to a simple equation,

$$
\begin{equation*}
\eta \dot{q}=f_{\mathrm{det}}(t)+\tilde{f}(t), \tag{5.74}
\end{equation*}
$$

with a ready solution for particle displacement during a finite time interval $t$ :

$$
\begin{equation*}
\Delta q(t) \equiv q(t)-q(0)=\langle\langle\Delta q(t)\rangle\rangle+\widetilde{q}(t), \quad\langle\langle\Delta q(t)\rangle\rangle=\frac{1}{\eta} \int_{0}^{t} \gamma_{\operatorname{det}}\left(t^{\prime}\right) d t^{\prime}, \quad \Delta \widetilde{q}(t)=\frac{1}{\eta} \int_{0}^{t} \widetilde{\gamma}\left(t^{\prime}\right) d t^{\prime} . \tag{5.75}
\end{equation*}
$$

Evidently, in the statistical average of the displacement, the fluctuation effects vanish, but this does not mean that the particle does not deviate from the deterministic trajectory $\langle\langle q(t)\rangle\rangle$ - just that is has equal probabilities to be shifted either of two possible directions from that trajectory. To see that, let us calculate the variance of the displacement:

$$
\begin{equation*}
\left\langle\left\langle\Delta \widetilde{q}^{2}(t)\right\rangle\right\rangle=\frac{1}{\eta^{2}} \int_{0}^{t} d t^{\prime} \int_{0}^{t} d t^{\prime \prime}\left\langle\widetilde{\mathcal{F}}\left(t^{\prime}\right) \widetilde{7}\left(t^{\prime \prime}\right)\right\rangle=\frac{1}{\eta^{2}} \int_{0}^{t} d t^{\prime} \int_{0}^{t} d t^{\prime \prime} K_{\mathcal{F}}\left(t^{\prime}-t^{\prime \prime}\right) . \tag{5.76}
\end{equation*}
$$

As we already know, at times $\tau \gg \tau_{c}$ (this correlation time, for typical molecular impacts, is of the order of a picosecond), correlation function may be well approximated by the delta-function - see Eq. (62). In this approximation, with $S_{\neq}(0)$ expressed by Eq. (73), and Eq. (76) yields

$$
\begin{equation*}
\left\langle\left\langle\Delta \widetilde{q}^{2}(t)\right\rangle\right\rangle=\frac{2 \pi}{\eta^{2}} S_{\neq}(0) \int_{0}^{t} d t^{\prime} \int_{0}^{t} d t^{\prime \prime} \delta\left(t^{\prime}-t^{\prime \prime}\right)=\frac{2 \pi}{\eta^{2}} \frac{\eta T}{\pi} \int_{0}^{t} d t^{\prime}=2 D t \tag{5.77}
\end{equation*}
$$

with

[^914]\[

$$
\begin{equation*}
D=\frac{T}{\eta} \tag{5.78}
\end{equation*}
$$

\]

## Einstein's relation

The final form of Eq. (77) describes the well-known law of diffusion ("random walk") of a 1D system, with the r.m.s. deviation from the point of origin growing as $(2 D t)^{1 / 2}$. Coefficient $D$ is this relation is called the coefficient of diffusion, and Eq. (78) describes the extremely simple Einstein relation between that coefficient and particle's damping. Often this relation is rewritten in SI units of temperature as $D=\mu_{m} k_{\mathrm{B}} T_{\mathrm{K}}$, where $\mu_{m} \equiv 1 / \eta$ is the mobility of the particle. The physical sense of $\mu_{m}$ becomes clear from rewriting the expression for the deterministic viscous motion $\langle\langle q(t)\rangle\rangle$ (particle's "drift") in the form:

$$
\begin{equation*}
v_{\mathrm{drift}} \equiv \frac{d\langle\langle q(t)\rangle\rangle}{d t}=\frac{1}{\eta} \not_{\mathrm{det}}(t)=\mu_{m} \not_{\mathrm{det}}(t), \tag{5.79}
\end{equation*}
$$

so that mobility is just velocity given to the particle by unit force. ${ }^{27}$
Another famous example of application of Eq. (73) is to the thermal (or "Johnson", or "JohnsonNyquist", or just "Nyquist") noise in resistive electron devices. Let us consider a two-terminal "probe" circuit, playing the role of the harmonic oscillator in our analysis above, connected to a resistor $R$ (Fig. 9), playing the role of noisy environment. (The noise is generated by the thermal motion of numerous electrons, randomly moving inside the resistor.) For this system, one convenient choice of conjugate variables (the generalized coordinate and generalized force) is, respectively, the electric charge $Q \equiv$ $\int I(t) d t$ that has passed through the "probe" circuit by time $t$, and voltage $V$ across its terminals, with the polarity shown in Fig. 9. (Indeed, the product $V d Q$ is the elementary work $d w$ done by the environment on the probe circuit.)


Fig. 5.9. Resistor $R$ of temperature $T$ as a noisy environment of a two-terminal probe circuit.

Making the corresponding replacements, $q \rightarrow Q$ and $\nrightarrow \vee$ in Eq. (64), we see that it becomes

$$
\begin{equation*}
\langle v\rangle=-\eta \dot{Q} \equiv-\eta I . \tag{5.80}
\end{equation*}
$$

Comparing this relation with Ohm's law, $R(-I)=\mathcal{R}_{2}^{8}$ we see that in this case, coefficient $\eta$ has the physical sense of the usual Ohmic resistance $R,{ }^{29}$ so that Eq. (73) becomes

[^915]\[

$$
\begin{equation*}
S_{v}(\omega)=\frac{R}{\pi} T . \tag{5.81a}
\end{equation*}
$$

\]

Using Eq. (61), and transferring to the SI units of temperature ( $T \rightarrow k_{\mathrm{B}} T_{\mathrm{K}}$ ), we can bring this famous Nyquist formula ${ }^{30}$ to its most popular form

Nyquist formula

$$
\begin{equation*}
\left\langle\tilde{V}^{2}\right\rangle_{\Delta v}=4 k_{\mathrm{B}} T_{\mathrm{K}} R \Delta v \tag{5.81b}
\end{equation*}
$$

Note that according to Eq. (65), this result is only valid at a negligible speed of change of the generalized coordinate $q$ (in this case, negligible current $I$ ), i.e. Eq. (81) expresses the voltage fluctuations as would be measured by an ideal voltmeter, with an input resistance much higher that $R$.

On the other hand, applying a different choice of generalized coordinate and force, $q \rightarrow \Phi, \nrightarrow I$ (where $\left.\Phi \equiv \int \mathscr{\varkappa} t\right) d t$ is the generalized magnetic flux, so that $d w=I d \Phi$ ), we get $\eta \rightarrow 1 / R$, and Eq. (73) yields the thermal fluctuations of the current through the resistor (as measured by an ideal ammeter, i.e. at $V \rightarrow 0)$ :

$$
\begin{equation*}
S_{I}(\omega)=\frac{1}{\pi R} T \text {, i.e. }\left\langle\widetilde{I}^{2}\right\rangle_{\Delta v}=\frac{4 k_{\mathrm{B}} T_{\mathrm{K}}}{R} \Delta v . \tag{5.81c}
\end{equation*}
$$

Note that Eqs. (81) as valid for noise in thermal equilibrium only. In electric circuits, which may be readily driven out of equilibrium by applied voltage $\langle V\rangle$, other types of noise are frequently important, notably the shot noise, which arises in short conductors, e.g., tunnel junctions, at applied voltages $\langle V\rangle \gg T / q$, due to the discreteness of charge carriers. ${ }^{31} \mathrm{~A}$ straightforward analysis using a simple model, described in the assignment of Exercise Problem 9, shows that this noise may be characterized by current fluctuations with low-frequency spectral density

$$
\begin{equation*}
S_{I}(\omega)=\frac{|q \bar{I}|}{2 \pi}, \quad \text { i.e. }\left\langle\widetilde{I}^{2}\right\rangle_{\Delta v}=2|q \bar{I}| \Delta v \tag{5.82}
\end{equation*}
$$

where $q$ is the electric charge of a single current carrier. This is the Schottky formula, valid for any relation between $I$ and $V$. Comparison of Eqs. (81c) and (82) for a device that obeys the Ohm law shows that the shot noise has the same intensity as the thermal noise with effective temperature

$$
\begin{equation*}
T_{\mathrm{ef}}=\frac{|q \bar{V}|}{2} \gg T \tag{5.83}
\end{equation*}
$$

This relation may be interpreted as a result of charge carrier overheating by the applied electric field, and explains why the Schottky formula (82) is only valid in conductors much shorter than the energy

[^916]relaxation length $l_{e}$ of the charge carriers. ${ }^{32}$ Another mechanism of the shot noise suppression, that becomes noticeable if system's transparency is high, is the Fermi-Dirac statistics of electrons. ${ }^{33}$

Returning to the bolometric Dicke radiometer (see Figs. 6-7 and their discussion), we may now use the Langevin equation formalism to finalize its analysis. For this system, the Langevin equation is just the usual equation of heat balance:

$$
\begin{equation*}
C_{V} \frac{d T}{d t}+g\left(T-T_{0}\right)=\mathcal{P}_{\operatorname{det}}(t)+\widetilde{\mathcal{P}}(t) \tag{5.84}
\end{equation*}
$$

where $\mathcal{P}_{\text {det }}=\langle\mathcal{P}\rangle$ describes the (deterministic) power of absorbed radiation, and $\widetilde{\mathcal{P}}$ presents the effective source of temperature fluctuations. Now we can use Eq. (84) to carry out a calculation of the spectral density $S_{T}(\omega)$ of temperature fluctuations absolutely similar to how this was done with Eq. (65), assuming that the frequency spectrum of the fluctuation source is much broader than the intrinsic bandwidth $1 / \tau=g / C_{V}$ of the bolometer, so that its spectral density at frequencies $\omega \tau \sim 1$ may be well approximated by its low-frequency value $S_{\mathcal{A}}(0)$ :

$$
\begin{equation*}
S_{T}(\omega)=\left|\frac{1}{-i \omega C_{V}+g}\right|^{2} S_{\mathcal{P}}(0) \tag{5.85}
\end{equation*}
$$

Then, requiring the variance of temperature fluctuations,

$$
\begin{equation*}
(\delta T)^{2} \equiv\left\langle\widetilde{T}^{2}\right\rangle=2 \int_{0}^{\infty} S_{T}(\omega) d \omega=2 S_{\mathcal{P}}(0) \int_{0}^{\infty}\left|\frac{1}{-i \omega C_{V}+g}\right|^{2} d \omega=2 S_{\mathcal{P}}(0) \frac{1}{C_{V}^{2}} \int_{0}^{\infty} \frac{d \omega}{\omega^{2}+\left(g / C_{V}\right)^{2}}=\frac{\pi S_{\mathcal{P}}(0)}{g C_{V}}, \tag{5.86}
\end{equation*}
$$

to coincide with our earlier "thermodynamic fluctuation" result (41), we get

$$
\begin{equation*}
S_{\mathcal{P}}(0)=\frac{g}{\pi} T_{0}^{2} . \tag{5.87}
\end{equation*}
$$

The r.m.s. value of the "power noise" $\widetilde{P}$ within bandwidth $\Delta v \ll 1 / \tau$ (Fig. 7) becomes equal to the deterministic signal power $\mathcal{P}_{\text {det }}$ (or more exactly, the main harmonic of its modulation law) at

$$
\begin{equation*}
\mathcal{P}_{\min }=\left(\left\langle\widetilde{\mathcal{P}}^{2}\right\rangle_{\Delta v}\right)^{1 / 2}=\left(2 S_{\mathcal{P}}(0) \Delta \omega\right)^{1 / 2}=2(g \Delta v)^{1 / 2} T_{0} . \tag{5.88}
\end{equation*}
$$

This result shows that our earlier prediction (45) may be improved by a substantial factor of the order of $(\Delta v / v)^{1 / 2}$, where the reduction of the output bandwidth is limited only by the signal accumulation time $\Delta t \sim 1 / \Delta v$, while the increase of $v$ is limited by the speed of (typically, mechanical) devices performing the power modulation. In practical systems this factor may improve the sensitivity by a couple orders of magnitude, enabling observation of extremely weak radiation. Maybe the most spectacular example are the recent measurements of the CMB radiation (discussed in Sec. 2.6), which corresponds to blackbody temperature $T_{\mathrm{K}} \approx 2.725 \mathrm{~K}$, with accuracy $\delta T_{\mathrm{K}} \sim 10^{-6} \mathrm{~K}$, using microwave

[^917]receivers with physical temperature of all their components much higher than $\delta T$. The observed weak $\left(\sim 10^{-5} \mathrm{~K}\right)$ anisotropy of the CMB radiation is a major experimental basis of all modern cosmology.

Let me also note that Eq. (73) may be readily generalized to the case when environment's response is different from the Ohmic model (64). This generalization is virtually evident from Eq. (66). Indeed, the second term in its left-hand part is just the Fourier component of the average response of the environment:

$$
\begin{equation*}
\left\langle\boldsymbol{\eta}_{\omega}\right\rangle=i \omega \eta q_{\omega} . \tag{5.89}
\end{equation*}
$$

Let the environment's response be still linear, but have an arbitrary dispersion,

$$
\begin{equation*}
\left\langle 7_{\omega}\right\rangle=\chi(\omega) q_{\omega}, \tag{5.90}
\end{equation*}
$$

where the function $\chi(\omega)$, called the generalized susceptibility of the environment, may be complex, i.e. have both the imaginary and real parts:

$$
\begin{equation*}
\chi(\omega)=\chi^{\prime}(\omega)+i \chi^{\prime \prime}(\omega) . \tag{5.91}
\end{equation*}
$$

Then Eq. (73) remains valid ${ }^{34}$ with the replacement $\eta \rightarrow \chi$ " $(\omega) / \omega$ :

$$
\begin{equation*}
S_{\mathcal{7}}(\omega)=\frac{\chi^{\prime \prime}(\omega)}{\pi \omega} T \tag{5.92}
\end{equation*}
$$

This fundamental relation ${ }^{35}$ is used not only to calculate the fluctuation intensity from the known generalized responsibility (i.e. the deterministic response of a complex system to a small perturbation), but sometimes in the opposite direction - to calculate the linear response from the known fluctuations. (The latter use is especially attractive at numerical simulations, such as molecular dynamics approaches, because it allows to avoid filtering a weak response from the noisy background.)

Now let us discuss what generalization of Eq. (92) is necessary to make that fundamental result suitable for arbitrary temperatures, $T \sim \hbar \omega$. The calculations we had performed started from the apparently classical equation of motion, Eq. (63). However, quantum mechanics shows ${ }^{36}$ that a similar equation is valid for the corresponding Heisenberg-picture operators, so that repeating all arguments leading to the Langevin equation (65), we may write its quantum-mechanical version

$$
\begin{equation*}
m \ddot{\hat{q}}+\eta \dot{\hat{q}}+\kappa \hat{q}=\hat{F}_{\mathrm{det}}+\hat{\tilde{\gamma}} \tag{5.93}
\end{equation*}
$$

[^918]This is the so-called the Heisenberg-Langevin (or "quantum Langevin") equation - in this particular case, for a harmonic oscillator.

The further operations, however, require certain caution, because the right-hand part of the equation is now an operator, and has some nontrivial properties. For example, the "values" of the Heisenberg operator, representing the same variable $f(t)$ at different times, do not necessarily commute:

$$
\begin{equation*}
\left[\hat{\tilde{f}}(t), \hat{\tilde{f}}\left(t^{\prime}\right)\right] \neq 0, \quad \text { if } t^{\prime} \neq t \tag{5.94}
\end{equation*}
$$

As a result, the function defined by Eq. (46) may not be an even function of time delay $\tau \equiv t^{\prime}-t$ even for a stationary process, making it inadequate for representation of the real correlation function - which has to obey Eq. (51). This technical difficulty may be circumvented by the introduction of the following symmetrized correlation function

$$
\begin{equation*}
K_{f}(\tau) \equiv \frac{1}{2}\langle\hat{\tilde{f}}(t) \hat{\tilde{f}}(t+\tau)+\hat{\tilde{f}}(t+\tau) \hat{\tilde{f}}(t)\rangle \equiv \frac{1}{2}\langle\{\hat{\tilde{f}}(t), \hat{\tilde{f}}(t+\tau)\}\rangle, \tag{5.95}
\end{equation*}
$$

(where $\{\ldots, \ldots\}$ denotes the anticommutator of the two operators), and, similarly, the symmetrical spectral density $S_{f}(\omega)$, defined by relation

$$
\begin{equation*}
S_{f}(\omega) \delta\left(\omega-\omega^{\prime}\right) \equiv \frac{1}{2}\left\langle\hat{f}_{\omega} \hat{f}_{\omega^{\prime}}^{*}+\hat{f}_{\omega^{\prime}}^{*} \hat{f}_{\omega}\right\rangle \equiv \frac{1}{2}\left\langle\left\{\hat{f}_{\omega}, \hat{f}_{\omega^{\prime}}^{*}\right\}\right\rangle, \tag{5.96}
\end{equation*}
$$

with $K_{f}(\tau)$ and $S_{f}(\omega)$ still related by the Fourier transform (59). ${ }^{37}$
Now we may repeat all the analysis that was carried out for the classical case, and get Eq. (71) again, but this expression has to be compared not with the equipartition theorem (72), but with its quantum-mechanical generalization (2.78), which, in our current notation, reads

$$
\begin{equation*}
\left\langle\left\langle\widetilde{q}^{2}\right\rangle\right\rangle=\frac{\hbar \omega_{0}}{2 \kappa} \operatorname{coth} \frac{\hbar \omega_{0}}{2 T} . \tag{5.97}
\end{equation*}
$$

As a result, we get the following quantum-mechanical generalization of Eq. (92):

$$
\begin{equation*}
S_{\neq}(\omega)=\frac{\hbar \chi^{\prime \prime}(\omega)}{2 \pi} \operatorname{coth} \frac{\hbar \omega}{2 T} \tag{5.98}
\end{equation*}
$$

Fluctuationdissipation theorem

This is the much-celebrated fluctuation-dissipation theorem, frequently referred to just as FDT. 38
As natural as it seems, this generalization poses a very interesting conceptual dilemma. Let, for the sake of clarity, temperature be relatively low, $T \ll \hbar \omega$; then Eq. (98) gives a temperatureindependent result

$$
\begin{equation*}
S_{\neq}(\omega)=\frac{\hbar \chi^{\prime \prime}(\omega)}{2 \pi} \tag{5.99}
\end{equation*}
$$

[^919]which is frequently called the quantum noise. According to the quantum Langevin equation (93), nothing but these fluctuations of the force exerted by the environment, with spectral density proportional to the imaginary part of susceptibility (i.e. damping), are the source of the ground-state "fluctuations" of the coordinate and momentum of a quantum harmonic oscillator, with r.m.s. values
\[

$$
\begin{equation*}
\delta q \equiv\left\langle\left\langle\widetilde{q}^{2}\right\rangle\right\rangle^{1 / 2}=\left(\frac{\hbar}{2 m \omega_{0}}\right)^{1 / 2}, \quad \delta p \equiv\left\langle\left\langle\widetilde{p}^{2}\right\rangle\right\rangle^{1 / 2}=m \omega_{0} \delta q=\left(\frac{\hbar m \omega_{0}}{2}\right)^{1 / 2}, \quad \text { i.e. } \delta q \cdot \delta p=\frac{\hbar}{2}, \tag{5.100}
\end{equation*}
$$

\]

and average energy $\hbar \omega_{0} / 2$. On the other hand, the basic quantum mechanics tells us that exactly these formulas describe the ground state of a dissipation-free oscillator, not coupled to any environment, and are a direct corollary of the Heisenberg uncertainty relation

$$
\begin{equation*}
\delta q \cdot \delta p \geq \frac{\hbar}{2} \tag{5.101}
\end{equation*}
$$

(The Gaussian wave packets, pertinent to a harmonic oscillator' ground state, turn the sign in Eq. (101) into pure equality.) So, what is the genuine source of Eqs. (100)?

The resolution of this paradox is that either interpretation of Eqs. (100) is legitimate, with their relative convenience depending on the particular application. (One can say that since the right-hand part of the quantum Langevin equation (93) is a quantum-mechanical operator, rather than a classical force, it "carries the uncertainty relation within itself".) However, this opportunistic resolution leaves the following question open: is the quantum noise (99) of the environment observable directly, without any probe oscillator subjected to it? An experimental resolution of this dilemma is not quite simple, because usual scientific instruments have their own zero-point fluctuations, which may be readily confused with those of the system under study. Fortunately, this difficulty may be overcome, for example, using unique frequency-mixing ("down-conversion") properties of Josephson junctions. ${ }^{39}$ Special low-temperature experiments using such down-conversion ${ }^{40}$ have confirmed that noise (99) is real and measurable. This has been one of the most convincing direct demonstrations of the reality of the zero-point energy $\hbar \omega / 2 .{ }^{41}$

Finally, let me mention briefly an alternative derivation ${ }^{42}$ of the fluctuation-theorem from the general quantum mechanics of open systems. This derivation is substantially longer, but gives an interesting sub-product,

$$
\begin{equation*}
\langle[\hat{\tilde{\gamma}}(t), \hat{\tilde{\gamma}}(t+\tau)]\rangle=i \hbar g(\tau) \tag{5.102}
\end{equation*}
$$

where $\mathfrak{g} \tau$ ) is the temporal Green's function of the environment (as "seen" by the system subjected to the generalized force $\mathcal{F}$ ), defined by equation

$$
\begin{equation*}
\langle\mathcal{\chi}(t)\rangle=\int_{0}^{\infty} g(\tau) q(t-\tau) d \tau=\int_{-\infty}^{t} g\left(t-t^{\prime}\right) q\left(t^{\prime}\right) d t^{\prime} . \tag{5.103}
\end{equation*}
$$

[^920]Plugging the Fourier transforms of all three functions participating in Eq. (103) into that relation, it is straightforward to check ${ }^{43}$ that the Green's function is just the Fourier image of the complex susceptibility $\chi(\omega)$, defined by Eq. (90):

$$
\begin{equation*}
\int_{0}^{\infty} g(\tau) e^{i \omega \tau} d \tau=\chi(\omega) \tag{5.104}
\end{equation*}
$$

here 0 is used as a lower limit instead of $(-\infty)$ just to emphasize that due to the causality principle, the Green's function has to be equal zero for $\tau<0$.

In order to reveal the real beauty of Eq. (102), we may use the Wiener-Khinchin theorem (59) to rewrite the fluctuation-dissipation theorem (98) in a form similar to Eq. (102):

$$
\begin{equation*}
\langle\{\hat{\tilde{\gamma}}(t), \hat{\tilde{\gamma}}(t+\tau)\}\rangle=2 K_{\neq 7}(\tau) \tag{5.105}
\end{equation*}
$$

where the correlation function $K_{\neq}(\tau)$ is most simply described by its Fourier transform, equal to $\pi S_{\neq}(\omega)$ :

$$
\begin{equation*}
\int_{0}^{\infty} K_{\ngtr}(\tau) \cos \omega \tau d \tau=\frac{\hbar \chi^{\prime \prime}(\omega)}{2} \operatorname{coth} \frac{\hbar \omega}{2 T} . \tag{5.106}
\end{equation*}
$$

The comparison of Eqs. (102) and (104), on one hand, and Eqs (105)-(106), on the other hand, shows that both the commutation and anticommutation properties of the Heisenberg-Langevin force operator at different moments of time are determined by the same generalized susceptibility $\chi(\omega)$, but the average anticommutator also depends on temperature, while the average commutator does not. ${ }^{44}$

### 5.6. The Kramers problem and the Smoluchowski equation

Returning to the classical case, it is evident that the Langevin equation (65) provides the means not only for the analysis of stationary fluctuations, but also for the description of an arbitrary time evolution of (classical) dynamic systems coupled to their environment - which, again, provides both dissipation and fluctuations. However, this approach suffers from two major handicaps.

First, this equation does enable us to find the statistical average of variable $q$, and the variance of its fluctuations (i.e., in the common mathematical terminology, the first and second moments of the probability distribution) as functions of time, but not the distribution $w(q, t)$ as such. This may not look like a big problem, because in most cases (in particular, in linear systems such as the harmonic oscillator) the distribution is Gaussian - see, e.g., Eq. (2.77).

The second, more painful, drawback of the Langevin approach is that it is instrumental only for the already mentioned "linear" systems - i.e., the systems whose dynamics is described by linear differential equations, such as Eq. (65). However, as we know from classical dynamics, many important problems (for example, the Kepler problem of planetary motion ${ }^{45}$ ) are reduced to 1 D motion in substantially anharmonic potentials $U_{\text {ef }}(q)$, leading to nonlinear equations of motion. If the energy of interaction between the system and its random environment is bilinear - i.e. is a product of variables

[^921]belonging to these sub-systems (as it is very frequently the case), we may repeat all arguments of the last section to derive the following generalized version of the Langevin equation
\[

$$
\begin{equation*}
m \ddot{q}+\eta \dot{q}+\frac{\partial U(q, t)}{\partial q}=\tilde{\not}(t), \tag{5.107}
\end{equation*}
$$

\]

valid for an arbitrary, possibly time-dependent potential $U(q, t){ }^{46}$ Unfortunately, the solution of this equation may be very hard. Indeed, the Fourier analysis carried out in the last section was essentially based on the linear superposition principle that is invalid for nonlinear equations.

If the fluctuation intensity is low, $|\delta q| \ll\langle q\rangle$, where $\langle q\rangle(t)$ is the deterministic solution of Eq. (107) in the absence of fluctuations, this equation may be linearized ${ }^{47}$ with respect to small fluctuations $\widetilde{q} \equiv q-\langle q\rangle$ to get a linear equation,

$$
\begin{equation*}
m \ddot{\tilde{q}}+\eta \dot{\widetilde{q}}+\kappa(t) \widetilde{q}=\tilde{\boldsymbol{q}}(t), \quad \text { with } \kappa(t) \equiv \frac{\partial^{2}}{\partial q^{2}} U(\langle q\rangle(t), t) \tag{5.108}
\end{equation*}
$$

This equation differs from Eq. (65) only by the time dependence of the effective spring constant $\kappa(t)$, and may be solved by the Fourier expansion of both fluctuations and function $\kappa(t)$. Such calculations are somewhat more cumbersome than have been performed above, but may be doable (especially if the unperturbed motion $\langle q\rangle(t)$ is periodic), and sometimes give useful analytical results. ${ }^{48}$

However, some important problems cannot be solved by the linearization. Perhaps, the most apparent example is the so-called Kramers problem ${ }^{49}$ of finding the lifetime of a metastable state of a 1D classical system in a potential well separated from the continuum motion region with a potential barrier (Fig. 10).


Fig. 5.10. The Kramers problem.

In the absence of fluctuations, the system, placed close to well's bottom ( $q=q_{1}$ ), would stay there forever. Fluctuations result not only in a finite spread of the probability density $w(q, t)$ around that point, but also in the gradual decrease of the total probability

$$
\begin{equation*}
W(t)=\int_{\substack{\text { wells } \\ \text { bottom }}} w(q, t) d q \tag{5.109}
\end{equation*}
$$

[^922]to find the system in the well, because of the growing probability of escape from the well, over the potential barrier, due to thermal activation. If the barrier height,
\[

$$
\begin{equation*}
U_{0} \equiv U\left(q_{2}\right)-U\left(q_{1}\right), \tag{5.110}
\end{equation*}
$$

\]

is much larger than temperature $T,{ }^{50}$ the Boltzmann distribution $w \propto \exp \{-U(q) / T\}$ should be approximately valid in most of the well, so that the probability for the system to overcome the barrier should scale as $\exp \left\{-U_{0} / T\right\}$. From these handwaving arguments, one may reasonably expect that if probability $W(t)$ that the system is still in the well by time $t$ should obey the usual "decay law"

$$
\begin{equation*}
\dot{W}=-\frac{W}{\tau}, \tag{5.111}
\end{equation*}
$$

then lifetime $\tau$ has to obey the general Arrhenius law, $\tau=\tau_{A} \exp \left\{U_{0} / T\right\}$. However, that relation needs to be proved, and the pre-exponential coefficient $\tau_{A}$ (frequently called the attempt time) needs to be calculated. This cannot be done by the linearization of Eq. (107), because the linearization is equivalent to a quadratic approximation of the potential $U(q)$, which evidently cannot describe the potential well and the potential barrier simultaneously - see Fig. 10.

This and other essentially nonlinear problems may be addressed using an alternative approach to fluctuation analysis, dealing directly with the time evolution of the probability density $w(q, t)$. Due to the shortage of time, I will review this approach a bit superficially, using mostly handwaving arguments, and refer the interested reader to special literature ${ }^{51}$ for strict mathematical proofs. Let us start from the effect of diffusion of a free 1D particle in the high damping limit, described by the Langevin equation (74), and assume that at all times the probability distribution stays Gaussian:

$$
\begin{equation*}
w(q, t)=\frac{1}{(2 \pi)^{1 / 2} \delta q(t)} \exp \left\{-\frac{\left(q-q_{0}\right)^{2}}{2 \delta q^{2}(t)}\right\} \tag{5.112}
\end{equation*}
$$

where $q_{0}$ is the initial position of the particle, and $\delta q(t)$ is the time-dependent distribution width, which grows in time in accordance with Eq. (77):

$$
\begin{equation*}
\delta q(t)=(2 D t)^{1 / 2} \tag{5.113}
\end{equation*}
$$

It is straightforward to check, by substitution, that this solution satisfies the following simple partial differential equation, ${ }^{52}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}=D \frac{\partial^{2} w}{\partial q^{2}} \tag{5.114}
\end{equation*}
$$

with the delta-functional initial condition

$$
\begin{equation*}
w(q, 0)=\delta\left(q-q_{0}\right) \tag{5.115}
\end{equation*}
$$

[^923]The simple and important equation of diffusion (114) may be naturally generalized to the 3D motion: ${ }^{53}$

Equation
of $3 D$
of 3D

$$
\begin{equation*}
\frac{\partial w}{\partial t}=D \nabla^{2} w \tag{5.116}
\end{equation*}
$$

Now let us compare this equation with the probability conservation law, ${ }^{54}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\nabla \cdot \mathbf{j}_{w}=0 \tag{5.117a}
\end{equation*}
$$

where vector $\mathbf{j}_{w}$ has the physical sense of the probability current density. (The validity of this relation is evident from its integral form,

$$
\begin{equation*}
\frac{d}{d t} \int_{V} w d^{3} r+\oint_{S} \mathbf{j}_{w} \cdot d^{2} \mathbf{r}=0 \tag{5.117b}
\end{equation*}
$$

that results from integration of Eq. (117a) over an arbitrary time-independent volume $V$ limited by surface $S$, and applying the divergence theorem ${ }^{55}$ to the second term.) The continuity relation (117a) coincides with Eq. (116), with $D$ given by Eq. (78), only if we take

$$
\begin{equation*}
\mathbf{j}_{w}=-D \nabla w=-\frac{T}{\eta} \nabla w . \tag{5.118}
\end{equation*}
$$

The first form of this relation allows a simple interpretation: the probability flow is proportional to the spatial gradient of probability density (i.e., in application to many ( $N$ ) similar and independent particles, just to the gradient of their concentration $n=N w$ ), with the sign corresponding to the flow from the higher to lower concentration. This flow is the very essence of the effect of diffusion.

The fundamental Eq. (117) has to be satisfied also for a force-driven particle at negligible diffusion $(D \rightarrow 0)$; in this case

$$
\begin{equation*}
\mathbf{j}_{w}=w \mathbf{v}, \tag{5.119}
\end{equation*}
$$

where $\mathbf{v}$ is the deterministic velocity of the particle. In the high-damping limit we are considering right now, $\mathbf{v}$ is just the drift velocity:

$$
\begin{equation*}
\mathbf{v}=\frac{1}{\eta} \boldsymbol{\gamma}_{\mathrm{det}}=-\frac{1}{\eta} \nabla U(\mathbf{r}) \tag{5.120}
\end{equation*}
$$

where $\boldsymbol{F}_{\text {det }}$ is the deterministic force described by potential energy $U(\mathbf{r})$. Now, as we have descriptions of $\mathbf{j}_{w}$ due to both drift and diffusion separately, we may rationally assume that in the general case when both effects are present, the corresponding components of the probability current just add up, so that

$$
\begin{equation*}
\mathbf{j}_{w}=\frac{1}{\eta}[w(-\nabla U)-T \nabla w], \tag{5.121}
\end{equation*}
$$

[^924]and Eq. (117a) takes the form
\[

$$
\begin{equation*}
\eta \frac{\partial w}{\partial t}=\nabla(w \nabla U)+T \nabla^{2} w \tag{5.122}
\end{equation*}
$$

\]

This is the Smoluchowski equation, ${ }^{56}$ which is closely related to the Boltzmann equation in multiparticle kinetics - to be discussed in the next chapter.

As a sanity check, let us see what does the Smoluchowski equation give in the stationary limit, $\partial w / \partial t \rightarrow 0$ (which evidently may be achieved only if the deterministic potential $U$ is time-independent.) Then Eq. (117a) yields $\mathbf{j}_{w}=$ const, where the constant describes the motion of the system as the whole. If such motion is absent, $\mathbf{j}_{w}=0$, then according to Eq. (121),

$$
\begin{equation*}
w \nabla U+T \nabla w=0, \quad \text { i.e. } \frac{\nabla w}{w}=-\frac{\nabla U}{T} . \tag{5.123}
\end{equation*}
$$

Since the left-hand part of the last form of the last relation is just $\nabla(\ln w)$, Eq. (123) may be immediately integrated, giving

$$
\begin{equation*}
\ln w=-\frac{U}{T}+\ln C, \quad \text { i.e. } w(\mathbf{r})=C \exp \left\{-\frac{U(\mathbf{r})}{T}\right\}, \tag{5.124}
\end{equation*}
$$

Multiplied by the number $N$ of similar, independent systems, with spatial density $n(\mathbf{r})=N w(\mathbf{r})$, this is just the Boltzmann distribution (3.26).

Now, as a less trivial example of the Smoluchowski equation's applications, let us use it to solve the 1 D Kramers problem (Fig. 10) in the corresponding high-damping limit, $m \ll \eta \tau_{A}$. It is straightforward to check that the 1D version of Eq. (121),

$$
\begin{equation*}
I_{w}=\frac{1}{\eta}\left[w\left(-\frac{\partial U}{\partial q}\right)-T \frac{\partial w}{\partial q}\right] \tag{5.125a}
\end{equation*}
$$

is equivalent to

$$
\begin{equation*}
I_{w}=-\frac{T}{\eta} \exp \left\{-\frac{U(q)}{T}\right\} \frac{\partial}{\partial q}\left(w \exp \left\{\frac{U(q)}{T}\right\}\right) \tag{5.125b}
\end{equation*}
$$

(where $I_{w}$ is the probability current at a certain location $q$, rather than its density), so that we can write

$$
\begin{equation*}
I_{w} \exp \left\{\frac{U(q)}{T}\right\}=-\frac{T}{\eta} \frac{\partial}{\partial q}\left(w \exp \left\{\frac{U(q)}{T}\right\}\right) \tag{5.126}
\end{equation*}
$$

As was discussed above, the notion of metastable state's lifetime is well defined only for sufficiently low temperatures

$$
\begin{equation*}
T \ll U_{0} . \tag{5.127}
\end{equation*}
$$

[^925]when the lifetime is relatively long, $\tau \gg \tau_{A}$, where $\tau_{A}$ has to be of the order of the time of the system relaxation inside the well. Since the first term of the continuity equation (117b) is of the order of $W / \tau$, in this limit the term, and hence the gradient of $I_{w}$, are negligibly small, so the probability current does not depend on $q$ in the potential barrier region. Let us integrate both sides of Eq. (126) over that region, using that fact:
\[

$$
\begin{equation*}
I_{w} \int_{q^{\prime}}^{q^{\prime \prime}} \exp \left\{\frac{U(q)}{T}\right\} d q=-\frac{T}{\eta}\left(w \exp \left\{\frac{U(q)}{T}\right\}\right)_{q^{\prime}}^{q^{\prime \prime}} \tag{5.128}
\end{equation*}
$$

\]

where the integration limits $q^{\prime}$ and $q^{\prime \prime}$ (Fig. 10) are selected so that so that

$$
\begin{equation*}
T \ll U\left(q^{\prime}\right)-U\left(q_{1}\right), U\left(q_{2}\right)-U\left(q^{\prime \prime}\right) \ll U_{0} . \tag{5.129}
\end{equation*}
$$

(Evidently, such selection is only possible if condition (127) is satisfied.) In this limit the contribution to the right-hand part from point $q^{\prime \prime}$ is negligible because the probability density behind the barrier is exponentially small. On the other hand, the probability at point $q$ ' is close to its stationary, Boltzmann value (124), so that

$$
\begin{equation*}
w\left(q^{\prime}\right) \exp \left\{\frac{U\left(q^{\prime}\right)}{T}\right\}=w\left(q_{1}\right) \exp \left\{\frac{U\left(q_{1}\right)}{T}\right\}, \tag{5.130}
\end{equation*}
$$

and Eq. (128) yields

$$
\begin{equation*}
I_{w}=\frac{T}{\eta} w\left(q_{1}\right) / \int_{q^{\prime}}^{q^{\prime \prime}} \exp \left\{\frac{U(q)-U\left(q_{1}\right)}{T}\right\} d q . \tag{5.131}
\end{equation*}
$$

We are almost done. The probability density $w\left(q_{1}\right)$ at the well's bottom may be expressed in terms of the total probability $W$ of the particle being in the well by using the normalization condition

$$
\begin{equation*}
W=\int_{\substack{\text { wells } \\ \text { bottom }}} w\left(q_{1}\right) \exp \left\{\frac{U\left(q_{1}\right)-U(q)}{T}\right\} d q \tag{5.132}
\end{equation*}
$$

the integration here may be limited by the region where the difference $U(q)-U\left(q_{1}\right)$ is larger then $T$ but still much smaller than $U_{0}-$ cf. Eq. (129). According to the Taylor expansion, the shape of any smooth potential well near its bottom may be well approximated by a quadratic parabola:

$$
\begin{equation*}
U\left(q \approx q_{1}\right)-U\left(q_{1}\right) \approx \frac{\kappa_{1}}{2}\left(q-q_{1}\right)^{2}, \quad \text { where }\left.\kappa_{1} \equiv \frac{d^{2} U}{d q^{2}}\right|_{q=q_{1}}>0 . \tag{5.133}
\end{equation*}
$$

With this approximation, Eq. (132) is reduced to the standard Gaussian integral: ${ }^{57}$

$$
\begin{equation*}
W=w\left(q_{1}\right) \int_{\substack{\text { wells } \\ \text { bottom }}} \exp \left\{-\frac{\kappa_{1}\left(q-q_{1}\right)^{2}}{2 T}\right\} d q \approx w\left(q_{1}\right) \int_{-\infty}^{+\infty} \exp \left\{\frac{\kappa_{1} \widetilde{q}^{2}}{2 T}\right\} d \widetilde{q}=w\left(q_{1}\right)\left(\frac{2 \pi T}{\kappa_{1}}\right)^{1 / 2} . \tag{5.134}
\end{equation*}
$$

To complete the calculation, we may use the similar approximation,

[^926]\[

$$
\begin{align*}
U\left(q \approx q_{2}\right)-U\left(q_{1}\right) & \approx\left[U\left(q_{2}\right)-\frac{\kappa_{2}}{2}\left(q-q_{2}\right)^{2}\right]-U\left(q_{1}\right)=U_{0}-\frac{\kappa_{2}}{2}\left(q-q_{2}\right)^{2}  \tag{5.135}\\
& \text { where } \kappa_{2} \equiv-\left.\frac{d^{2} U}{d q^{2}}\right|_{q=q_{2}}>0
\end{align*}
$$
\]

to work out the remaining integral in Eq. (131), because in the limit (129) this integral is dominated by the contribution from a region very close to the barrier top, where approximation (135) is asymptotically exact. As a result, we get

$$
\begin{equation*}
\int_{q^{\prime}}^{q^{\prime \prime}} \exp \left\{\frac{U(q)-U\left(q_{1}\right)}{T}\right\} d q \approx \exp \left\{\frac{U_{0}}{T}\right\}\left(\frac{2 \pi T}{\kappa_{2}}\right)^{1 / 2} \tag{5.136}
\end{equation*}
$$

Plugging Eqs. (136), and $w\left(q_{1}\right)$ expressed from Eq. (134), into Eq. (131), we finally get

$$
\begin{equation*}
I_{w}=W \frac{\left(\kappa_{1} \kappa_{2}\right)^{1 / 2}}{2 \pi \eta} \exp \left\{-\frac{U_{0}}{T}\right\} \tag{5.137}
\end{equation*}
$$

This expression should be compared with the 1D version of Eq. (117b) for the segment $\left[-\infty, q^{\prime}\right]$. Since this interval covers the region near $q_{1}$ where most of the probability density resides, and $I_{q}(-\infty)=$ 0 , the result is merely

$$
\begin{equation*}
\frac{d W}{d t}+I_{w}\left(q^{\prime}\right)=0 \tag{5.138}
\end{equation*}
$$

In our approximation, $I_{w}\left(q^{\prime}\right)$ does not depend on the exact position of point $q^{\prime}$, and is given by Eq. (137), so that plugging it into Eq. (138), we recover the exponential decay law (111), with lifetime

$$
\begin{equation*}
\tau=\frac{2 \pi \eta}{\left(\kappa_{1} \kappa_{2}\right)^{1 / 2}} \exp \left\{\frac{U_{0}}{T}\right\}=2 \pi\left(\tau_{1} \tau_{2}\right)^{1 / 2} \exp \left\{\frac{U_{0}}{T}\right\}, \quad \text { where } \tau_{1,2} \equiv \frac{\eta}{\kappa_{1,2}} \tag{5.139}
\end{equation*}
$$

Thus the metastable state lifetime is indeed described by the Arrhenius law, with the attempt time scaling as the geometric mean of system's "relaxation times" near the potential well bottom $\left(\tau_{1}\right)$ and the potential barrier top $\left(\tau_{2}\right) .{ }^{58}$ Let me leave for reader's exercise to prove that if the potential profile near well's bottom and/or top is sharp, the pre-exponential factor in Eq. (139) should be modified, but the Arrhenius exponent is not affected.

### 5.7. The Fokker-Planck equation

Expression (139) is just a particular, high-damping limit of a more general result obtained by Kramers. In order to recover all of it, we need to generalize the Smoluchowski equation to arbitrary values of damping $\eta$. In this case, the probability density $w$ is a function of not only the particle's position $\mathbf{q}$ (and time $t$ ), but also its momentum $\mathbf{p}$ - see Eq. (2.11). Thus the continuity equation (117a) needs to be generalized to 6D phase space. Such generalization is natural:

[^927]\[

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\nabla_{q} \cdot \mathbf{j}_{q}+\nabla_{p} \cdot \mathbf{j}_{p}=0 \tag{5.140}
\end{equation*}
$$

\]

where $\mathbf{j}_{q}$ (which was called $\mathbf{j}_{w}$ in the last section) is the probability current density in the coordinate space, while $\mathbf{j}_{p}$ is the current density in the momentum space, and $\nabla_{p}$ is the gradient operator in that space,

$$
\begin{equation*}
\nabla_{p} \equiv \sum_{j=1}^{3} \mathbf{n}_{j} \frac{\partial}{\partial p_{j}} \tag{5.141}
\end{equation*}
$$

while $\nabla_{q}$ is the usual gradient operator in the coordinate space, that was denoted as $\nabla$ in the previous section - with index $q$ added here just for additional clarity. At negligible fluctuations ( $T \rightarrow 0$ ), $\mathbf{j}_{p}$ in the momentum space may be evaluated using the natural analogy with $\mathbf{j}_{q}$ - see Eq. (119). In our new notation, that relation takes the following form,

$$
\begin{equation*}
\mathbf{j}_{q}=w \mathbf{v}=w \dot{\mathbf{q}}=w \frac{\mathbf{p}}{m}, \tag{5.142}
\end{equation*}
$$

so it is naturally to take

$$
\begin{equation*}
\mathbf{j}_{p}=w \dot{\mathbf{p}}=w\langle\boldsymbol{\gamma}\rangle=w\left(-\nabla_{q} U-\eta \mathbf{v}\right)=w\left(-\nabla_{q} U-\eta \frac{\mathbf{p}}{m}\right) . \tag{5.143}
\end{equation*}
$$

As a sanity check, it is straightforward to verify that the diffusion-free equation resulting from the combination of Eqs. (140), (142) and (143),

$$
\begin{equation*}
\left.\frac{\partial w}{\partial t}\right|_{\mathrm{drift}}=-\nabla_{q} \cdot\left(w \frac{\mathbf{p}}{m}\right)+\nabla_{p} \cdot\left[w\left(\nabla_{q} U+\eta \frac{\mathbf{p}}{m}\right)\right] \tag{5.144}
\end{equation*}
$$

allows the following particular solution

$$
\begin{equation*}
w(\mathbf{q}, \mathbf{p}, t)=\delta(\mathbf{q}-\langle\mathbf{q}\rangle(t)) \delta(\mathbf{p}-\langle\mathbf{p}\rangle(t)) \tag{5.145}
\end{equation*}
$$

where the statistical-average coordinate and momentum satisfy the deterministic equations of motion,

$$
\begin{equation*}
\langle\dot{\mathbf{q}}\rangle=\frac{\langle\mathbf{p}\rangle}{m}, \quad\langle\dot{\mathbf{p}}\rangle=-\nabla_{q} U-\eta \frac{\langle\mathbf{p}\rangle}{m}, \tag{5.146}
\end{equation*}
$$

describing particle's drift, with the appropriate deterministic initial conditions.
In order to understand how the diffusion may be accounted for, let us consider a statistical ensemble of free $\left(\nabla_{q} U=0, \eta \rightarrow 0\right)$ particles that are uniformly distributed in direct space (so that $\nabla_{q} w=$ 0 ), but possibly localized in the momentum space. For this case, the right-hand part of Eq. (144) vanishes, i.e. the time evolution of the probability density $w$ may be only due to diffusion. In the corresponding limit $\langle\boldsymbol{\eta}\rangle \rightarrow 0$, the Langevin equation (107) for each Cartesian coordinate is reduced to

$$
\begin{equation*}
m \ddot{q}_{j}=\widetilde{\mathcal{F}}_{j}(t), \text { i.e. } \dot{p}_{j}=\widetilde{\mathcal{F}}_{j}(t) \tag{5.147}
\end{equation*}
$$

This equation is similar to the high-damping 1D equation (74) (with $\not_{\mathrm{det}}=0$ ), with replacement $q \rightarrow$ $p_{j} / \eta$, and hence the corresponding contribution to $\partial w / \partial t$ may be described by the second term of Eq. (122) with that replacement:

$$
\begin{equation*}
\left.\frac{\partial w}{\partial t}\right|_{\text {diffusion }}=D \nabla_{p / \eta}^{2} w=\frac{T}{\eta} \eta^{2} \nabla_{p}^{2} w=\eta T \nabla_{p}^{2} w . \tag{5.148}
\end{equation*}
$$

Now the reasonable assumption that in the arbitrary case the drift and diffusion contributions to $\partial w / \partial t$ just add up, immediately leads us to the full Fokker-Planck equation: ${ }^{59}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}=-\nabla_{q} \cdot\left(w \frac{\mathbf{p}}{m}\right)+\nabla_{p} \cdot\left[w\left(\nabla_{q} U+\eta \frac{\mathbf{p}}{m}\right)\right]+\eta T \nabla_{p}^{2} w . \tag{5.149}
\end{equation*}
$$

As a sanity check, let us use this equation to find the stationary probability distribution of momentum of free particles, at arbitrary damping $\eta$, in the momentum space, assuming their uniform distribution in the direct space, $\nabla_{q}=0$. In the stationary case $\partial w / \partial t=0$, so that Eq. (149) is reduced to

$$
\begin{equation*}
\nabla_{p} \cdot\left[w\left(\eta \frac{\mathbf{p}}{m}\right)\right]+\eta T \nabla_{p}^{2} w=0 . \tag{5.150}
\end{equation*}
$$

The damping coefficient $\eta$ cancels, and the first integration over momentum yields

$$
\begin{equation*}
\frac{\mathbf{p}}{m} w+T \nabla_{p} w=\mathbf{j} \tag{5.152}
\end{equation*}
$$

where $\mathbf{j}$ is a vector constant describing a possible motion of the system as the whole. In the absence of such motion, $\mathbf{j}=0$, the second integration over momentum gives

$$
\begin{equation*}
w=\text { const } \times \exp \left\{-\frac{p^{2}}{2 m T}\right\}, \tag{5.153}
\end{equation*}
$$

i.e. the Maxwell distribution (3.5). However, result (153) is more general than that obtained in Sec. 3.1, because it shows that the distribution stays the same even at nonvanishing damping.

It is also easy to show that if the damping is large (in the sense assumed in the last section), the solution of the Fokker-Planck equation tends to the following product

$$
\begin{equation*}
w(\mathbf{q}, \mathbf{p}, t) \rightarrow \text { const } \times \exp \left\{-\frac{p^{2}}{2 m T}\right\} \times w(\mathbf{q}, t) \tag{5.154}
\end{equation*}
$$

where the direct-space distribution $\mathrm{w}(\mathbf{q}, t)$ obeys the Smoluchowski equation (122). However, in the general case, solutions of Eq. (149) may be rather complex, ${ }^{60}$ so I would mention (rather than derive) only one of them, that of the Kramers problem (Fig. 10). Acting virtually exactly as in Sec. 6, one can show at arbitrary damping (but still in the limit (127), $T \ll U_{0}$, with the additional restriction $\tau \gg m / \gamma$ ), the metastable state's lifetime is again given by the Arrhenius formula (139), with the same exponent $\exp \left\{U_{0} / T\right\}$, but with the reciprocal time constants $1 / \tau_{1,2}$ replaced with

$$
\omega_{1,2}^{\prime} \equiv\left[\omega_{1,2}^{2}+\left(\frac{\eta}{2 m}\right)^{2}\right]^{1 / 2}-\frac{\eta}{2 m} \rightarrow \begin{cases}\omega_{1,2}, & \text { for } \eta \ll m \omega_{1,2}  \tag{5.155}\\ 1 / \tau_{1,2}, & \text { for } m \omega_{1,2} \ll \eta\end{cases}
$$

[^928]where $\omega_{1,2} \equiv\left(\kappa_{1,2} / m\right)^{1 / 2}$, while $\kappa_{1,2}$ are the effective spring constants defined by Eqs. (133) and (135). Thus, in the most important particular limit of low damping, Eq. (139) is replaced with the famous formula

Kramers
formula for low damping

$$
\begin{equation*}
\tau=\frac{2 \pi}{\left(\omega_{1} \omega_{2}\right)^{1 / 2}} \exp \left\{\frac{U_{0}}{T}\right\} \tag{5.156}
\end{equation*}
$$

This Kramers' result for the classical thermal activation of the virtually-Hamiltonian system over the potential barrier may be compared with that for its quantum-mechanical tunneling through the barrier. ${ }^{61}$ Even the simplest, WKB approximation for the latter time,

$$
\begin{equation*}
\tau_{Q}=\tau_{A} \exp \left\{-2 \int_{\kappa^{2}(q)>0} \kappa(q) d q\right\}, \quad \text { with } \frac{\hbar^{2} \kappa^{2}(q)}{2 m} \equiv U(q)-E \text {, } \tag{5.157}
\end{equation*}
$$

shows that generally those two lifetimes have different dependences on the barrier shape. For example, for a nearly-rectangular potential barrier, the exponent that determines the classical lifetime (156) depends (linearly) only on the barrier height $U_{0}$, while that defining the quantum lifetime is proportional to the barrier width, while scaling as a square root of $U_{0}$. However, in the important case of "soft" potential profiles, which are typical for the case of barely emerging (or nearly disappearing) quantum wells (Fig. 11) the classical and quantum results may be simply related.


Fig. 5.11. Cubic-parabolic potential profile and its parameters.

Indeed, such potential profile $U(q)$ may be well approximated by 4 leading terms of its Taylor expansion, with the highest term proportional to $\left(q-q_{0}\right)^{3}$, near some point $q_{0}$ in the vicinity of the well. In this approximation, the second derivative $d^{2} U / d q^{2}$ vanishes at the point $q_{0}=\left(q_{1}+q_{2}\right) / 2$, exactly between the well's bottom and the barrier's top (in Fig. 11, $q_{1}$ and $q_{2}$ ). Selecting the origin at this point, we may reduce the approximation to just two terms: ${ }^{62}$

$$
\begin{equation*}
U(q)=a q-\frac{b}{3} q^{3}, \tag{5.158}
\end{equation*}
$$

with $a b>0$. Using a straightforward calculus, we can find all important parameters of this cubicparabola: the positions of its minimum and maximum:

$$
\begin{equation*}
q_{2}=-q_{1}=(a / b)^{1 / 2} \tag{5.159}
\end{equation*}
$$

the barrier height over the well's bottom:

[^929]\[

$$
\begin{equation*}
U_{0} \equiv U\left(q_{2}\right)-U\left(q_{1}\right)=\frac{4}{3}\left(\frac{a^{3}}{b}\right)^{1 / 2}, \tag{5.160}
\end{equation*}
$$

\]

and the effective spring constants:

$$
\begin{equation*}
\kappa_{1}=\kappa_{2} \equiv\left|\frac{d^{2} U}{d q^{2}}\right|_{q_{1,2}}=2(a b)^{1 / 2} \tag{5.161}
\end{equation*}
$$

The last expression shows that for this potential profile, frequencies $\omega_{1,2}$ participating in Eq. (161) are equal to each other, so that this result may be rewritten as

$$
\begin{equation*}
\tau=\frac{2 \pi}{\omega_{0}} \exp \left\{\frac{U_{0}}{T}\right\}, \quad \text { with } \omega_{0}^{2} \equiv \frac{2(a b)^{1 / 2}}{m} \tag{5.162}
\end{equation*}
$$

On the other hand, for the same profile, the WKB approximation (157) (which is accurate when the height of the metastable state energy over the well's bottom, $E-U\left(q_{1}\right) \approx \hbar \omega_{0} / 2$, is much less than the barrier height $U_{0}$ ) yields ${ }^{63}$

Comparison of the dominating, exponential factors in these two results shows that the thermal activation yields lower lifetime (i.e., dominates the metastable state decay) if temperature is above the crossover value

$$
\begin{equation*}
T_{c}=\frac{36}{5} \hbar \omega_{0}=7.2 \hbar \omega_{0} \tag{5.164}
\end{equation*}
$$

This expression for the cubic-parabolic barrier may be compared with the similar crossover for a quadratic-parabolic barrier, ${ }^{64}$ for which $T_{c}=2 \pi \hbar \omega_{0} \approx 6.28 \hbar \omega_{0}$. We see that the numerical factors for these two different soft potential profiles are very substantial, but rather close.

### 5.8. Back to the correlation function

Unfortunately I will not have time to review solutions of other problems using the Smoluchowski and Fokker-Planck equations, but have to mention one conceptual issue. Since it is intuitively clear that these equations provide the complete statistical information about the system under analysis, one may wonder whether they may be used to find the temporal characteristics of the system, which were discussed in Secs. $4-5$ using the Langevin formalism. For any statistical average of a function taken at the same time instant, the answer is evidently yes - cf. Eq. (2.11):

$$
\begin{equation*}
\langle f(\mathbf{q}(t), \mathbf{p}(t))\rangle=\int f(\mathbf{q}, \mathbf{p}) w(\mathbf{q}, \mathbf{p}, t) d^{3} q d^{3} p, \tag{5.165}
\end{equation*}
$$

[^930]but what if the function depends on variables taken at different times, for example the components of the correlation function $K_{f}(\tau)$ defined by Eq. (49)?

To answer this question, let us start from the discrete variable case when Eq. (165) takes form (2.7), which, for our current purposes, may be rewritten as

$$
\begin{equation*}
\langle f(t)\rangle=\sum_{m} f_{m} W_{m}(t) . \tag{5.166}
\end{equation*}
$$

In plain English, this is a sum of all possible values of the function, each multiplied by its probability as a function of time. But this means that average $\left\langle f(t) f\left(t^{\prime}\right)\right\rangle$ may be calculated as the sum of all possible products $f_{m} f_{m}$, multiplied by the joint probability for measurement outcome $m$ at moment $t$, and outcome $m^{\prime}$ at moment $t$ '. The joint probability may be presented as a product of $W_{m}(t)$ by the conditional probability $W\left(m^{\prime}, t^{\prime} \mid m, t\right)$. Since the correlation function is well defined only for stationary systems, in the last expression we can take $t=0$, i.e. find the conditional probability as the result, $W_{m} \cdot(\tau)$, of solution of the equation describing system's probability evolution, at time $\tau=t^{\prime}-t$ (rather than $t^{\prime}$ ), with the special initial condition

$$
\begin{equation*}
W_{m^{\prime}}(0)=\delta_{m^{\prime}, m} \tag{5.167}
\end{equation*}
$$

On the other hand, since the average $\langle f(t) f(t+\tau)\rangle$ of a stationary process should not depend on $t$, instead of $W_{m}(t)$ we may take the stationary probability distribution $W_{m}(\infty)$, independent of the initial conditions, and may be found as the same special solution, but at time $\tau \rightarrow \infty$. As a result, we may write

$$
\begin{equation*}
\langle f(t) f(t+\tau)\rangle=\sum_{m, m^{\prime}} f_{m} W_{m}(\infty) f_{m^{\prime}} W_{m^{\prime}}(\tau) \tag{5.168}
\end{equation*}
$$

This expression looks simple, but note that this recipe requires to solve the time evolution equations for each $W_{m} \cdot(\tau)$ for all possible initial conditions (167). To see how this recipe works in practice, let us revisit the simplest two-level system (see, e.g., Fig. 4.13 reproduced in Fig. 12 below in a notation more convenient for our current purposes), and calculate the correlation function of its energy fluctuations.


Fig. 5.12. Dynamics of a two-level system.

The stationary probabilities for this system (i.e. the probabilities for $\tau \rightarrow \infty$ ) have been calculated in Chapter 2, and then again in Sec. 4.4. In our current notation (Fig. 12),

$$
\begin{equation*}
W_{0}(\infty)=\frac{1}{1+e^{-\Delta / T}}, \quad W_{1}(\infty)=\frac{1}{e^{\Delta / T}+1}, \quad\langle E\rangle=W_{0}(\infty) \times 0+W_{1}(\infty) \times \Delta=\frac{\Delta}{e^{\Delta / T}+1} . \tag{5.169}
\end{equation*}
$$

In order to calculate the conditional probabilities $W_{m} \cdot(\tau)$ with initial conditions (167) (according to Eq. (168), we need all 4 of them, for $m, m^{\prime}=0,1$ ), we may use master equations (4.100), in our current notation reading

$$
\begin{equation*}
\frac{d W_{1}}{d \tau}=-\frac{d W_{0}}{d \tau}=\Gamma_{\uparrow} W_{0}-\Gamma_{\downarrow} W_{1} . \tag{5.170}
\end{equation*}
$$

Since Eq. (170) conserves the total probability, $W_{0}+W_{1}=1$, only one probability (say, $W_{1}$ ) is an independent variable, and for it, Eq. (170) gives a simple, linear differential equation,

$$
\begin{equation*}
\frac{d W_{1}}{d \tau}=\Gamma_{\uparrow}-\Gamma_{\Sigma} W_{1}, \quad \text { where } \Gamma_{\Sigma} \equiv \Gamma_{\uparrow}+\Gamma_{\downarrow} \tag{5.171}
\end{equation*}
$$

This equation may be readily integrated for an arbitrary initial condition:

$$
\begin{equation*}
W_{1}(\tau)=W_{1}(0) e^{-\Gamma_{\Sigma} \tau}+W_{1}(\infty)\left(1-e^{-\Gamma_{\Sigma} \tau}\right), \tag{5.172}
\end{equation*}
$$

where $W_{1}(\infty)$ is given by the second of Eqs. (169). (It is straightforward to check that the solution for $W_{0}(\tau)$ may be presented in the similar form, with the corresponding change of the state index.) Now everything is ready to calculate average $\langle E(t) E(t+\tau)\rangle$ using Eq. (168), with $f_{m, m^{\prime}}=E_{0,1}$. Thanks to our (smart :-) choice of energy origin, of 4 terms in the double sum (168), all 3 terms that include at least one factor $E_{0}=0$ vanish, and we have only one term left:

$$
\begin{align*}
\langle E(t) E(t+\tau)\rangle & =\left.E_{1} W_{1}(\infty) E_{1} W_{1}(\tau)\right|_{W_{1}(0)=1}=E_{1}^{2} W_{1}(\infty)\left[W_{1}(0) e^{-\Gamma_{\Sigma} \tau}+W_{1}(\infty)\left(1-e^{-\Gamma_{\Sigma} \tau}\right)\right] W_{W_{1}}(0)=1 \\
& =\frac{\Delta^{2}}{e^{\Delta / T}+1}\left[e^{-\Gamma_{\Sigma} \tau}+\frac{1}{e^{\Delta / T}+1}\left(1-e^{-\Gamma_{\Sigma} \tau}\right)\right]=\frac{\Delta^{2}}{\left(e^{\Delta / T}+1\right)^{2}}\left(1+e^{\Delta / T} e^{-\Gamma_{\Sigma} \tau}\right) . \tag{5.173}
\end{align*}
$$

From here and the last of Eqs. (169), the correlation function of energy fluctuations is ${ }^{65}$

$$
\begin{align*}
K_{E}(\tau) & \equiv\langle\widetilde{E}(t) \widetilde{E}(t+\tau)\rangle=\langle(E(t)-\langle E(t)\rangle)(E(t+\tau)-\langle E(t)\rangle)\rangle=\langle E(t) E(t+\tau)\rangle-\langle E(t)\rangle\langle E(t+\tau)\rangle \\
& =\langle E(t) E(t+\tau)\rangle-\langle E\rangle^{2}=\Delta^{2} \frac{e^{\Delta / T}}{\left(e^{\Delta / T}+1\right)^{2}} e^{-\Gamma_{\Sigma} \tau} \tag{5.174}
\end{align*}
$$

Since transition rates $\Gamma \uparrow$ and $\Gamma \downarrow$ have to obey the detailed balance relation (4.103), $\Gamma \downarrow / \Gamma \uparrow=\exp \{\Delta / T\}$, and hence

$$
\begin{equation*}
\frac{e^{\Delta / T}}{\left(e^{\Delta / T}+1\right)^{2}}=\frac{\Gamma_{\downarrow} / \Gamma_{\uparrow}}{\left(\Gamma_{\downarrow} / \Gamma_{\uparrow}+1\right)^{2}}=\frac{\Gamma_{\uparrow} \Gamma_{\downarrow}}{\left(\Gamma_{\uparrow}+\Gamma_{\downarrow}\right)^{2}}=\frac{\Gamma_{\uparrow} \Gamma_{\downarrow}}{\Gamma_{\Sigma}^{2}}, \tag{5.175}
\end{equation*}
$$

expression (174) may be presented also in a simpler form:

$$
\begin{equation*}
K_{E}(\tau)=\Delta^{2} \frac{\Gamma_{\uparrow} \Gamma_{\downarrow}}{\Gamma_{\Sigma}^{2}} e^{-\Gamma_{\Sigma} \tau} \tag{5.176}
\end{equation*}
$$

We see that the correlation function of energy decays exponentially with time, with the net rate $\Gamma_{\Sigma}$, while its variance, equal to $K_{E}(0)$, does not depend on the transition rates. Now using the WienerKhinchin theorem (58) to calculate its spectral density, we get

[^931]\[

$$
\begin{equation*}
S_{E}(\omega)=\frac{1}{\pi} \int_{0}^{\infty} \Delta^{2} \frac{\Gamma_{\uparrow} \Gamma_{\downarrow}}{\Gamma_{\Sigma}^{2}} e^{-\Gamma_{\Sigma} \tau} \cos \omega \tau d \tau=\frac{\Delta^{2}}{\pi \Gamma_{\Sigma}} \frac{\Gamma_{\uparrow} \Gamma_{\downarrow}}{\Gamma_{\Sigma}^{2}+\omega^{2}} \tag{5.177}
\end{equation*}
$$

\]

Such dependence on frequency ${ }^{66}$ is very typical for discrete-state systems described by master equations. It is interesting that the most widely accepted explanation of the $1 / f$ noise (also called the "flicker" or "excess" noise), which was mentioned in Sec. 5, is that it is a result of thermally-activated jumps between metastable states of a statistical ensemble of such two-level systems, with an exponentially-broad statistical distribution of transition rates $\Gamma_{\uparrow, \downarrow}$. Such a broad distribution follows from the Kramers formula (156), which is approximately valid for lifetimes of states of systems with double-well potential profiles (Fig. 13), for a statistical ensemble with a smooth statistical distribution of energy gaps $\Delta$. Such profiles are typical, in particular, for electrons in disordered (amorphous) solidstate materials that, indeed, feature high $1 / f$ noise.


Fig. 5.13. Typical doublewell potential profile.

Returning to the Fokker-Planck equation, we may use the evident generalization of Eq. (168) to the continuous-variable case:

Correlation function of continuousstate system

$$
\begin{equation*}
\langle f(t) f(t+\tau)\rangle=\int d^{3} q d^{3} p \int d^{3} q^{\prime} d^{3} p^{\prime} f(\mathbf{q}, \mathbf{p}) w(\mathbf{q}, \mathbf{p}, \infty) f\left(\mathbf{q}^{\prime}, \mathbf{p}^{\prime}\right) w\left(\mathbf{q}^{\prime}, \mathbf{p}^{\prime}, \tau\right) \tag{5.178}
\end{equation*}
$$

were both probability density distributions are solutions of the equation with the delta-functional initial condition

$$
\begin{equation*}
w\left(\mathbf{q}^{\prime}, \mathbf{p}^{\prime}, 0\right)=\delta\left(\mathbf{q}^{\prime}-\mathbf{q}\right) \delta\left(\mathbf{p}^{\prime}-\mathbf{p}\right) \tag{5.179}
\end{equation*}
$$

For the Smoluchowski equation, valid in the high-damping limit, the expressions are similar, albeit with a lower dimensionality:

$$
\begin{gather*}
\langle f(t) f(t+\tau)\rangle=\int d^{3} q \int d^{3} q^{\prime} f(\mathbf{q}) w(\mathbf{q}, \infty) f\left(\mathbf{q}^{\prime}\right) w\left(\mathbf{q}^{\prime}, \tau\right)  \tag{5.180}\\
w\left(\mathbf{q}^{\prime}, 0\right)=\delta\left(\mathbf{q}^{\prime}-\mathbf{q}\right) \tag{5.181}
\end{gather*}
$$

To see this formalism in action, let us use it to find the correlation function $K_{q}(\tau)$ of a linear relaxator, i.e. an overdamped 1D harmonic oscillator with $m \omega_{0} \ll \eta$. In this limit, the coordinate averaged over the heat baths obeys a linear equation,

$$
\begin{equation*}
\eta\langle\dot{q}\rangle+\kappa\langle q\rangle=0, \tag{5.182}
\end{equation*}
$$

which describes its exponential relaxation from a certain initial condition $q_{0}$ to the equilibrium position $q=0$, with the reciprocal time constant $\Gamma=\kappa / \eta$ :

[^932]\[

$$
\begin{equation*}
\langle q\rangle(t)=q_{0} e^{-\Gamma t} . \tag{5.183}
\end{equation*}
$$

\]

The deterministic equation (182) corresponds to the quadratic potential energy $U(q)=\kappa q^{2} / 2$, so that the 1D version of the Smoluchowski equation (122) takes the following form:

$$
\begin{equation*}
\eta \frac{\partial w}{\partial t}=\kappa \frac{\partial}{\partial q}(w q)+T \frac{\partial^{2} w}{\partial q^{2}} . \tag{5.184}
\end{equation*}
$$

It is straightforward to check, by substitution, that this equation, rewritten for function $w\left(q^{\prime}, \tau\right)$, with the delta-functional initial condition (181), $w\left(q^{\prime}, 0\right)=\delta\left(q^{\prime}-q\right)$, is satisfied by a Gaussian function,

$$
\begin{equation*}
w\left(q^{\prime}, \tau\right)=\frac{1}{(2 \pi)^{1 / 2} \delta q(\tau)} \exp \left\{-\frac{\left(q^{\prime}-\langle q\rangle(\tau)\right)^{2}}{2 \delta q^{2}(\tau)}\right\} \tag{5.185}
\end{equation*}
$$

with its center, $\langle q\rangle(\tau)$, moving in accordance with Eq. (183), and the time-dependent variance

$$
\begin{equation*}
\delta q^{2}(\tau)=\delta q^{2}(\infty)\left(1-e^{-2 \Gamma \tau}\right), \quad \text { where } \delta q^{2}(\infty)=\left\langle q^{2}\right\rangle=\frac{T}{\kappa} \tag{5.186}
\end{equation*}
$$

(As a sanity check, the last equality coincides with the equipartition theorem's result.) Finally, the first probability under the integral in Eq. (180) may be found from Eq. (185) in the limit $\tau \rightarrow \infty$ (in which $\langle q\rangle(\tau) \rightarrow 0)$, by replacing $q^{\prime}$ for $q$ :

$$
\begin{equation*}
w(q, \infty)=\frac{1}{(2 \pi)^{1 / 2} \delta q(\infty)} \exp \left\{-\frac{q^{2}}{2 \delta q^{2}(\infty)}\right\} . \tag{5.187}
\end{equation*}
$$

Now, all components of recipe (180) are ready, and we can write it, for $f(q)=q$, as

$$
\begin{equation*}
\langle q(t) q(t+\tau)\rangle=\frac{1}{2 \pi \delta q(\tau) \delta q(\infty)} \int_{-\infty}^{+\infty} d q \int_{-\infty}^{+\infty} d q^{\prime} q \exp \left\{-\frac{q^{2}}{2 \delta q^{2}(\infty)}\right\} q^{\prime} \exp \left\{-\frac{\left(q^{\prime}-q e^{-\Gamma \tau}\right)^{2}}{2 \delta q^{2}(\tau)}\right\} \tag{5.188}
\end{equation*}
$$

The integral over $q^{\prime}$ may be worked our first, by the replacing that integration variable with ( $q^{\prime \prime}+q e^{-\Gamma \tau}$ ) and hence $d q$ ' with $d q$ ":

$$
\begin{equation*}
\langle q(t) q(t+\tau)\rangle=\frac{1}{2 \pi \delta q(\tau) \delta q(\infty)} \int_{-\infty}^{+\infty} q \exp \left\{-\frac{q^{2}}{2 \delta q^{2}(\infty)}\right\} d q \int_{-\infty}^{+\infty}\left(q^{\prime \prime}+q e^{-\Gamma \tau}\right) \exp \left\{-\frac{q^{\prime \prime 2}}{2 \delta q^{2}(\tau)}\right\} d q^{\prime \prime} \tag{5.189}
\end{equation*}
$$

The integral of the first term in parentheses $\left(q^{\prime \prime}+q e^{-\Gamma \tau}\right)$ equals zero (as that of an odd function in symmetric integration limits), while that with the second term is the standard Gaussian integral, giving

$$
\begin{equation*}
\langle q(t) q(t+\tau)\rangle=\frac{1}{(2 \pi)^{1 / 2} \delta q(\infty)} e^{-\Gamma \tau} \int_{-\infty}^{+\infty} q^{2} \exp \left\{-\frac{q^{2}}{2 \delta q^{2}(\infty)}\right\} d q=\frac{2 T}{\pi^{1 / 2} \kappa} e^{-\Gamma \tau} \int_{-\infty}^{+\infty} \xi^{2} \exp \left\{-\xi^{2}\right\} d \xi \tag{5.190}
\end{equation*}
$$

The last integral ${ }^{67}$ is just $\pi^{1 / 2} / 2$, so that taking into account that for this stationary system centered at the coordinate origin, the ensemble average $\langle q\rangle=0,{ }^{68}$ we finally get a very simple result,

[^933]Correlation function of linear relaxator

$$
\begin{equation*}
K_{q}(\tau) \equiv\langle\widetilde{q}(t) \widetilde{q}(t+\tau)\rangle=\langle q(t) q(t+\tau)\rangle-\langle q\rangle^{2}=\langle q(t) q(t+\tau)\rangle=\frac{T}{\kappa} e^{-\Gamma \tau} \tag{5.191}
\end{equation*}
$$

As a sanity check, for $\tau=0$ it yields $K_{q}(0) \equiv\left\langle q^{2}\right\rangle=T / \kappa$, in accordance with Eq. (186). As $\tau$ is increased the correlation function decreases monotonically - see the solid-line sketch in Fig. 8.

So, the solution of this very simple problem has required straightforward but somewhat bulky calculations. On the other hand, the same result may be obtained literally in one line, using the Langevin formalism - namely, as the Fourier transform (59) of the spectral density (68) in the corresponding limit $m \omega \ll \eta$, with $S_{\neq}(\omega)$ given by Eq. (73):69

$$
\begin{equation*}
K_{q}(\tau)=2 \int_{0}^{\infty} S_{q}(\omega) \cos \omega \tau d \omega=2 \int_{0}^{\infty} \frac{\eta T}{\pi} \frac{1}{\kappa^{2}+(\eta \omega)^{2}} \cos \omega \tau d \omega=2 \frac{T \Gamma}{\pi} \int_{0}^{\infty} \frac{\cos \xi}{(\Gamma \tau)^{2}+\xi^{2}} d \xi=\frac{T}{\kappa} e^{-\Gamma \tau} \tag{5.192}
\end{equation*}
$$

This example illustrates well that for linear systems (and small fluctuations in nonlinear systems) the Langevin approach is usually much simpler that the one based on the Fokker-Planck or Smoluchowski equations. However, again, the latter approach is indispensable for the analysis of fluctuations of arbitrary intensity in nonlinear systems.

To conclude this chapter, I have to emphasize again that the Fokker-Planck and Smoluchowski equations give a quantitative description of time evolution of nonlinear Brownian systems with finite dissipation in the classical limit. The description of quantum properties of such dissipative ("open") and nonlinear quantum systems is more complex, ${ }^{70}$ and only a few simple problems of such theory have been solved so far, ${ }^{71}$ typically using a particular model of the environment, e.g., as a large set of harmonic oscillators with different statistical distributions of their parameters, leading to different frequency dependence of susceptibility $\chi(\omega)$.

### 5.10. Exercise problems

5.1. Considering the first 30 digits of number $\pi=3.1415 \ldots$ as a statistical ensemble of integers $k$ (equal to $3,1,4,1,5, \ldots$ ), calculate
(i) average $\langle k\rangle$, and
(ii) the r.m.s. fluctuation $\delta k$.

Compare the results with those for an ensemble of completely random integers $0,1, ., 9$, and comment.
5.2. For a set of $N$ non-interacting Ising "spins" $s_{j}= \pm 1$, placed into magnetic field $h$, calculate the relative fluctuation of system's magnetization.

Hint: The total magnetic moment of an Ising system is assumed to be proportional to the sum

[^934]$$
\mathcal{S} \equiv \sum_{j=1}^{N} s_{j},
$$
so that the requested relative fluctuation may be calculated just as $\delta S \ll S T$.
5.3. For a field-free, two-site Ising system with energy values $E_{m}=-J s_{1} s_{2}$, in the thermal equilibrium at temperature $T$, find the variance of energy fluctuations. Explore the low-temperature and high-temperature limits of the result.
5.4. For the 1 D , three-site Ising ring with ferromagnetic coupling (and no external field), calculate the correlation coefficient $\left\langle s_{\left.j^{\prime} j_{j}\right\rangle}\right\rangle$ for both $j=j^{\prime}$ and $j \neq j^{\prime}$.
5.5. Within the framework of Weiss' molecular-field theory, calculate the variance of spin fluctuations in the $d$-dimensional Ising model. Use the result to derive the conditions of quantitative validity of the theory.
5.6. Calculate the variance of fluctuations of the energy of a quantum harmonic oscillator of frequency $\omega$, in thermal equilibrium at temperature $T$, and express it via the average value of the energy.
5.7. Express the r.m.s. fluctuation of the occupancy $N_{k}$ of a certain energy level $\varepsilon_{k}$ by:
(i) a classical particle,
(ii) a fermion, and
(iii) a boson,
in the thermodynamic equilibrium, via the average occupancy $\left\langle N_{k}\right\rangle$, and compare the results.
5.8.* Starting from the Maxwell distribution of velocities, calculate constant $C$ in the (approximate) expression $K_{P}(\tau)=C \delta(\tau)$, for the correlation function of fluctuations of pressure $P(t)$ of an ideal gas of $N$ classical particles. Compare the result with that of Problem 3.2, and estimate the pressure fluctuation variance.

Hint: You may like to consider a cylindrically-shaped container of volume $V=L A$ (see Fig. on the right) to calculate fluctuations of force acting on its plane lid of area $A$, and then recalculate them into fluctuations of pressure $P$.

5.9. Perhaps the simplest model of diffusion is the 1D discrete random walk: each time interval $\tau$, a particle leaps, with equal probability, to any of two neighboring sites of a 1D lattice with the spatial period $a$. Prove that particle's displacement during time interval $t \gg$ $\tau$, obeys Eq. (77), and calculate the corresponding diffusion coefficient $D$.
5.10.* Calculate the low-frequency spectral density of current $I(t)$ due to random passage of charged particles between two conducting electrodes - see Fig. on the right. Assume that the particles are emitted by one of the electrodes at random times, and are fully absorbed by the counterpart electrode.

5.11.* Within the rotating-wave approximation (RWA), ${ }^{72}$ calculate major statistical properties of fluctuations of the phase of classical self-oscillations, at:
(i) the free run of the oscillator, and
(ii) its phase locking by an external sinusoidal force, assuming that the fluctuations are caused by a weak, broadband noise with spectral density $S_{f}(\omega)$.
5.12. Calculate the correlation function of the coordinate of a 1 D harmonic oscillator with small Ohmic damping at thermal equilibrium.
5.13. Consider a very long, uniform, two-wire transmission line (see Fig. on the right), that allows the propagation of TEM waves with negligible attenuation, in thermal equilibrium with the environment at temperature $T$. Find variance $\left\langle V^{2}\right\rangle_{\Delta v}$ of electromagnetic fluctuations of voltage $V$ between the wires
 within a small frequency interval $\Delta v$.

Hint: As an E\&M reminder, ${ }^{73}$ TEM waves propagate with a frequency-independent velocity (equal to $c$ if the wires are in vacuum), with voltage $V$ and current $I$ (see Fig. above) related as $\mathcal{Z}(x, t) / I(x, t)= \pm \mathcal{Z}$, where $\mathcal{Z}$ is a frequency-independent constant ("wave impedance").
5.14. Now consider a similar line terminated, at one end, with an impedance-matching resistor $R$ $=\boldsymbol{Z}$. Find variance $\left\langle\boldsymbol{V}^{2}\right\rangle_{\Delta v}$ of the voltage across the resistor, and discuss the relation between the result and the Nyquist theorem (81).

Hint: Take into account that resistor with $R=\boldsymbol{Z}$ absorbs incident TEM waves without reflection.
5.15. An overdamped classical 1D particle escapes from a potential well with a smooth bottom, but a sharp edge - see Fig. on the right. Find the appropriate modification of the Kramers formula (139).

5.16. A particle may occupy any of $N$ similar sites. Particle's interaction with environment induces its random, incoherent jumps from the occupied site to any other one with the same rate $\Gamma$. Find the correlation function and the spectral density of fluctuations of the instant occupancy $n(t)$ (equal to either 1 or 0 ) of any particular site.

[^935]

## Chapter 6. Elements of Kinetics

This chapter gives a brief introduction to the basic notions of physical kinetics. Its main focus is on the Boltzmann equation, especially within the relaxation-time approximation, which allows, in particular, an approximate but reasonable and simple description of transport phenomena (such as the electric current and thermoelectric effects) in gases, including electron gases in metals and semiconductors.

### 6.1. The Liouville theorem

Physical kinetics is the branch of statistical physics that deals with systems out of thermodynamic equilibrium. Major tasks of kinetics include:
(i) for autonomous systems (those out of external fields): transient processes (relaxation) leading from an arbitrary initial state of a system to the thermodynamic equilibrium;
(ii) for systems in time-dependent external fields (say, in a sinusoidal "ac" field): the periodic oscillations of system's parameters; and
(iii) for systems in time-independent ("dc") external fields: dc transport effects.

In the last case, we are dealing with stationary $(\partial / \partial t=0$ everywhere $)$, but non-equilibrium situations, in which the effect of an external field, continuously driving the system out of the equilibrium, is balanced by the simultaneous relaxation - the trend toward the equilibrium. Perhaps the most important effect of this class is the dc current in conductors, which alone justifies the inclusion of the basic notions of kinetics into any set of core physics courses.

Actually, the reader who has reached this point of the notes, already has a good taste of physical kinetics, because the subject of the last part of Chapter 5 was the kinetics of a "Brownian particle", i.e. of a "heavy" system interacting with environment consisting of many "lighter" components. Indeed, the equations discussed in that part - whether the Smoluchowski equation (5.122) or the Fokker-Planck equation (5.149) - are valid if the environment is in thermodynamic equilibrium, but the system of our interest is not necessarily so. As a result, we could use those equations to discuss such non-equilibrium phenomena as the Kramers problem for the metastable state lifetime.

This chapter is devoted to the more traditional subject of kinetics: a system of very many similar particles - generally, interacting with each other, but not too strongly, so that the energy of the system still may be partitioned into a sum of the components, with the component interactions considered as a weak perturbation. Actually, we have already started the job of describing such a system in Sec. 5.8, in the course of deriving the Fokker-Planck equation for a single classical particle. Indeed, in the absence of particle interactions (i.e. when it is unimportant whether the particle is light or heavy), the probability current densities in the coordinate and momentum spaces are given, respectively, by Eqs. (5.142) and (5.143), so that the continuity equation (5.140) takes the form

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\nabla_{q} \cdot(w \dot{\mathbf{q}})+\nabla_{p} \cdot(w \dot{\mathbf{p}})=0 . \tag{6.1}
\end{equation*}
$$

If similar particles do not interact, this equation for single-particle probability density $w(\mathbf{q}, \mathbf{p}, t)$ is valid for each of them, and the result of its solution may be used to calculate any average of the system as a whole.

Let us rewrite Eq. (1) in the Cartesian component form,

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\sum_{j}\left[\frac{\partial}{\partial q_{j}}\left(w \dot{q}_{j}\right)+\frac{\partial}{\partial p_{j}}\left(w \dot{p}_{j}\right)\right]=0 \tag{6.2}
\end{equation*}
$$

where index $j$ lists all degrees of freedom of the particle, and assume that its motion in an external field may be described by a Hamiltonian function $\not \forall\left(q_{j}, p_{j}, t\right)$. Plugging into Eq. (2) the Hamiltonian equations of motion: ${ }^{1}$

$$
\begin{equation*}
\dot{q}_{j}=\frac{\partial \mathcal{H}}{\partial p_{j}}, \quad \dot{p}_{j}=-\frac{\partial \mathcal{H}}{\partial q_{j}}, \tag{6.3}
\end{equation*}
$$

we get

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\sum_{j}\left[\frac{\partial}{\partial q_{j}}\left(w \frac{\partial \mathcal{H}}{\partial p_{j}}\right)-\frac{\partial}{\partial p_{j}}\left(w \frac{\partial \mathcal{H}}{\partial q_{j}}\right)\right]=0 . \tag{6.4}
\end{equation*}
$$

At the parentheses' differentiation, the mixed terms $w \partial^{2} \nexists \partial \partial q_{j} \partial p_{j}$ and $w \partial^{2} \nexists \partial \partial p_{j} \partial q_{j}$ cancel, and using Eq. (3) again, we get the so-called Liouville theorem ${ }^{2}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\sum_{j}\left(\frac{\partial w}{\partial q_{j}} \dot{q}_{j}+\frac{\partial w}{\partial p_{j}} \dot{p}_{j}\right)=0 \tag{6.5}
\end{equation*}
$$

Liouville theorem

Since the left-hand part of this equation is just the full derivative of the probability density considered as a function of the generalized coordinates $q_{j}(t)$ of a particle, its generalized momenta components $p_{j}(t)$, and (possibly) time $t$, the Liouville theorem (5) may be presented in a surprisingly simple form:

$$
\begin{equation*}
\frac{d w(\mathbf{q}, \mathbf{p}, t)}{d t}=0 \tag{6.6}
\end{equation*}
$$

Physically it means that the probability $d W=w d^{3} q d^{3} p$ to find a Hamiltonian particle in a small volume of the coordinate-momentum space $[\mathbf{q}, \mathbf{p}]$, with the center moving in accordance to the deterministic law (3), does not change with time - see Fig. 1.


Fig. 6.1. Cartoon representation of the Liouville theorem in the 6 D space $[\mathbf{q}, \mathbf{p}]$.

[^936]At the first glance, this may not look surprising, because according to the fundamental Einstein relation (5.78), one needs non-Hamiltonian forces (such as kinematic friction, i.e. drag) to have diffusion. On the other hand, it is striking that the Liouville theorem is valid even for (Hamiltonian) systems with deterministic chaos, ${ }^{3}$ in which the deterministic trajectories corresponding to slightly different initial conditions become increasingly mixed with time.

For an ideal gas of 3D particles, we may select the usual Cartesian coordinates $r_{j}$ (with $j=1,2$, 3) for the generalized coordinates $q_{j}$, so that $p_{j}$ become the Cartesian components $m v_{j}$ of the usual (linear) momentum, and the elementary volume is just $d^{3} r d^{3} p-$ see Fig. 1. In this case Eqs. (3) are just

$$
\begin{equation*}
\dot{r}_{j}=\frac{p_{j}}{m} \equiv v_{j}, \quad \dot{p}_{j}=7_{j}, \tag{6.7}
\end{equation*}
$$

so that the Liouville theorem may be rewritten as

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\sum_{j=1}^{3}\left(v_{j} \frac{\partial w}{\partial r_{j}}+7_{j} \frac{\partial w}{\partial p_{j}}\right)=0 \tag{6.8}
\end{equation*}
$$

and conveniently presented in the vector form ${ }^{4}$

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\mathbf{v} \cdot \nabla w+\boldsymbol{7} \cdot \nabla_{p} w=0 \tag{6.9}
\end{equation*}
$$

where I have returned to using unindexed symbol $\nabla$ for the vector differentiation in the coordinate space.

### 6.2. The Boltzmann equation

The situation becomes much more complex if particles interact. Generally, a system of $N$ similar particles in 3D space has to be described by probability density $w$ being a function of $6 N+1$ arguments ( $3 N$ Cartesian coordinates, plus $3 N$ momentum components, plus time). Analytical or numerical solution of any equation describing time evolution of such a function for a typical ensemble of $N \sim 10^{23}$ particles is evidently a hopeless task. Hence, kinetics of realistic ensembles has to rely on making reasonable approximations that would simplify the situation.

One of the most useful approximation (sometimes called Stosszahlansatz, German for the "collision number assumption") was suggested by L. Boltzmann for a gas of particles that move freely most of the time, but interact during short time intervals, when a particle comes close to either an immobile scattering center (say, an impurity in a conductor) or to another particle of the gas. Such a brief scattering event changes particle's momentum, and may be approximately described by the addition of a special term (called the scattering integral) to the right-hand part of Eq. (9):

Boltzmann equation

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\mathbf{v} \cdot \nabla w+\boldsymbol{\mathcal { F }} \cdot \nabla_{p} w=\left.\frac{\partial w}{\partial t}\right|_{\text {scattering }} \tag{6.10}
\end{equation*}
$$

while still keeping $w$ a function of only 7 arguments: 3 coordinate components of vector $\mathbf{r}$ and 3 components of momentum $\mathbf{p}$ (all of just one particle), plus time $t$. This is the Boltzmann transport equation.

[^937]The concrete form of the scattering integral depends on the scattering object. If scattering centers do not belong to the ensemble under consideration (again, for example, an impurity atom in a conductor - see Fig. 2), then the scattering integral may be obtained by an evident generalization of the master equation (4.100): ${ }^{5}$

$$
\begin{equation*}
\left.\frac{\partial w}{\partial t}\right|_{\text {scattering }}=\int d^{3} p^{\prime}\left[\Gamma_{\mathbf{p}^{\prime} \rightarrow \mathbf{p}} w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)-\Gamma_{\mathbf{p} \rightarrow \mathbf{p}^{\prime}} w(\mathbf{r}, \mathbf{p}, t)\right] \tag{6.11}
\end{equation*}
$$

where the physical sense of $\Gamma_{\mathbf{p} \rightarrow \mathbf{p}}$, is the rate (i.e. the probability per unit time) for the particle to be scattered from the state with momentum $\mathbf{p}$ into the state with momentum $\mathbf{p}$ '.


Fig. 6.2. Particle scattering event.

Most elastic interactions are reciprocal, i.e. obey the following relation (closely related to the reversibility of time in Hamiltonian systems): $\Gamma_{\mathbf{p} \rightarrow \mathbf{p}^{\prime}}=\Gamma_{\mathbf{p}^{\prime} \rightarrow \mathbf{p}}$, so that Eq. (11) may be rewritten as ${ }^{6}$

$$
\begin{equation*}
\left.\frac{\partial w}{\partial t}\right|_{\text {scatteering }}=\int d^{3} p^{\prime} \Gamma_{\mathbf{p} \rightarrow \mathbf{p}^{\prime}}\left[w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)-w(\mathbf{r}, \mathbf{p}, t)\right] . \tag{6.12}
\end{equation*}
$$

With such scattering integral, Eq. (10) stays linear in $w$, but becomes an integro-differential equation, typically harder to solve than differential equations.

The equation becomes even more complex if the scattering is due to mutual interaction of the particle members of the system (Fig. 3).


Fig. 6.3. Particle-particle scattering event.

[^938]In this case, the probability of the scattering event scales as a product of two single-particle probabilities, and the simplest form of the scattering integral is ${ }^{7}$

$$
\begin{equation*}
\left.\frac{\partial w}{\partial t}\right|_{\text {scatteering }}=\int d^{3} p^{\prime} \int d^{3} p \cdot\left[\Gamma_{\mathbf{p}^{\prime} \rightarrow \mathbf{p}, \mathbf{p}^{\prime} \rightarrow \mathbf{p}}, w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right) w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)-\Gamma_{\mathbf{p} \rightarrow \mathbf{p}^{\prime}, \mathbf{p}, \rightarrow \mathbf{p},{ }^{\prime}} w(\mathbf{r}, \mathbf{p}, t) w(\mathbf{r}, \mathbf{p}, t)\right] . \tag{6.13}
\end{equation*}
$$

The integration dimensionality in Eq. (13) takes into account the fact that due to the conservation of the total momentum at scattering,

$$
\begin{equation*}
\mathbf{p}+\mathbf{p}=\mathbf{p}^{\prime}+\mathbf{p}^{\prime}, \tag{6.14}
\end{equation*}
$$

one of the momenta is not an independent argument, so that the integration in Eq. (13) may be restricted to a $6 \mathrm{D} p$-space rather than the 9 D one. For the reciprocal interaction, Eq. (13) may also be a bit simplified, but it still keeps Eq. (10) a nonlinear integro-differential transport equation, excluding such powerful solution methods as the Fourier expansion (which hinges on the linear superposition principle).

This is why most useful results based on the Boltzmann transport equation hinge on its further simplifications, most notably the relaxation-time approximation - RTA for short. ${ }^{8}$ This approximation is based on noticing that in the absence of spatial gradients $(\nabla=0)$, and external forces ( $\boldsymbol{7}=0)$, Eq. (10) yields

$$
\begin{equation*}
\frac{\partial w}{\partial t}=\left.\frac{\partial w}{\partial t}\right|_{\text {scattering }} \tag{6.15}
\end{equation*}
$$

so that the thermally-equilibrium probability distribution $w_{0}(\mathbf{r}, \mathbf{p}, t)$ has to turn any scattering integral into zero. Hence at small deviations from the equilibrium,

$$
\begin{equation*}
\widetilde{w}(\mathbf{r}, \mathbf{p}, t) \equiv w(\mathbf{r}, \mathbf{p}, t)-w_{0}(\mathbf{r}, \mathbf{p}, t) \rightarrow 0, \tag{6.16}
\end{equation*}
$$

the scattering integral should be proportional to the deviation $\widetilde{w}$, and its simplest reasonable model is
 approximation (RTA)
$\left.\frac{\partial w}{\partial t}\right|_{\text {scatteering }}=-\frac{\widetilde{w}}{\tau}$
where $\tau$ is a phenomenological constant (which, according to Eq. (15), has to be positive for system's stability) called the relaxation time. Its physical meaning will be more clear in the next section.

The relaxation-time approximation is quite reasonable if the angular distribution of the scattering rate is dominated by small angles between vectors $\mathbf{p}$ and $\mathbf{p}^{\prime}$ - as it is, for example, for the Rutherford scattering by a Coulomb center. ${ }^{9}$ Indeed, in this case the two functions $w$, participating in Eq. (12) are close to each other, so that the loss of the second momentum argument ( $\mathbf{p}$ ') is not too essential. However, while using the Boltzmann-RTA equation, which results from combining Eqs. (10) and (17),

$$
\begin{equation*}
\frac{\partial w}{\partial t}+\mathbf{v} \cdot \nabla w+\boldsymbol{7} \cdot \nabla_{p} w=-\frac{\widetilde{w}}{\tau} \tag{6.18}
\end{equation*}
$$

[^939]the reader should always remember this is just an approximation, sometimes giving completely wrong results. For example, it prescribes the same time scale, $\tau$, to the relaxation of the net momentum of the system, and to its energy relaxation, while in many real systems the latter process (that requires inelastic interactions) may be substantially longer. Naturally, in the following sections I will describe only those applications of the RTA approximation that give a reasonable description of reality.

### 6.3. The Ohm law and the Drude formula

Despite its shortcomings, Eq. (18) is adequate for quite a few applications. Perhaps the most important of them is deriving the Ohm law for dc current is a gas of charged particles, whose only important deviation from ideality is the scattering in the form of Eq. (17), and hence described, in equilibrium, by the equilibrium probability $w_{0}$ of an ideal gas (see Sec. 3.1):

$$
\begin{equation*}
w_{0}(\mathbf{r}, \mathbf{p}, t)=\frac{g}{(2 \pi \hbar)^{3}}\langle N(\varepsilon)\rangle, \tag{6.19}
\end{equation*}
$$

where $g$ is the degeneracy factor (say, $g=2$ for electrons due to their spin), and $\langle N(\varepsilon)\rangle$ is the average occupancy of a quantum state with momentum $\mathbf{p}$, that obeys either the Fermi-Dirac or the Bose-Einstein distribution:

$$
\begin{equation*}
\langle N(\varepsilon)\rangle=\frac{1}{e^{(\varepsilon-\mu) / T} \pm 1}, \quad \varepsilon=\varepsilon(\mathbf{p}) \tag{6.20}
\end{equation*}
$$

(Up to a point, our calculations will be valid for both statistics, and hence, in the limit $\mu / T \rightarrow-\infty$, for a classical gas as well.)

Now let a uniform, dc electric field $\boldsymbol{\varepsilon}$ be applied to the gas, exerting force $\boldsymbol{\mathcal { F }}=q \boldsymbol{\mathcal { E }}$ on each particle with electric charge $q$. Then the stationary solution to Eq. (18), with $\partial / \partial t=0$, should also be stationary and spatially-uniform $(\nabla=0)$, so that this equation is reduced to

$$
\begin{equation*}
q \varepsilon \cdot \nabla_{p} w=-\frac{\widetilde{w}}{\tau} . \tag{6.21}
\end{equation*}
$$

Let us assume the electric field to be relatively low as well, so that the perturbation $\widetilde{w}$ it produces is relatively small. (I will quantify this condition later on.) Then in the left-hand side of Eq. (21) we can neglect that perturbation, by replacing $w$ with $w_{0}$, because that side already has a small factor (乎). As a result, this equation yields

$$
\begin{equation*}
\widetilde{w}=-\tau q \varepsilon \cdot \nabla_{p} w_{0}=-\tau q \varepsilon \cdot\left(\nabla_{p} \varepsilon\right) \frac{\partial w_{0}}{\partial \varepsilon}, \tag{6.22}
\end{equation*}
$$

where the partial derivative sign marks the implied local constancy of parameters $\mu$ and $T$, i.e. their independence of momentum $\mathbf{p}$. But gradient $\nabla_{p} \varepsilon$ is nothing else than particle's velocity $\mathbf{v}$ - for a quantum particle, its group velocity. ${ }^{10}$ (This fact is easy to verify for the isotropic and parabolic dispersion law, pertinent to classical particles moving in free space,

[^940]\[

$$
\begin{equation*}
\varepsilon(\mathbf{p})=\frac{p^{2}}{2 m}=\frac{p_{1}^{2}+p_{2}^{2}+p_{3}^{2}}{2 m} . \tag{6.23}
\end{equation*}
$$

\]

Indeed, in this case the Cartesian components of vector $\nabla_{p} \varepsilon$ are

$$
\begin{equation*}
\left(\nabla_{p} \varepsilon\right)_{j} \equiv \frac{\partial \varepsilon}{\partial p_{j}}=\frac{p_{j}}{m}=v_{j} \tag{6.24}
\end{equation*}
$$

so that $\nabla_{p} \varepsilon=\mathbf{v}$.) Hence, Eq. (22) may be rewritten as

$$
\begin{equation*}
\widetilde{w}=-\tau q \varepsilon \cdot \mathbf{v} \frac{\partial w_{0}}{\partial \varepsilon} . \tag{6.25}
\end{equation*}
$$

Let us use this result to calculate the electric current density $\mathbf{j}$. The contribution of each quantum state to the current density is $q \mathbf{v} w$, so that the total density is

$$
\begin{equation*}
\mathbf{j}=\int q \mathbf{v} w d^{3} p=q \int \mathbf{v}\left(w_{0}+\widetilde{w}\right) d^{3} p . \tag{6.26}
\end{equation*}
$$

Since in the equilibrium state (with $w=w_{0}$ ), the current has to be zero, integral of the first term in the parentheses has to vanish. For the integral of the second term, plugging in Eq. (25), and also using Eq. (19), we get

$$
\begin{equation*}
\mathbf{j}=q^{2} \tau \int \mathbf{v}(\boldsymbol{\varepsilon} \cdot \mathbf{v})\left(-\frac{\partial w_{0}}{\partial \varepsilon}\right) d^{3} p=\frac{g q^{2} \tau}{(2 \pi \hbar)^{3}} \int \mathbf{v}(\varepsilon \cdot \mathbf{v})\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d^{2} p_{\perp} d p_{| |} \tag{6.27}
\end{equation*}
$$

where $d^{2} p_{\perp}$ is the elementary area of the constant energy surface in the momentum space, while $d p \|$ is the momentum differential's component normal to that surface. This result ${ }^{11}$ is valid even for particles with an arbitrary dispersion law $\varepsilon(\mathbf{p})$ (that may be rather complicated, for example, for particles moving in space-periodic potentials ${ }^{12}$ ), and may give, in particular, a fair description of conductivity's anisotropy in crystals.

For classical particles whose dispersion law is isotropic and parabolic, as in Eq. (23), the constant energy surface is a sphere of radius $p$, so that $d^{2} p_{\perp}=p^{2} d \Omega=p^{2} \sin \theta d \theta d \varphi$, while $d p \|=d p$. In spherical coordinates with the polar axis direction along vector $\mathcal{\varepsilon}$, we get $(\boldsymbol{\varepsilon} \cdot \mathbf{v})=\mathcal{E} v \cos \theta$. Now separating vector $\mathbf{v}$ outside the parentheses into a component $v \cos \theta$ directed along vector $\varepsilon$, and two perpendicular components, $v \sin \theta \cos \varphi$ and $v \sin \theta \sin \varphi$, we see that the integrals of the last two components over angle $\varphi$ give zero. Hence, as we could expect, in the isotropic case the net current is directed along the electric field and obeys the linear Ohm law, ${ }^{13}$

$$
\begin{equation*}
\mathbf{j}=\sigma \mathcal{\varepsilon} \tag{6.28}
\end{equation*}
$$

with a field-independent electric conductivity

[^941]\[

$$
\begin{equation*}
\sigma=\frac{g q^{2} \tau}{(2 \pi \hbar)^{3}} \int_{0}^{2 \pi} d \varphi \int_{0}^{\pi} \sin \theta d \theta \cos ^{2} \theta \int_{0}^{\infty} p^{2} d p v^{2}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) \tag{6.29}
\end{equation*}
$$

\]

Since $\sin \theta d \theta$ is just $-d(\cos \theta)$, the integral over $\theta$ equals $(2 / 3)$. The integral over $d \varphi$ is of course just $2 \pi$, while that over $p$ may be readily transformed to one over particle's energy $\varepsilon(\mathbf{p})=p^{2} / 2 m$ : $v d p=p d p / m=$ $d \varepsilon$, so that $p^{2} d p v^{2}=p^{2} v d \varepsilon=(2 m \varepsilon)(2 \varepsilon / m)^{1 / 2} d \varepsilon=\left(8 m \varepsilon^{3}\right)^{1 / 2} d \varepsilon$. As a result, the conductivity equals

$$
\begin{equation*}
\sigma=\frac{g q^{2} \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \int_{0}^{\infty}\left(8 m \varepsilon^{3}\right)^{1 / 2}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon . \tag{6.30}
\end{equation*}
$$

Note that $\sigma$ is proportional to $q^{2}$ and hence does not depend on the particle charge sign; this is why the Hall effect in external magnetic field, which lacks this ambivalence, is typically used to determine the charge of current carriers (electrons or holes) in semiconductors.

So far, the calculations have been valid for any gas (Bose, Fermi, or classical), an arbitrary temperature. Let us work out the remaining integral over energy for the most important case of a degenerate Fermi (say, electron) gas, with $T \ll \varepsilon_{F} .{ }^{14}$ As was discussed in Sec. 3.3, in this limit, factor ($\partial\langle N(\varepsilon))\rangle / \partial \varepsilon)$ is essentially Dirac's delta-function $\delta\left(\varepsilon-\varepsilon_{\mathrm{F}}\right)$, so that the conductivity does not depend on temperature: ${ }^{15}$

$$
\begin{equation*}
\sigma=\frac{g q^{2} \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3}\left(8 m \varepsilon_{F}^{3}\right)^{1 / 2}=\frac{q^{2} \tau}{m} \frac{g}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3}\left(2 m \varepsilon_{F}\right)^{3 / 2}=\frac{q^{2} \tau}{m} \frac{g}{(2 \pi \hbar)^{3}} \frac{4 \pi p_{\mathrm{F}}^{3}}{3} . \tag{6.31}
\end{equation*}
$$

But the last fraction in this product is just the volume of the Fermi sphere in the momentum space, so that the product of the last two fractions is the total number of quantum states filled at $T=0$ (per unit volume), i.e. the total density $n \equiv N / V$ of electrons in the gas. Hence, Sommerfeld's result is reduced to the Drude formula, ${ }^{16}$

$$
\begin{equation*}
\sigma=\frac{q^{2} \tau}{m} n \tag{6.32}
\end{equation*}
$$

[^942]which should be well familiar to the reader from an undergraduate physics course, with $\tau$ being a scale of time intervals between scattering events.

This calculation poses with an important conceptual question. The very structure of Eq. (30) implies that the only quantum states contributing to electric conductance are those where the derivative $(-\partial\langle N(\varepsilon)\rangle / \partial \varepsilon)$ is significant. At $T \ll \varepsilon_{\mathrm{F}}$, these are the states at the very surface of the Fermi sphere. On

[^943]the other hand, the classical derivation of Eq. (32) involves all electrons. ${ }^{17}$ So, what exactly electrons are responsible for conductance: all of them, or only those on the Fermi surface?

For the resolution of this paradox, let us return to Eq. (22) and analyze the physical meaning of that result. For that, let us compare it with the following model distribution:

$$
\begin{equation*}
w_{\text {model }} \equiv w_{0}(\mathbf{r}, \mathbf{p}-\widetilde{\mathbf{p}}, t), \tag{6.33}
\end{equation*}
$$

where $\widetilde{\mathbf{p}}$ is some constant, small vector, which describes a small shift of the unperturbed distribution $w_{0}$ in the momentum space as a whole. Performing the Taylor expansion of Eq. (33) in this small parameter, and keeping only two leading terms, we get

$$
\begin{equation*}
w_{\text {model }} \approx w_{0}(\mathbf{r}, \mathbf{p}, t)+\widetilde{w}_{\text {model }}, \quad \widetilde{w}_{\text {model }}=-\widetilde{\mathbf{p}} \cdot \nabla_{p} w_{0}(\mathbf{r}, \mathbf{p}, t) . \tag{6.34}
\end{equation*}
$$

Comparing the model perturbation with the first form of Eq. (22), we see that they coincide, provided that

$$
\begin{equation*}
\widetilde{\mathbf{p}}=q \boldsymbol{\varepsilon} \tau=\boldsymbol{\tau} \tau \tag{6.35}
\end{equation*}
$$

This means that Eq. (22) describes a small shift of the equilibrium distribution of electrons by $q \mathcal{E} \tau$ (in $p$ space) along the direction of electric field, ${ }^{18}$ and gives the picture of the electron transport in a degenerate gas, shown in Fig. 4.


Fig. 6.4. Filling of momentum states in a degenerate electron gas: (a) in the absence and (b) in the presence of external electric field $\boldsymbol{\varepsilon}$. Arrows show representative scattering events.

At $\boldsymbol{\varepsilon}=0$, the system is in equilibrium, so that the quantum states inside the Fermi sphere ( $\mathbf{p}<$ $\mathbf{p}_{\mathrm{F}}$ ), are occupied, while those outside of it are empty (Fig. 4a). Electron scattering events happen only between states within a very thin layer $\left(\left|p^{2} / 2 m-\varepsilon_{\mathrm{F}}\right| \sim T\right)$ at the Fermi surface, because only in this layer

[^944]the states are partially occupied, so that both components of the product $w(\mathbf{r}, \mathbf{p}, t)[1-w(\mathbf{r}, \mathbf{p}, t)]$, mentioned in Sec. 1, do not vanish. These scattering events, on the average, do not change the equilibrium probability distribution, because they are uniformly spread over the Fermi surface.

In the instant the electric field has been turned on, it starts to accelerate all electrons in its direction, i.e. the whole Fermi sphere starts moving in the momentum space, along the field's direction in the real space. For elastic scattering events (with $\left|p^{\prime}\right|=|p|$ ), this creates an addition of occupied states at the leading front of the accelerating sphere, and an addition of free states on its trailing edge (Fig. 4b). As a result, now there are more scattering events bringing electrons from the leading edge to the trailing edge of the sphere than in the opposite direction. This creates the average backflow of states occupancy in the momentum space. These two trends eventually cancel each other, and the Fermi sphere approaches a stationary (though not equilibrium!) state, with the shift (35) relatively to its thermalequilibrium position.

Thus Fig. 4b presents a clear answer to the question which of the two different interpretations of the Drude formula is correct, and due to electrons' indistinguishability, the answer is: either. On one hand, we can look at the electric current at a result of shift (35) of all electrons in the momentum space. On the other hand, each filled quantum state deep inside the sphere gives exactly the same contribution into the net current density as it did without the field. All these internal contributions to the net current cancel each other, so that the applied field changes the situation only at the Fermi surface. Thus it is equally legitimate to say that only the surface states are responsible for the nonvanishing net current. ${ }^{19}$

Let me also mention the second paradox related to the Drude formula, which is often misunderstood (not only by students :-). As was emphasized above, $\tau$ is finite even at elastic scattering that by itself does not change the total energy of the electron gas. The question is how can such scattering may be responsible for Ohmic resistivity $\rho \equiv 1 / \sigma$, and hence for the Joule heat production, with power density $\mathcal{P} V=\mathbf{j} \cdot \varepsilon=\rho j^{2}$ ? The answer is that the Drude and Sommerfeld formulas describe just the "bottleneck" of the Joule heat formation. In the scattering picture (Fig. 4b) the elastically scattered electron states are predominantly located above the (shifted) Fermi surface, and eventually need to relax onto it via some inelastic process that releases their additional energy in the form of heat (in solid state materials, described by phonons - see Sec. 2.6). The rate and other features of these inelastic phenomena do not participate in the Drude formula directly, but for keeping the theory valid (in particular, keeping the probability distribution $w$ close to its equilibrium value $w_{0}$ ), their intensity has to be sufficient to avoid gas overheating by the applied field. This gives an additional restriction on the simple theory described above. In some semiconductors, the charge carrier overheating effects, resulting in deviations from the Ohm law, i.e. from the linear relation (28) between $\mathbf{j}$ and $\boldsymbol{\varepsilon}$, may be readily observed already at rather modest applied electric fields.

### 6.4. Electrochemical potential and the drift-diffusion equation

Now let us generalize our calculation to the case when transport takes place in the presence of a time-independent spatial gradient of the probability distribution, $\nabla w \neq 0$, caused for example by that of the particle concentration $n=N / V$ (and hence, according to Eq. (3.40), of the chemical potential $\mu$ ),

[^945]while still considering temperature $T$ constant. For this generalization, we should just keep the second term in the left-hand part of Eq. (18). If the gradient of $w$ is sufficiently small, we can repeat arguments of the last section and replace $w$ with $w_{0}$ in this term as well. With the applied electric field $\boldsymbol{\varepsilon}$ presented as $(-\nabla \phi)$, where $\phi$ is the electrostatic potential, Eq. (25) now becomes
\[

$$
\begin{equation*}
\widetilde{w}=\tau \mathbf{v} \cdot\left(\frac{\partial w_{0}}{\partial \varepsilon} q \nabla \phi-\nabla w_{0}\right) . \tag{6.36}
\end{equation*}
$$

\]

Since in any of distributions (20), $\langle N(\varepsilon)\rangle$ is a function of $\varepsilon$ and $\mu$ only in combination $(\varepsilon-\mu)$, it obeys the following relation,

$$
\begin{equation*}
\frac{\partial\langle N(\varepsilon)\rangle}{\partial \mu}=-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon} \tag{6.37}
\end{equation*}
$$

Using this relation, the gradient of $w_{0} \propto\langle N(\varepsilon)\rangle$ may be presented as ${ }^{20}$

$$
\begin{equation*}
\nabla w_{0}=-\frac{\partial w_{0}}{\partial \varepsilon} \nabla \mu, \quad \text { for } T=\mathrm{const} \tag{6.38}
\end{equation*}
$$

so that Eq. (36) becomes

$$
\begin{equation*}
\widetilde{w}=\tau \frac{\partial w_{0}}{\partial \varepsilon} \mathbf{v} \cdot(q \nabla \phi+\nabla \mu)=\tau \frac{\partial w_{0}}{\partial \varepsilon} \mathbf{v} \cdot q \nabla \Phi \tag{6.39}
\end{equation*}
$$

where the following sum,

chemical potential

$$
\begin{equation*}
\Phi \equiv \phi+\frac{\mu}{q} \tag{6.40}
\end{equation*}
$$

is called the electrochemical potential. ${ }^{21}$ Now repeating the calculation of the electric current, carried out in the last section, we get the following generalization of the Ohm law (28):

$$
\begin{equation*}
\mathbf{j}=\sigma(-\nabla \Phi)=\sigma \mathcal{E} \tag{6.41}
\end{equation*}
$$

where the effective electric field $\mathcal{E}$ is the (minus) gradient of the electrochemical potential, rather of the electrostatic potential:

Effective electric field

$$
\begin{equation*}
\mathcal{E} \equiv-\nabla \Phi=\varepsilon-\frac{\nabla \mu}{q} \tag{6.42}
\end{equation*}
$$

The physics of this extremely important result ${ }^{22}$ may be explained in two ways. First, let us have a look at the energy spectrum of a uniform, degenerate Fermi gas confined in a volume of finite size. In order to ensure such a confinement, we need a piecewise-constant potential $U(\mathbf{r})$ - a "hard-wall, flat-

[^946]bottom potential well" - see Fig. 5a. (In a solid conductor, such profile is readily provided by the crystal lattice of positively charged ions of the crystal lattice.) The well should be of a sufficient depth $U_{0}>\varepsilon_{\text {F }}$ $\equiv \mu_{T=0}$ in order to provide the confinement of the overwhelming majority of the particles, with energies below or slightly above the Fermi level $\varepsilon_{\mathrm{F}}$. This means that there should be a substantial energy gap,
\[

$$
\begin{equation*}
\psi \equiv U_{0}-\mu \gg T \tag{6.43}
\end{equation*}
$$

\]

between the Fermi energy of a particle inside the well, and its potential energy outside the well. (The latter value is usually called the vacuum level.) The difference defined by Eq. (43) is called the workfunction; ${ }^{23}$ for most metals, its is between 4 and 5 eV , so that relation $\psi \gg T$ is well fulfilled for the room temperatures ( $T \sim 0.025 \mathrm{eV}$ ) - and actually for all temperatures up to material's evaporation point.


Fig. 6.5. Potential profiles of (a) a single conductor and (b,c) a system of two closely located conductors, for two different biasing conditions: (b) zero electrostatic field ("flat-band"), and (c) zero voltage $V \equiv \Delta \Phi$.

Now let us consider two conductors, with different values of $\psi$, separated by a small gap $d$ - see Fig. 5b,c. Panel (b) shows the case when the electric field $\mathcal{E}=-\nabla \phi$ in the free-space gap between the conductors equals zero, i.e. their electrostatic potentials $\phi$ are equal. ${ }^{24}$ If there is an opportunity for particles to cross the gap (e.g., by either the thermally-activated hopping over the potential barrier, discussed in Secs. 5.6-5.7, or quantum-mechanical tunneling through it), there will be an average flux of particles from the conductor with the higher Fermi level to that with the lower Fermi level, ${ }^{25}$ because the chemical equilibrium requires their equality - see Secs. 1.5 and 2.7. If the particles have an electric charge (as electrons do), the equilibrium will be automatically achieved by them recharging the effective capacitor formed by the conductors, until the electrostatic energy difference $q \Delta \phi$ reaches the value reproducing that of the workfunctions (Fig. 5c). According to Eq. (43), at the recharging, sum ( $\psi+\mu$ ) of each conductor has to stay constant, so that for the equilibrium potential difference ${ }^{26}$ we may write

$$
\begin{equation*}
q \Delta \phi=\Delta \psi=-\Delta \mu \tag{6.44}
\end{equation*}
$$

[^947]At this equilibrium, the electric field in the gap between the conductors is

$$
\begin{equation*}
\varepsilon \equiv-\frac{\Delta \phi}{d} \mathbf{n}=\frac{\Delta \mu}{q d} \mathbf{n}=\frac{\nabla \mu}{q} ; \tag{6.45}
\end{equation*}
$$

in Fig. 5c the field is clearly visible as the tilt of the electric potential profile. Comparing Eq. (45) with definition (42) of the effective electric field $\mathcal{E}$, we see that the transport equilibrium, i.e. the absence of current, is achieved exactly when $\mathcal{E}=0$, in accordance with Eq. (41).

Another interpretation of Eq. (41) may be achieved by modifying Eq. (38) for the particular case of a classical gas. Indeed, the gas' local density $n \equiv N / V$ obeys Eq. (3.32), which may be presented as

$$
\begin{equation*}
n(\mathbf{r})=\text { const } \times \exp \left\{\frac{\mu(\mathbf{r})}{T}\right\} \tag{6.46}
\end{equation*}
$$

Taking the spatial gradient of the both parts of this relation (at constant $T$ ), we get

$$
\begin{equation*}
\nabla n=\operatorname{const} \times \frac{1}{T} \exp \left\{\frac{\mu}{T}\right\} \nabla \mu=\frac{n}{T} \nabla \mu, \tag{6.47}
\end{equation*}
$$

so that $\nabla \mu=(T / n) \nabla n$, and Eq. (41), with $\sigma$ given by Eq. (32), may be recast as

$$
\begin{equation*}
\mathbf{j}=\sigma(-\nabla \Phi)=\frac{q^{2} \tau}{m} n\left(-\nabla \phi-\frac{1}{q} \nabla \mu\right)=q \frac{\tau}{m}(n q \varepsilon-T \nabla n) . \tag{6.48}
\end{equation*}
$$

Hence the current may be viewed as consisting of two independent parts: one due to the "usual" electric field $\varepsilon=-\nabla \phi$, and another due to the particle diffusion - see Eq. (5.118) and its discussion. This is exactly the physics of the "mysterious" term $\nabla \mu$ in Eq. (42), though it may be presented in the simple form (48) only in the classical limit.

Besides being very useful for practice, ${ }^{27}$ Eq. (48) gives us a pleasant surprise. Namely, plugging it into the continuity equation for electric charge,

$$
\begin{equation*}
\frac{\partial(q n)}{\partial t}+\nabla \cdot \mathbf{j}=0 \tag{6.49}
\end{equation*}
$$

we get (after the division of all terms by $q \tau / m$ ) the so-called drift-diffusion equation:28

Drift-
diffusion
equation

$$
\begin{equation*}
\frac{m}{\tau} \frac{\partial n}{\partial t}=\nabla(n \nabla U)+T \nabla^{2} n, \quad \text { with } U \equiv q \phi \tag{6.50}
\end{equation*}
$$

Comparing it with Eq. (5.122), we see that the drift-diffusion equation is identical to the Smoluchowski equation, ${ }^{29}$ if we identify ratio $\tau / m$ with mobility $\mu_{m}=1 / \eta$ :

$$
\begin{equation*}
\frac{\tau}{m} \leftrightarrow \mu_{\mathrm{m}} \equiv \frac{1}{\eta}, \tag{6.51}
\end{equation*}
$$

[^948]and hence the following combination, $\tau T / m$, with the diffusion constant $D$ - see (5.78). As a result, Eq. (48) is frequently rewritten as an expression for the particle flow density $\mathbf{j}_{n} \equiv n \mathbf{j}_{w}=\mathbf{j} /$ q:
\[

$$
\begin{equation*}
\mathbf{j}_{n}=n \mu_{m} q \boldsymbol{\varepsilon}-D \nabla n . \tag{6.52}
\end{equation*}
$$

\]

This similarity may look surprising. Indeed, our (or rather Einstein's :-) treatment of the Brownian motion in Chapter 5 was based on a strong hierarchy of the total system, consisting of a large "Brownian particle" in an environment of many smaller particles - "molecules". On the other hand, in this chapter we are considering a gas of similar particles. Nevertheless, the equations describing the dynamics of their probability distribution, are the same - at least within the framework of the Boltzmann transport equation with the relaxation-time approximation (17) of the scattering integral.

The origin of this similarity is that Eq. (12) is applicable to Brownian particles as well, with each "scattering" event being the particle's hit by a random molecule. Since, due to the mass hierarchy, the particle momentum change at each such event is small, the scattering integral has to be local, i.e. depend only on $w$ at the same momentum $\mathbf{p}$ as the left-hand part of the Boltzmann equation, so that the relaxation time approximation (17) is absolutely natural. But the same is true for collisions of similar particles, if they are dominated by small-angle scattering, as true, for example, for Coulomb scattering. ${ }^{30}$

Returning to the electric field duality ( $\mathcal{E} \leftrightarrow \mathcal{\mathcal { E }}$ ), recovered in our analysis, it raises a natural question: which of these fields we are speaking about in the everyday and laboratory practice? Upon some contemplation, the reader should agree that most of our electric field measurements are done indirectly, by measuring corresponding voltages - with voltmeters. A vast majority of these instruments belong to the electrodynamic variety that is based on the measurement of a small current flowing through the voltmeter. As Eq. (41) shows, electrodynamic voltmeters measure the electrochemical potential difference $\Delta \Phi$. However, there exist a rare breed of electrostatic voltmeters (also called "electrometers") that measure the electrostatic potential difference $\Delta \phi$ between two conductors. One way to implement such an instrument is to use a usual, electrodynamic voltmeter, but with the reference point set at the flat-band condition (Fig. 5b) between the conductors. This condition may be detected by vanishing electric charge on the adjacent surfaces of the conductors, and hence by the absence of its modulation in time, caused by a specially arranged periodic variation of the distance between the surfaces. Another (less sensitive but also less invasive) way to detect the flat-band condition is to measure the voltage at which the force of electrostatic interaction between two conductors, which is proportional to $\varepsilon^{2} \propto(\Delta \phi)^{2}$, vanishes.

### 6.5. Thermoelectric effects

Now let us extend our analysis even further, to the effects of a finite (though small) temperature gradient. Again, since for any of statistics (20), the average occupancy $\langle N(\varepsilon)\rangle$ is a function of just one combination of all its arguments, $\xi \equiv(\varepsilon-\mu) / T$, its partial derivatives obey not only Eq. (37), but also the following relation:

$$
\begin{equation*}
\frac{\partial\langle N(\varepsilon)\rangle}{\partial T}=-\frac{\varepsilon-\mu}{T^{2}} \frac{\partial\langle N(\varepsilon)\rangle}{\partial \xi}=\frac{\varepsilon-\mu}{T} \frac{\partial\langle N(\varepsilon)\rangle}{\partial \mu} . \tag{6.53}
\end{equation*}
$$

[^949]As a result, Eq. (38) is generalized as

$$
\begin{equation*}
\nabla w_{0}=-\frac{\partial w_{0}}{\partial \varepsilon}\left(\nabla \mu+\frac{\varepsilon-\mu}{T} \nabla T\right) \tag{6.54}
\end{equation*}
$$

giving the following generalization of Eq. (39):

$$
\begin{equation*}
\widetilde{w}=\tau \frac{\partial w_{0}}{\partial \varepsilon} \mathbf{v} \cdot\left(q \nabla \Phi+\frac{\varepsilon-\mu}{T} \nabla T\right) . \tag{6.55}
\end{equation*}
$$

Now, repeating the current density calculation, we get a result which is traditionally presented as

$$
\begin{equation*}
\mathbf{j}=\sigma(-\nabla \Phi)+\sigma S(-\nabla T) \tag{6.56}
\end{equation*}
$$

where constant $S$, called the Seebeck coefficient ${ }^{31}$ (or the "thermoelectric power", or just "thermopower") is defined by the following relation:

$$
\begin{equation*}
\sigma S=\frac{g q \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \int_{0}^{\infty}\left(8 m \varepsilon^{3}\right)^{1 / 2} \frac{(\varepsilon-\mu)}{T}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon \tag{6.57}
\end{equation*}
$$

Working out this integral for the most important case of a degenerate Fermi gas, with $T \ll \varepsilon_{\mathrm{F}}$, we have to be careful, because the center of the sharp peak of the last factor under the integral coincides with the zero point of the previous factor, $(\varepsilon-\mu) / T$. This uncertainty may be resolved using the Sommerfeld expansion formula (3.59). Indeed, for a smooth function $f(\varepsilon)$ defined by Eq. (3.60), so that $f(0)=0$, we may use (3.61) to rewrite the formula as

$$
\begin{equation*}
\int_{0}^{\infty} f(\varepsilon)\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon=f(\mu)+\left.\frac{\pi^{2}}{6} T^{2} \frac{d^{2} f(\varepsilon)}{d \varepsilon^{2}}\right|_{\varepsilon=\mu} . \tag{6.58}
\end{equation*}
$$

In particular, for integral (57), we may take $f(\varepsilon) \equiv\left(8 m \varepsilon^{3}\right)^{1 / 2}(\varepsilon-\mu) / T$. (Evidently, for this function, condition $f(0)=0$ is satisfied.) Then $f(\mu)=0, d^{2} f /\left.d \varepsilon^{2}\right|_{\varepsilon=\mu}=3(8 m \mu)^{1 / 2} / T \approx 3\left(8 m \varepsilon_{\mathrm{F}}\right)^{1 / 2} / T$, and Eq. (57) yields

$$
\begin{equation*}
\sigma S=\frac{g q \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \frac{\pi^{2}}{6} T^{2} \frac{3\left(8 m \varepsilon_{F}\right)^{1 / 2}}{T} \tag{6.59}
\end{equation*}
$$

Comparing the result with Eq. (31), for constant $S$ we get a simple expression independent of $\tau$. ${ }^{32}$

$$
\begin{equation*}
\mathcal{S}=\frac{\pi^{2}}{2 q} \frac{T}{\varepsilon_{F}}=\frac{c_{V}}{q}, \tag{6.60}
\end{equation*}
$$

where $c_{v} \equiv C_{V} / N$ is the heat capacity of the gas per unit particle, given by Eq. (3.70).

[^950]In order to understand the physical meaning of the Seebeck coefficient, it is sufficient to consider a conductor carrying no current. For this case, Eq. (56) yields

$$
\begin{equation*}
\nabla(\Phi+S T)=0 \tag{6.61}
\end{equation*}
$$

Thus, the temperature gradient creates the oppositely directed gradient of the effective electric potential $\Phi$, i.e. the effective field $\mathcal{E}$ defined by Eq. (42). This is the Seebeck effect. Figure 6 shows the standard way of its measurement, using a usual (electrodynamic) voltmeter that measures the difference of potentials $\Phi$, and a connection (in this context, called thermocouple) of two different materials, with different coefficients $S$. Integrating Eq. (61) around the loop from point $A$ to point $B$, and neglecting the temperature drop across the voltmeter, we get the following simple expression for the thermally-induced difference of the electrochemical potential, frequently also called the either the thermoelectric power or "thermo e.m.f.":

$$
\begin{align*}
V & \equiv \Phi_{\mathrm{B}}-\Phi_{\mathrm{A}}=\int_{\mathrm{A}}^{\mathrm{B}} \nabla \Phi \cdot d \mathbf{r}=-\int_{\mathrm{A}}^{\mathrm{B}} \Omega \nabla T \cdot d \mathbf{r}=-\varsigma_{1} \int_{\mathrm{A}^{\prime}}^{\mathrm{A}^{\prime \prime}} \nabla T \cdot d \mathbf{r}-\varsigma_{2}\left(\int_{\mathrm{A}^{\prime \prime}}^{\mathrm{B}} \nabla T \cdot d \mathbf{r}+\int_{\mathrm{A}}^{\mathrm{A}^{\prime}} \nabla T \cdot d \mathbf{r}\right)  \tag{6.62}\\
& =-\varsigma_{1}\left(T^{\prime \prime}-T^{\prime}\right)-\varsigma_{2}\left(T^{\prime}-T^{\prime \prime}\right)=\left(\varsigma_{1}-\varsigma_{2}\right)\left(T^{\prime}-T^{\prime \prime}\right) .
\end{align*}
$$

(Note that according to Eq. (62), any attempt to measure such voltage across any two points of a uniform conductor would give results depending on the voltmeter lead materials, due to the unintentional gradient of temperature in them.)


Using thermocouples is a popular, inexpensive method of temperature measurement - especially in the few-hundred- ${ }^{\circ} \mathrm{C}$ range (where gas- and fluid-based thermometers are not too practicable), if a $1^{\circ} \mathrm{C}$-scale accuracy is sufficient. The "responsivity" $\left(S_{1}-S_{2}\right)$ of a typical popular thermocouple, chromel-constantan, ${ }^{33}$ is about $70 \mu \mathrm{~V} /{ }^{\circ} \mathrm{C}$. In order to understand why typical values of $S$ are so small, let us discuss Seebeck effect's physics. Superficially, it is very simple: particles, heated by an external source, diffuse from it toward the colder parts of the conductor, carrying electrical current with them if they are charged. However, this naïve argument neglects the fact that at $\mathbf{j}=0$, there should be no total flow of particles. For a more accurate interpretation, note that the Seebeck effect is described by the factor $(\varepsilon-\mu) / T$ in integral (57), which changes sign at the Fermi surface, i.e. at the same energy where the term $(-\partial\langle N(\varepsilon)\rangle / \partial \varepsilon)$, describing the state availability for transport (due to their intermediate occupancy

[^951]$0<\langle N(\varepsilon)\rangle<1$ ), reaches its peak. The only reason why that integral does not vanish completely, and hence $S \neq 0$, is the growth of first factor under the integral (which describes the number of available quantum states) with $\varepsilon$, so the hotter particles (with $\varepsilon>\mu$ ) are more numerous and carry more heat then the colder ones.

The Seebeck effect is of course not the only result of temperature gradient; the same diffusion of hotter particles also causes a flow of heat from the region of higher $T$ to those with lower $T$, i.e. the effect of thermal conductivity, well known from our everyday practice. The heat (i.e. thermal energy) flow density may be calculated similarly to that of the electric current - see Eq. (26), with the natural replacement of the electric charge $q$ of each particle with the thermal energy $(\varepsilon-\mu)$ of its state: ${ }^{34}$

$$
\begin{equation*}
\mathbf{j}_{h}=\int(\varepsilon-\mu) \mathbf{v} w d^{3} p \tag{6.63}
\end{equation*}
$$

Again, at equilibrium $\left(w=w_{0}\right)$ the heat flow vanishes, so that $w$ may be replaced with its perturbation $\widetilde{w}$, which already has been calculated - see Eq. (55). The substitution of that expression into Eq. (63), and its transformation exactly similar to the one perform above for the electric current $\mathbf{j}$, yields ${ }^{35}$

$$
\begin{equation*}
\mathbf{j}_{h}=\sigma \Pi(-\nabla \Phi)+\kappa(-\nabla T), \tag{6.64}
\end{equation*}
$$

with coefficients $\Pi$ and $\kappa$ defined by equalities

Peltier coefficient and thermal conductivity

$$
\begin{align*}
& \sigma \Pi=\frac{g q \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \int_{0}^{\infty}\left(8 m \varepsilon^{3}\right)^{1 / 2}(\varepsilon-\mu)\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon  \tag{6.65}\\
& \kappa=\frac{g \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \int_{0}^{\infty}\left(8 m \varepsilon^{3}\right)^{1 / 2} \frac{(\varepsilon-\mu)^{2}}{T}\left(-\frac{\partial\langle N(\varepsilon)\rangle}{\partial \varepsilon}\right) d \varepsilon \tag{6.66}
\end{align*}
$$

Besides the missing factor $T$ in the denominator, integral in Eq. (65) is the same as in Eq. (57), so that constant $\Pi$ (called the Peltier coefficient), is simply and fundamentally related to the Seebeck coefficient: ${ }^{36}$
$\Pi$ vs. $s$

$$
\begin{equation*}
\Pi=S T . \tag{6.67}
\end{equation*}
$$

[^952]On the other hand, integral (66) may be readily calculated, for the most important case of a degenerate Fermi gas, using the Sommerfeld expansion (58) with $f(\varepsilon) \equiv\left(8 m \varepsilon^{3}\right)^{1 / 2}(\varepsilon-\mu)^{2} / T$, for which $f(\mu)=0$ and $d^{2} f /\left.d \varepsilon^{2}\right|_{\varepsilon=\mu}=2\left(8 m \mu^{3}\right)^{1 / 2} / T \approx 2\left(8 m \varepsilon_{F}^{3}\right)^{1 / 2} / T$, so that

$$
\begin{equation*}
\kappa=\frac{g \tau}{(2 \pi \hbar)^{3}} \frac{4 \pi}{3} \frac{\pi^{2}}{6} T^{2} \frac{2\left(8 m \varepsilon_{F}^{3}\right)^{1 / 2}}{T} . \tag{6.68}
\end{equation*}
$$

Comparing the result with the first form of Eq. (31), we get the so called Wiedemann-Franz law ${ }^{37}$

$$
\begin{equation*}
\kappa=\frac{\pi^{2}}{3} \frac{T}{q^{2}} \sigma \tag{6.69}
\end{equation*}
$$

This relation between the electric conductivity $\sigma$ and thermal conductivity $\kappa$ is more general than our formal derivation might imply. Indeed, it is straightforward to show that the Wiedemann-Franz law is also valid for an arbitrary dispersion law anisotropy (i.e. arbitrary Fermi surface shape) and, moreover, well beyond the relaxation-time approximation. (For example, it is also valid for scattering integral (12) with an arbitrary angular dependence of rate $\Gamma$, provided that scattering is elastic.) Experiments show that the law is well obeyed by most metals, but only at relatively low temperatures $T$ $\ll T_{\mathrm{D}}$, when the thermal conductance due to electrons is well above the one due to lattice vibrations, i.e. phonons - see Sec. 2.6. (Note also that Eq. (69) is not valid for classical gases - see Problem 2.)

Now let us discuss the less evident, first term of Eq. (64). It describes the so-called Peltier effect, which may be measured in the geometry similar to that shown in Fig. 6, but driven by an external voltage source - see Fig. 7.


Fig. 7. The Peltier effect.

The voltage drives certain dc current $I=j A$ (where $A$ is conductor's cross-section area), necessarily the same in the whole loop. However, according to Eq. (64), if materials 1 and 2 are

[^953]different, power $\mathcal{P}=j_{\mathrm{H}} A$ of the heat flow is different in two parts of the loop. Indeed, if the whole system is kept at the same temperature $(\nabla T=0)$, integration of the equation over the cross-section yields
\[

$$
\begin{equation*}
\frac{(\mathcal{P})_{1,2}}{I}=\frac{\left(j_{h}\right)_{1,2}}{j}=\frac{(\sigma \Pi)_{1,2}}{\sigma_{1,2}}=\Pi_{1,2} . \tag{6.70}
\end{equation*}
$$

\]

This means that in order to sustain the constant temperature, the following power difference,

Peltier effect

$$
\begin{equation*}
\Delta \mathcal{P}=\left(\Pi_{1}-\Pi_{2}\right) I \tag{6.71}
\end{equation*}
$$

has to be extracted from one junction of the two materials, and inserted into another junction. If a constant temperature is not maintained, the former junction is heated, while the latter one is cooled (on the top of the bulk, Joule heating), thus implementing a thermoelectric heat pump / refrigerator. Such refrigerators, with no moving parts and gas/fluid materials, are very convenient for modest (by a few tens ${ }^{\circ} \mathrm{C}$ ) cooling of relatively small components of various systems - from sensitive radiation detectors in spacecraft, all the way to cold drinks in vending machines. It is straightforward to use above formulas to show that the efficiency of active materials used in such thermoelectric refrigerators may be characterized by the following dimensionless figure-of-merit,

$$
\begin{equation*}
Z T \equiv \frac{\sigma S^{2}}{\kappa} T \tag{6.72}
\end{equation*}
$$

For the best thermoelectric materials found so far, $Z T$ is in the range from 2 to 3 , providing the coefficient of performance, defined by Eq. (1.69), of the order of 0.5 - a few times lower than that of traditional, mechanical refrigerators. The search for composite materials (including those with nanoparticles) with higher values of $Z T$ is one of very active fields of applied solid state physics. ${ }^{38}$

Let me finish this chapter (and this course, and this series :-) by emphasizing again that due to time/space restrictions I was able to barely scratch the surface of physical kinetics. ${ }^{39}$

### 6.6. Exercise problems

6.1. Use the relaxation-time approximation of the Boltzmann equation to prove the Drude formula for the complex conductivity at frequency $\omega$,

$$
\sigma(\omega)=\frac{\sigma(0)}{1-i \omega \tau}
$$

where $\sigma(0)$ is the dc conductivity given by Eq. (6.30) of the lecture notes, and give a physical interpretation of the formula.

[^954]6.2. Use the variable separation method to calculate the time evolution of the particle density distribution in space, provided that at $t=0$, the particles are released from their uniform distribution in a wide box of thickness $2 a$ :
\[

n= $$
\begin{cases}n_{0}, & \text { for }-a \leq x \leq+a, \\ 0, & \text { otherwise }\end{cases}
$$
\]

6.3. For the 1 D version of the diffusion equation (i.e. of the drift-diffusion equation (6.50) with $\tau T / m \equiv D$, and without the drift-inducing field, $\nabla U=0$ ),

$$
\frac{\partial n}{\partial t}=D \frac{\partial^{2} n}{\partial x^{2}}, \quad \text { for }-\infty<x<+\infty
$$

find an appropriate spatial-temporal Green's function, and use it to solve the previous problem.
6.4.* Calculate the electric conductance of a narrow, uniform conducting channel between two bulk conductors, in the low-voltage and low-temperature limit, neglecting the electron interaction and scattering inside the channel.
6.5. Calculate the electric conductivity $\sigma$, the thermal conductivity $\kappa$, as well as the thermoelectric coefficients $\mathcal{S}$ and $\Pi$, for a classical, ideal gas of electrically charged particles. Compare the results with those for the degenerate Fermi gas, derived in the lecture notes.
6.6. Derive a partial differential equation describing the time evolution of temperature distribution in a medium with negligible thermal expansion and with temperature-independent specific heat $c_{V}$ and thermal conductivity $\kappa$, given by the Fourier law

$$
\mathbf{j}_{h}=-\kappa \nabla T .
$$

6.7. Use the equation derived in the previous problem to calculate the time evolution of temperature in the center of a uniform solid sphere of radius $R$, initially heated to temperature $T_{i}$, and at $t$ $=0$ placed into a heat bath that keeps its surface at temperature $T_{0}$.
6.8. Suggest a reasonable definition of the entropy production rate (per unit volume), and calculate this rate for a stationary thermal conduction, assuming that it obeys the Fourier law, in a material with negligible thermal expansion. Give a physical interpretation of the result. Does the stationary temperature distribution in a sample correspond to the minimum of the total entropy production in it?


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## Essential Graduate Physics

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Appendix MA

## Selected Mathematical Formulas

that are used in this lecture course series, but not always remembered by students (and some instructors :-)

## 1. Constants

- Euclidean circle’s length-to-diameter ratio:

$$
\begin{equation*}
\pi=3.141592653 \ldots ; \quad \pi^{1 / 2} \approx 1.77 \tag{1.1}
\end{equation*}
$$

- Natural logarithm base:

$$
\begin{equation*}
e \equiv \lim _{n \rightarrow \infty}\left(1+\frac{1}{n}\right)^{n}=2.718281828 \ldots ; \tag{1.2a}
\end{equation*}
$$

from that value, the logarithm base conversion factors are as follows ( $\xi>0$ ):

$$
\begin{equation*}
\frac{\ln \xi}{\log _{10} \xi}=\ln 10 \approx 2.303, \quad \frac{\log _{10} \xi}{\ln \xi}=\frac{1}{\ln 10} \approx 0.434 \tag{1.2b}
\end{equation*}
$$

- The Euler (or "Euler-Mascheroni") constant:

$$
\begin{equation*}
\gamma \equiv \lim _{n \rightarrow \infty}\left(1+\frac{1}{2}+\frac{1}{3}+\ldots+\frac{1}{n}-\ln n\right)=0.5771566490 \ldots ; \quad e^{\gamma} \approx 1.781 \tag{1.3}
\end{equation*}
$$

## 2. Combinatorics, sums, and series

(i) Combinatorics

- The number of different permutations, i.e. ordered sequences of $k$ elements selected from a set of $n$ distinct elements ( $n \geq k$ ), is

$$
\begin{equation*}
{ }^{n} P_{k} \equiv n \cdot(n-1) \cdot \ldots \cdot(n-k+1)=\frac{n!}{(n-k)!} \tag{2.1a}
\end{equation*}
$$

in particular, the number of different permutations of all elements of the set $(n=k)$ is

$$
\begin{equation*}
{ }^{k} P_{k}=k \cdot(k-1) \cdot \ldots \cdot 2 \cdot 1=k! \tag{2.1b}
\end{equation*}
$$

- The number of different combinations, i.e. unordered sequences of $k$ elements from a set of $n \geq$ $k$ distinct elements, is equal to the binomial coefficient

$$
\begin{equation*}
{ }^{n} C_{k} \equiv\binom{n}{k} \equiv \frac{{ }^{n} P_{k}}{{ }^{k} P_{k}}=\frac{n!}{k!(n-k)!} \tag{2.2}
\end{equation*}
$$

In an alternative, very popular "ball/box language", ${ }^{n} C_{k}$ is the number of different ways to put in a box, in an arbitrary order, $k$ balls selected from $n$ distinct balls.

- A generalization of the binomial coefficient notion is the multinomial coefficient,

$$
\begin{equation*}
{ }^{n} C_{k_{1}, k_{2}, \ldots k_{l}} \equiv \frac{n!}{k_{1}!k_{2}!\ldots k_{l}!}, \quad \text { with } n=\sum_{j=1}^{l} k_{j} \tag{2.3}
\end{equation*}
$$

which, in the standard mathematical language, is a number of different permutations in a multiset of $l$ distinct element types from an $n$-element set which contains $k_{j}(j=1,2, \ldots l)$ elements of each type. In the "ball/box language", the coefficient (2.3) is the number of different ways to distribute $n$ balls between $l$ distinct boxes, each time keeping the number ( $k_{j}$ ) of balls in the $j$-th box fixed, but ignoring their order inside the box. The binomial coefficient ${ }^{n} C_{k}$ (2.2), is a particular case of the multinomial coefficient (2.3) for $l=2$ - counting the explicit box for the first one, and the remaining space for the second box, so that if $k_{1} \equiv k$, then $k_{2}=n-k$.

- One more important combinatorial quantity is the number $M_{n}{ }^{(k)}$ of ways to place $n$ indistinguishable balls into $k$ distinct boxes. It may be readily calculated from Eq. (2.2) as the number of different ways to select $(k-1)$ partitions between the boxes in an imagined linear row of $(k-1+n)$ "objects" (balls in the boxes and partitions between them):

$$
\begin{equation*}
M_{n}^{(k)}={ }^{n-1+k} C_{k-1} \equiv \frac{(k-1+n)!}{(k-1)!n!} . \tag{2.4}
\end{equation*}
$$

(ii) Sums and series

- Arithmetic progression:

$$
\begin{equation*}
r+2 r+\ldots+n r \equiv \sum_{k=1}^{n} k r=\frac{n(r+n r)}{2} ; \tag{2.5a}
\end{equation*}
$$

in particular, at $r=1$ it is reduced to the sum of $n$ first natural numbers:

$$
\begin{equation*}
1+2+\ldots+n \equiv \sum_{k=1}^{n} k=\frac{n(n+1)}{2} \tag{2.5b}
\end{equation*}
$$

- Sums of squares and cubes of $n$ first natural numbers:

$$
\begin{gather*}
1^{2}+2^{2}+\ldots+n^{2} \equiv \sum_{k=1}^{n} k^{2}=\frac{n(n+1)(2 n+1)}{6} ;  \tag{2.6a}\\
1^{3}+2^{3}+\ldots+n^{3} \equiv \sum_{k=1}^{n} k^{3}=\frac{n^{2}(n+1)^{2}}{4}, \tag{2.6b}
\end{gather*}
$$

- The Riemann zeta function:

$$
\begin{equation*}
\zeta(s) \equiv 1+\frac{1}{2^{s}}+\frac{1}{3^{s}}+\ldots=\sum_{k=1}^{\infty} \frac{1}{k^{s}} \tag{2.7a}
\end{equation*}
$$

the particular values frequently met in applications are

$$
\begin{equation*}
\zeta\left(\frac{3}{2}\right) \approx 2.612, \quad \zeta(2)=\frac{\pi^{2}}{6}, \quad \zeta\left(\frac{5}{2}\right) \approx 1.341, \quad \zeta(3) \approx 1.202, \quad \zeta(4)=\frac{\pi^{4}}{90}, \quad \zeta(5) \approx 1.037 \tag{2.7b}
\end{equation*}
$$

- Finite geometric progression (for real $\lambda \neq 1$ ):

$$
\begin{equation*}
1+\lambda+\lambda^{2}+\ldots+\lambda^{n-1} \equiv \sum_{k=0}^{n-1} \lambda^{k}=\frac{1-\lambda^{n}}{1-\lambda} ; \tag{2.8a}
\end{equation*}
$$

in particular, if $\lambda^{2}<1$, the progression has a finite limit at $n \rightarrow \infty$ (called the geometric series):

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \sum_{k=0}^{n-1} \lambda^{k}=\sum_{k=0}^{\infty} \lambda^{k}=\frac{1}{1-\lambda} . \tag{2.8b}
\end{equation*}
$$

- Binomial sum (or the "binomial theorem"):

$$
\begin{equation*}
(1+a)^{n}=\sum_{k=0}^{n}{ }^{n} C_{k} a^{k}, \tag{2.9}
\end{equation*}
$$

where ${ }^{n} C_{k}$ are the binomial coefficients defined by Eq. (2.2).

- The Stirling formula:

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \ln (n!)=n(\ln n-1)+\frac{1}{2} \ln (2 \pi n)+\frac{1}{12 n}-\frac{1}{360 n^{3}}+\ldots \tag{2.10}
\end{equation*}
$$

for most applications in physics, the first term ${ }^{1}$ is sufficient.

- The Taylor (or "Taylor-Maclaurin") series: for any infinitely differentiable function $f(\xi)$ :

$$
\begin{equation*}
\lim _{\tilde{x} \rightarrow 0} f(\xi+\tilde{\xi})=f(\xi)+\frac{d f}{d \xi}(\xi) \tilde{\xi}+\frac{1}{2!} \frac{d^{2} f}{d \xi^{2}}(\xi) \tilde{\xi}^{2}+\ldots=\sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^{k} f}{d \xi^{k}}(\xi) \tilde{\xi}^{k} \tag{2.11a}
\end{equation*}
$$

note that for many functions this series converges only within a limited, sometimes small range of deviations $\tilde{x}$. For a function of several arguments, $f\left(\xi_{1}, \xi_{2}, \ldots, \xi_{N}\right)$, the first terms of the Taylor series are

$$
\begin{equation*}
\lim _{\tilde{\xi}_{k} \rightarrow 0} f\left(\xi_{1}+\tilde{\xi}_{1}, \xi_{2}+\tilde{\xi}_{2}, \ldots\right)=f\left(\xi_{1}, \xi_{2}, \ldots\right)+\sum_{k=1}^{N} \frac{\partial f}{\partial \xi_{k}}\left(\xi_{1}, \xi_{2}, \ldots\right) \tilde{\xi}_{k}+\frac{1}{2!} \sum_{k, k^{\prime}=1}^{N} \frac{\partial^{2} f}{\partial_{k} \xi \partial \xi_{k^{\prime}}} \widetilde{\xi}_{k} \tilde{\xi}_{k^{\prime}}+\ldots \tag{2.11b}
\end{equation*}
$$

- The Euler-Maclaurin formula, valid for any infinitely differentiable function $f(\xi)$ :

$$
\begin{align*}
\sum_{k=1}^{n} f(k)= & \int_{0}^{n} f(\xi) d \xi+\frac{1}{2}[f(n)-f(0)]+\frac{1}{6} \cdot \frac{1}{2!}\left[\frac{d f}{d \xi}(n)-\frac{d f}{d \xi}(0)\right] \\
& -\frac{1}{30} \cdot \frac{1}{4!}\left[\frac{d^{3} f}{d \xi^{3}}(n)-\frac{d^{3} f}{d \xi^{3}}(0)\right]+\frac{1}{42} \cdot \frac{1}{6!}\left[\frac{d^{5} f}{d \xi^{5}}(n)-\frac{d^{5} f}{d \xi^{5}}(0)\right]+\ldots \tag{2.12a}
\end{align*}
$$

[^955]the coefficients participating in this formula are the so-called Bernoulli numbers: ${ }^{2}$
\[

$$
\begin{equation*}
B_{1}=\frac{1}{2}, \quad B_{2}=\frac{1}{6}, \quad B_{3}=0, \quad B_{4}=\frac{1}{30}, \quad B_{5}=0, \quad B_{6}=\frac{1}{42}, \quad B_{7}=0, \quad B_{8}=\frac{1}{30}, \ldots . \tag{2.12b}
\end{equation*}
$$

\]

## 3. Basic trigonometric functions

- Trigonometric functions of the sum and the difference of two arguments: ${ }^{3}$

$$
\begin{align*}
\cos (a \pm b) & =\cos a \cos b \mp \sin a \sin b  \tag{3.1a}\\
\sin (a \pm b) & =\sin a \cos b \pm \cos a \sin b . \tag{3.1b}
\end{align*}
$$

- Sums of two functions of arbitrary arguments:

$$
\begin{align*}
& \cos a+\cos b=2 \cos \frac{a+b}{2} \cos \frac{b-a}{2}  \tag{3.2a}\\
& \cos a-\cos b=2 \sin \frac{a+b}{2} \sin \frac{b-a}{2},  \tag{3.2b}\\
& \sin a \pm \sin b=2 \sin \frac{a \pm b}{2} \cos \frac{ \pm b-a}{2} \tag{3.2c}
\end{align*}
$$

- Trigonometric function products:

$$
\begin{align*}
& 2 \cos a \cos b=\cos (a+b)+\cos (a-b)  \tag{3.3a}\\
& 2 \sin a \cos b=\sin (a+b)+\sin (a-b)  \tag{3.3b}\\
& 2 \sin a \sin b=\cos (a-b)-\cos (a+b) \tag{3.3c}
\end{align*}
$$

For the particular case of equal arguments, $b=a$, these three formulas yield the following expressions for the squares of trigonometric functions, and their product:

$$
\begin{equation*}
\cos ^{2} a=\frac{1}{2}(1+\cos 2 a), \quad \sin a \cos a=\frac{1}{2} \sin 2 a, \quad \sin ^{2} a=\frac{1}{2}(1-\cos 2 a) . \tag{3.3d}
\end{equation*}
$$

- Cubes of trigonometric functions:

$$
\begin{equation*}
\cos ^{3} a=\frac{3}{4} \cos a+\frac{1}{4} \cos 3 a, \quad \sin ^{3} a=\frac{3}{4} \sin a-\frac{1}{4} \sin 3 a . \tag{3.4}
\end{equation*}
$$

- Trigonometric functions of a complex argument:

$$
\begin{align*}
& \sin (a+i b)=\sin a \cosh b+i \cos a \sinh b, \\
& \cos (a+i b)=\cos a \cosh b-i \sin a \sinh b . \tag{3.5}
\end{align*}
$$

[^956]- Sums of trigonometric functions of $n$ equidistant arguments:

$$
\sum_{k=1}^{n}\left\{\begin{array}{c}
\sin  \tag{3.6}\\
\cos
\end{array}\right\} k \xi=\left\{\begin{array}{l}
\sin \\
\cos
\end{array}\right\}\left(\frac{n+1}{2} \xi\right) \sin \left(\frac{n}{2} \xi\right) / \sin \left(\frac{\xi}{2}\right) .
$$

## 4. General differentiation

- Full differential of a product of two functions:

$$
\begin{equation*}
d(f g)=(d f) g+f(d g) \tag{4.1}
\end{equation*}
$$

- Full differential of a function of several independent arguments, $f\left(\xi_{1}, \xi_{2}, \ldots, \xi_{n}\right)$ :

$$
\begin{equation*}
d f=\sum_{k=1}^{n} \frac{\partial f}{\partial \xi_{k}} d \xi_{k} . \tag{4.2}
\end{equation*}
$$

- Curvature of the Cartesian plot of a 1D function $f(\xi)$ :

$$
\begin{equation*}
\kappa \equiv \frac{1}{R}=\frac{\left|d^{2} f / d \xi^{2}\right|}{\left[1+(d f / d \xi)^{2}\right]^{3 / 2}} \tag{4.3}
\end{equation*}
$$

## 5. General integration

- Integration by parts - immediately follows from Eq. (4.1):

$$
\begin{equation*}
\int_{g(A)}^{g(B)} f d g=\left.f g\right|_{A} ^{B}-\int_{f(A)}^{f(B)} g d f . \tag{5.1}
\end{equation*}
$$

- Numerical (approximate) integration of 1D functions: the simplest trapezoidal rule,

$$
\begin{equation*}
\int_{a}^{b} f(\xi) d \xi \approx h\left[f\left(a+\frac{h}{2}\right)+f\left(a+\frac{3 h}{2}\right)+\ldots+f\left(b-\frac{h}{2}\right)\right]=h \sum_{n=1}^{N} f\left(a-\frac{h}{2}+n h\right), \quad h \equiv \frac{b-a}{N} . \tag{5.2}
\end{equation*}
$$

has relatively low accuracy (error of the order of $\left(h^{3} / 12\right) d^{2} f / d \xi^{2}$ per step), so that the following Simpson formula,

$$
\begin{equation*}
\int_{a}^{b} f(\xi) d \xi \approx \frac{h}{3}[f(a)+4 f(a+h)+2 f(a+2 h)+\ldots+4 f(b-h)+f(b)], \quad h \equiv \frac{b-a}{2 N}, \tag{5.3}
\end{equation*}
$$

whose error per step scales as $\left(h^{5} / 180\right) d^{4} f / d \xi^{4}$, is used much more frequently. ${ }^{4}$

[^957]
## 6. A few 1D integrals ${ }^{5}$

(i) Indefinite integrals

- Integrals with $\left(1+\xi^{2}\right)^{1 / 2}$ :

$$
\begin{gather*}
\int\left(1+\xi^{2}\right)^{1 / 2} d \xi=\frac{\xi}{2}\left(1+\xi^{2}\right)^{1 / 2}+\frac{1}{2} \ln \left|\xi+\left(1+\xi^{2}\right)^{1 / 2}\right|  \tag{6.1}\\
\int \frac{d \xi}{\left(1+\xi^{2}\right)^{1 / 2}}=\ln \left|\xi+\left(1+\xi^{2}\right)^{1 / 2}\right|  \tag{6.2a}\\
\int \frac{d \xi}{\left(1+\xi^{2}\right)^{3 / 2}}=\frac{\xi}{\left(1+\xi^{2}\right)^{1 / 2}} . \tag{6.2b}
\end{gather*}
$$

- Miscellaneous indefinite integrals:

$$
\begin{gather*}
\int \frac{d \xi}{\xi\left(\xi^{2}+2 a \xi-1\right)^{1 / 2}}=\cos ^{-1} \frac{a \xi-1}{|\xi|\left(a^{2}+1\right)^{1 / 2}}  \tag{6.3a}\\
\int \frac{(\sin \xi-\xi \cos \xi)^{2}}{\xi^{5}} d \xi=\frac{2 \xi \sin 2 \xi+\cos 2 \xi-2 \xi^{2}-1}{8 \xi^{4}},  \tag{6.3b}\\
\int \frac{d \xi}{a+b \cos \xi}=\frac{2}{\left(a^{2}-b^{2}\right)^{1 / 2}} \tan ^{-1}\left[\frac{(a-b)}{\left(a^{2}-b^{2}\right)^{1 / 2}} \tan \frac{\xi}{2}\right], \quad \text { for } a^{2}>b^{2}  \tag{6.3c}\\
\int \frac{d \xi}{1+\xi^{2}}=\tan ^{-1} \xi \tag{6.3d}
\end{gather*}
$$

(ii) Semi-definite integrals:

- Integrals with $1 /\left(e^{\xi} \pm 1\right)$ :

$$
\begin{align*}
& \int_{a}^{\infty} \frac{d \xi}{e^{\xi}+1}=\ln \left(1+e^{-a}\right)  \tag{6.4a}\\
& \int_{a>0}^{\infty} \frac{d \xi}{e^{\xi}-1}=\ln \frac{1}{1-e^{-a}} \tag{6.4b}
\end{align*}
$$

(iii) Definite integrals

- Integrals with $1 /\left(1+\xi^{2}\right):{ }^{6}$

$$
\begin{equation*}
\int_{0}^{\infty} \frac{d \xi}{1+\xi^{2}}=\frac{\pi}{2} \tag{6.5a}
\end{equation*}
$$

[^958]\[

$$
\begin{equation*}
\int_{0}^{\infty} \frac{d \xi}{\left(1+\xi^{2}\right)^{3 / 2}}=1 ; \tag{6.5b}
\end{equation*}
$$

\]

more generally,

$$
\begin{equation*}
\int_{0}^{\infty} \frac{d \xi}{\left(1+\xi^{2}\right)^{n}}=\frac{\pi}{2} \frac{(2 n-3)!!}{(2 n-2)!!} \equiv \frac{\pi}{2} \frac{1 \cdot 3 \cdot 5 \ldots(2 n-3)}{2 \cdot 4 \cdot 6 \ldots(2 n-2)}, \quad \text { for } n=2,3, \ldots \tag{6.5c}
\end{equation*}
$$

- Integrals with $\left(1-\xi^{2 n}\right)^{1 / 2}$ :

$$
\begin{align*}
& \int_{0}^{1} \frac{d \xi}{\left(1-\xi^{2 n}\right)^{1 / 2}}=\frac{\pi^{1 / 2}}{2 n} \Gamma\left(\frac{1}{2 n}\right) / \Gamma\left(\frac{n+1}{2 n}\right),  \tag{6.6a}\\
& \int_{0}^{1}\left(1-\xi^{2 n}\right)^{1 / 2} d \xi=\frac{\pi^{1 / 2}}{4 n} \Gamma\left(\frac{1}{2 n}\right) / \Gamma\left(\frac{3 n+1}{2 n}\right), \tag{6.6b}
\end{align*}
$$

where $\Gamma(s)$ is the gamma-function, which is most often defined (for $\operatorname{Re} s>0$ ) by the following integral:

$$
\begin{equation*}
\int_{0}^{\infty} \xi^{s-1} e^{-\xi} d \xi=\Gamma(s) \tag{6.7a}
\end{equation*}
$$

The key property of this function is the recurrence relation, valid for any $s \neq 0,-1,-2, \ldots$, is

$$
\begin{equation*}
\Gamma(s+1)=s \Gamma(s) . \tag{6.7b}
\end{equation*}
$$

Since, according to Eq. (6.7a), $\Gamma(1)=1$, Eq. (6.7b) for non-negative integers takes the form

$$
\begin{equation*}
\Gamma(n+1)=n!, \text { for } n=0,1,2, \ldots \tag{6.7c}
\end{equation*}
$$

(where $0!\equiv 1$ ). Because of this, for integer $s=n+1 \geq 1$, Eq. (6.7a) is reduced to

$$
\begin{equation*}
\int_{0}^{\infty} \xi^{n} e^{-\xi} d \xi=n! \tag{6.7d}
\end{equation*}
$$

Other frequently met values of the gamma-function are those for positive semi-integer arguments:

$$
\begin{equation*}
\Gamma\left(\frac{1}{2}\right)=\pi^{1 / 2}, \quad \Gamma\left(\frac{3}{2}\right)=\frac{1}{2} \pi^{1 / 2}, \quad \Gamma\left(\frac{5}{2}\right)=\frac{1}{2} \cdot \frac{3}{2} \pi^{1 / 2}, \quad \Gamma\left(\frac{7}{2}\right)=\frac{1}{2} \cdot \frac{3}{2} \cdot \frac{5}{2} \pi^{1 / 2}, \ldots . \tag{6.7e}
\end{equation*}
$$

- Integrals with $1 /\left(e^{\xi} \pm 1\right)$ :

$$
\begin{gather*}
\int_{0}^{\infty} \frac{\xi^{s-1} d \xi}{e^{\xi}+1}=\left(1-2^{1-s}\right) \Gamma(s) \zeta(s), \quad \text { for } s>0,  \tag{6.8a}\\
\int_{0}^{\infty} \frac{\xi^{s-1} d \xi}{e^{\xi}-1}=\Gamma(s) \zeta(s), \quad \text { for } s>1, \tag{6.8b}
\end{gather*}
$$

where $\zeta(s)$ is the Riemann zeta-function - see Eq. (2.6). Particular cases: for $s=2 n$,

$$
\begin{equation*}
\int_{0}^{\infty} \frac{\xi^{2 n-1} d \xi}{e^{\xi}+1}=\frac{2^{2 n-1}-1}{2 n} \pi^{2 n} B_{2 n} \tag{6.8c}
\end{equation*}
$$

$$
\begin{equation*}
\int_{0}^{\infty} \frac{\xi^{2 n-1} d \xi}{e^{\xi}-1}=\frac{(2 \pi)^{2 n}}{4 n} B_{2 n} \tag{6.8d}
\end{equation*}
$$

where $B_{n}$ are the Bernoulli numbers - see Eq. (2.12). For the particular case $s=1$ (when Eq. (6.8a) yields uncertainty),

$$
\begin{equation*}
\int_{0}^{\infty} \frac{d \xi}{e^{\xi}+1}=\ln 2 . \tag{6.8e}
\end{equation*}
$$

- Integrals with $\exp \left\{-\xi^{2}\right\}$ :

$$
\begin{equation*}
\int_{0}^{\infty} \xi^{s} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma\left(\frac{s+1}{2}\right), \text { for } s>-1 \text {; } \tag{6.9a}
\end{equation*}
$$

for applications the most important particular values of $s$ are 0 and 2:

$$
\begin{align*}
& \int_{0}^{\infty} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma\left(\frac{1}{2}\right)=\frac{\pi^{1 / 2}}{2}  \tag{6.9b}\\
& \int_{0}^{\infty} \xi^{2} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma\left(\frac{3}{2}\right)=\frac{\pi^{1 / 2}}{4} \tag{6.9c}
\end{align*}
$$

though we will also run into the cases $s=4$ and $s=6$ :

$$
\begin{equation*}
\int_{0}^{\infty} \xi^{4} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma\left(\frac{5}{2}\right)=\frac{3 \pi^{1 / 2}}{8}, \quad \int_{0}^{\infty} \xi^{6} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma\left(\frac{7}{2}\right)=\frac{15 \pi^{1 / 2}}{16} ; \tag{6.9d}
\end{equation*}
$$

for odd integer values $s=2 n+1$ (with $n=0,1,2, \ldots$ ), Eq. (6.9a) takes a simpler form:

$$
\begin{equation*}
\int_{0}^{\infty} \xi^{2 n+1} e^{-\xi^{2}} d \xi=\frac{1}{2} \Gamma(n+1)=\frac{n!}{2} . \tag{6.9e}
\end{equation*}
$$

- Integrals with cosine and sine functions:

$$
\begin{gather*}
\int_{0}^{\infty} \cos \left(\xi^{2}\right) d \xi=\int_{0}^{\infty} \sin \left(\xi^{2}\right) d \xi=\left(\frac{\pi}{8}\right)^{1 / 2} .  \tag{6.10}\\
\int_{0}^{\infty} \frac{\cos \xi}{a^{2}+\xi^{2}} d \xi=\frac{\pi}{2 a} e^{-a} .  \tag{6.11}\\
\int_{0}^{\infty}\left(\frac{\sin \xi}{\xi}\right)^{2} d \xi=\frac{\pi}{2} \tag{6.12}
\end{gather*}
$$

- Integrals with logarithms:

$$
\begin{gather*}
\int_{0}^{1} \ln \frac{a+\left(1-\xi^{2}\right)^{1 / 2}}{a-\left(1-\xi^{2}\right)^{1 / 2}} d \xi=\pi\left[a-\left(a^{2}-1\right)^{1 / 2}\right], \quad \text { for } a \geq 1  \tag{6.13}\\
\int_{0}^{1} \ln \frac{1+(1-\xi)^{1 / 2}}{\xi^{1 / 2}} d \xi=1 \tag{6.14}
\end{gather*}
$$

- Integral representations of the Bessel functions of integer order:

$$
\begin{gather*}
J_{n}(\alpha)=\frac{1}{2 \pi} \int_{-\pi}^{+\pi} e^{i(\alpha \sin \xi-n \xi)} d \xi, \quad \text { so that } e^{i \alpha \sin \xi}=\sum_{k=-\infty}^{\infty} J_{k}(\alpha) e^{i k \xi} ;  \tag{6.15a}\\
I_{n}(\alpha)=\frac{1}{\pi} \int_{0}^{\pi} e^{\alpha \cos \xi} \cos n \xi d \xi \tag{6.15b}
\end{gather*}
$$

## 7. 3D vector products

(i) Definitions:

- Scalar ("dot-") product:

$$
\begin{equation*}
\mathbf{a} \cdot \mathbf{b}=\sum_{j=1}^{3} a_{j} b_{j}, \tag{7.1}
\end{equation*}
$$

where $a_{j}$ and $b_{j}$ are vector components in any orthogonal coordinate system. In particular, the vector squared (the same as its norm squared) is:

$$
\begin{equation*}
a^{2} \equiv \mathbf{a} \cdot \mathbf{a}=\sum_{j=1}^{3} a_{j}^{2} \equiv\|\mathbf{a}\|^{2} \tag{7.2}
\end{equation*}
$$

- Vector ("cross-") product:

$$
\mathbf{a} \times \mathbf{b} \equiv \mathbf{n}_{1}\left(a_{2} b_{3}-a_{3} b_{2}\right)+\mathbf{n}_{2}\left(a_{3} b_{1}-a_{1} b_{3}\right)+\mathbf{n}_{3}\left(a_{1} b_{2}-a_{2} b_{1}\right)=\left|\begin{array}{lll}
\mathbf{n}_{1} & \mathbf{n}_{2} & \mathbf{n}_{3}  \tag{7.3}\\
a_{1} & a_{2} & a_{3} \\
b_{1} & b_{2} & b_{3}
\end{array}\right|,
$$

where $\left\{\mathbf{n}_{j}\right\}$ is the set of mutually perpendicular unit vectors ${ }^{7}$ along the corresponding coordinate system axes. ${ }^{8}$ In particular, Eq. (7.3) yields

$$
\begin{equation*}
\mathbf{a} \times \mathbf{a}=0 . \tag{7.4}
\end{equation*}
$$

(ii) Corollaries (readily verified by Cartesian components):

- Double vector product (the so-called bac minus cab rule):

$$
\begin{equation*}
\mathbf{a} \times(\mathbf{b} \times \mathbf{c})=\mathbf{b}(\mathbf{a} \cdot \mathbf{c})-\mathbf{c}(\mathbf{a} \cdot \mathbf{b}) . \tag{7.5}
\end{equation*}
$$

- Mixed scalar-vector product (called the operand rotation rule):

$$
\begin{equation*}
\mathbf{a} \cdot(\mathbf{b} \times \mathbf{c})=\mathbf{b} \cdot(\mathbf{c} \times \mathbf{a})=\mathbf{c} \cdot(\mathbf{a} \times \mathbf{b}) . \tag{7.6}
\end{equation*}
$$

- Scalar product of vector products:

$$
\begin{equation*}
(\mathbf{a} \times \mathbf{b}) \cdot(\mathbf{c} \times \mathbf{d})=(\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d})-(\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}) ; \tag{7.7a}
\end{equation*}
$$

in the particular case of two similar operands (say, $\mathbf{a}=\mathbf{c}$ and $\mathbf{b}=\mathbf{d}$ ), the last formula is reduced to

[^959]\[

$$
\begin{equation*}
(\mathbf{a} \times \mathbf{b})^{2}=(a b)^{2}-(\mathbf{a} \cdot \mathbf{b})^{2} . \tag{7.7b}
\end{equation*}
$$

\]

## 8. Differentiation in 3D Cartesian coordinates

- Definition of the del (or "nabla") vector-operator $\nabla$ : ${ }^{9}$

$$
\begin{equation*}
\nabla \equiv \sum_{j=1}^{3} \mathbf{n}_{j} \frac{\partial}{\partial r_{j}} \tag{8.1}
\end{equation*}
$$

where $r_{j}$ is a set of linear and orthogonal (called Cartesian) coordinates along directions $\mathbf{n}_{j}$. In accordance with this definition, the operator $\nabla$ acting on a scalar function of coordinates, $f(\mathbf{r}),{ }^{10}$ gives its gradient, i.e. a new vector:

$$
\begin{equation*}
\nabla f \equiv \sum_{j=1}^{3} \mathbf{n}_{j} \frac{\partial f}{\partial r_{j}} \equiv \operatorname{grad} f \tag{8.2}
\end{equation*}
$$

- The scalar product of del by a vector function of coordinates (a vector field),

$$
\begin{equation*}
\mathbf{f}(\mathbf{r}) \equiv \sum_{j=1}^{3} \mathbf{n}_{j} f_{j}(\mathbf{r}), \tag{8.3}
\end{equation*}
$$

compiled formally following Eq. (7.1), is a scalar function - the divergence of the initial function:

$$
\begin{equation*}
\nabla \cdot \mathbf{f} \equiv \sum_{j=1}^{3} \frac{\partial f_{j}}{\partial r_{j}} \equiv \operatorname{div} \mathbf{f}, \tag{8.4}
\end{equation*}
$$

while the vector product of $\nabla$ and $\mathbf{f}$, formed in a formal accordance with Eq. (7.3), is a new vector - the curl (in European tradition, called rotor and denoted rot) of $\mathbf{f}$ :

$$
\nabla \times \mathbf{f} \equiv\left|\begin{array}{ccc}
\mathbf{n}_{1} & \mathbf{n}_{2} & \mathbf{n}_{3}  \tag{8.5}\\
\frac{\partial}{\partial r_{1}} & \frac{\partial}{\partial r_{2}} & \frac{\partial}{\partial r_{3}} \\
f_{1} & f_{2} & f_{3}
\end{array}\right|=\mathbf{n}_{1}\left(\frac{\partial f_{3}}{\partial r_{2}}-\frac{\partial f_{2}}{\partial r_{3}}\right)+\mathbf{n}_{2}\left(\frac{\partial f_{1}}{\partial r_{3}}-\frac{\partial f_{3}}{\partial r_{1}}\right)+\mathbf{n}_{3}\left(\frac{\partial f_{2}}{\partial r_{1}}-\frac{\partial f_{1}}{\partial r_{2}}\right) \equiv \text { curl f. }
$$

- One more frequently met "product" is $(\mathbf{f} \cdot \nabla) \mathbf{g}$, where $\mathbf{f}$ and $\mathbf{g}$ are two arbitrary vector functions of $\mathbf{r}$. This product should be also understood in the sense implied by Eq. (7.1), i.e. as a vector whose $j$-th Cartesian component is

$$
\begin{equation*}
[(\mathbf{f} \cdot \nabla) \mathbf{g}]_{j}=\sum_{j^{\prime}=1}^{3} f_{j^{\prime}} \frac{\partial g_{j}}{\partial r_{j^{\prime}}} \tag{8.5}
\end{equation*}
$$

## 9. The Laplace operator $\nabla^{2} \equiv \nabla \cdot \nabla$

- Expression in Cartesian coordinates - in the formal accordance with Eq. (7.2):

[^960]\[

$$
\begin{equation*}
\nabla^{2}=\sum_{j=1}^{3} \frac{\partial^{2}}{\partial r_{j}^{2}} \tag{9.1}
\end{equation*}
$$

\]

- According to its definition, the Laplace operator acting on a scalar function of coordinates gives a new scalar function:

$$
\begin{equation*}
\nabla^{2} f \equiv \nabla \cdot(\nabla f)=\operatorname{div}(\operatorname{grad} f)=\sum_{j=1}^{3} \frac{\partial^{2} f}{\partial r_{j}^{2}} \tag{9.2}
\end{equation*}
$$

- On the other hand, acting on a vector function (8.3), operator $\nabla^{2}$ returns another vector:

$$
\begin{equation*}
\nabla^{2} \mathbf{f}=\sum_{j=1}^{3} \mathbf{n}_{j} \nabla^{2} f_{j} \tag{9.3}
\end{equation*}
$$

Note that Eqs. (9.1)-(9.3) are only valid in Cartesian (i.e. orthogonal and linear) coordinates, but generally not in other (even orthogonal) coordinates - see, e.g., Eqs. (10.3), (10.6), (10.9), and (10.12) below.

## 10. Operators $\nabla$ and $\nabla^{2}$ in the most important systems of orthogonal coordinates ${ }^{11}$

(i) Cylindrical ${ }^{12}$ coordinates $\{\rho, \varphi, z\}$ (see Fig. below) may be defined by their relations with the Cartesian coordinates:


- Gradient of a scalar function:

$$
\begin{equation*}
\nabla f=\mathbf{n}_{\rho} \frac{\partial f}{\partial \rho}+\mathbf{n}_{\varphi} \frac{1}{\rho} \frac{\partial f}{\partial \varphi}+\mathbf{n}_{z} \frac{\partial f}{\partial z} \tag{10.2}
\end{equation*}
$$

- The Laplace operator of a scalar function:

$$
\begin{equation*}
\nabla^{2} f=\frac{1}{\rho} \frac{\partial}{\partial \rho}\left(\rho \frac{\partial f}{\partial \rho}\right)+\frac{1}{\rho^{2}} \frac{\partial^{2} f}{\partial \varphi^{2}}+\frac{\partial^{2} f}{\partial z^{2}}, \tag{10.3}
\end{equation*}
$$

- Divergence of a vector function of coordinates ( $\mathbf{f}=\mathbf{n}_{\rho} f_{\rho}+\mathbf{n}_{\varphi} f_{\varphi}+\mathbf{n}_{z} f_{z}$ ):

$$
\begin{equation*}
\nabla \cdot \mathbf{f}=\frac{1}{\rho} \frac{\partial\left(\rho f_{\rho}\right)}{\partial \rho}+\frac{1}{\rho} \frac{\partial f_{\varphi}}{\partial \varphi}+\frac{\partial f_{z}}{\partial z} . \tag{10.4}
\end{equation*}
$$

[^961]- Curl of a vector function:

$$
\begin{equation*}
\nabla \times \mathbf{f}=\mathbf{n}_{\rho}\left(\frac{1}{\rho} \frac{\partial f_{z}}{\partial \varphi}-\frac{\partial f_{\varphi}}{\partial z}\right)+\mathbf{n}_{\varphi}\left(\frac{\partial f_{\rho}}{\partial z}-\frac{\partial f_{z}}{\partial \rho}\right)+\mathbf{n}_{z} \frac{1}{\rho}\left(\frac{\partial\left(\rho f_{\varphi}\right)}{\partial \rho}-\frac{\partial f_{\rho}}{\partial \varphi}\right) \tag{10.5}
\end{equation*}
$$

- The Laplace operator of a vector function:

$$
\begin{equation*}
\nabla^{2} \mathbf{f}=\mathbf{n}_{\rho}\left(\nabla^{2} f_{\rho}-\frac{1}{\rho^{2}} f_{\rho}-\frac{2}{\rho^{2}} \frac{\partial f_{\varphi}}{\partial \varphi}\right)+\mathbf{n}_{\varphi}\left(\nabla^{2} f_{\varphi}-\frac{1}{\rho^{2}} f_{\varphi}+\frac{2}{\rho^{2}} \frac{\partial f_{\rho}}{\partial \varphi}\right)+\mathbf{n}_{z} \nabla^{2} f_{z} \tag{10.6}
\end{equation*}
$$

(ii) Spherical coordinates $\{r, \theta, \varphi\}$ (see Fig. below) may be defined as:


- Gradient of a scalar function:

$$
\begin{equation*}
\nabla f=\mathbf{n}_{r} \frac{\partial f}{\partial r}+\mathbf{n}_{\theta} \frac{1}{r} \frac{\partial f}{\partial \theta}+\mathbf{n}_{\varphi} \frac{1}{r \sin \theta} \frac{\partial f}{\partial \varphi} . \tag{10.8}
\end{equation*}
$$

- The Laplace operator of a scalar function:

$$
\begin{equation*}
\nabla^{2} f=\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial f}{\partial r}\right)+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial f}{\partial \theta}\right)+\frac{1}{(r \sin \theta)^{2}} \frac{\partial^{2} f}{\partial \varphi^{2}} \tag{10.9}
\end{equation*}
$$

- Divergence of a vector function $\mathbf{f}=\mathbf{n}_{r} f_{r}+\mathbf{n}_{\theta} f_{\theta}+\mathbf{n}_{\varphi} f_{\varphi}$ :

$$
\begin{equation*}
\nabla \cdot \mathbf{f}=\frac{1}{r^{2}} \frac{\partial\left(r^{2} f_{r}\right)}{\partial r}+\frac{1}{r \sin \theta} \frac{\partial\left(f_{\theta} \sin \theta\right)}{\partial \theta}+\frac{1}{r \sin \theta} \frac{\partial f_{\varphi}}{\partial \varphi} . \tag{10.10}
\end{equation*}
$$

- Curl of a similar vector function:

$$
\begin{equation*}
\nabla \times \mathbf{f}=\mathbf{n}_{r} \frac{1}{r \sin \theta}\left(\frac{\partial\left(f_{\varphi} \sin \theta\right)}{\partial \theta}-\frac{\partial f_{\theta}}{\partial \varphi}\right)+\mathbf{n}_{\theta} \frac{1}{r}\left(\frac{1}{\sin \theta} \frac{\partial f_{r}}{\partial \varphi}-\frac{\partial\left(r f_{\varphi}\right)}{\partial r}\right)+\mathbf{n}_{\varphi} \frac{1}{r}\left(\frac{\partial\left(r f_{\theta}\right)}{\partial r}-\frac{\partial f_{r}}{\partial \theta}\right) \tag{10.11}
\end{equation*}
$$

- The Laplace operator of a vector function:

$$
\begin{align*}
\nabla^{2} \mathbf{f} & =\mathbf{n}_{r}\left(\nabla^{2} f_{r}-\frac{2}{r^{2}} f_{r}-\frac{2}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(f_{\theta} \sin \theta\right)-\frac{2}{r^{2} \sin \theta} \frac{\partial f_{\varphi}}{\partial \varphi}\right) \\
& +\mathbf{n}_{\theta}\left(\nabla^{2} f_{\theta}-\frac{1}{r^{2} \sin ^{2} \theta} f_{\theta}+\frac{2}{r^{2}} \frac{\partial f_{r}}{\partial \theta}-\frac{2 \cos \theta}{r^{2} \sin ^{2} \theta} \frac{\partial f_{\varphi}}{\partial \varphi}\right)  \tag{10.12}\\
& +\mathbf{n}_{\varphi}\left(\nabla^{2} f_{\varphi}-\frac{1}{r^{2} \sin ^{2} \theta} f_{\varphi}+\frac{2}{r^{2} \sin \theta} \frac{\partial f_{r}}{\partial \varphi}+\frac{2 \cos \theta}{r^{2} \sin ^{2} \theta} \frac{\partial f_{\theta}}{\partial \varphi}\right) .
\end{align*}
$$

## 11. Products involving $\nabla$

(i) Useful zeros:

- For any scalar function $f(\mathbf{r})$,

$$
\begin{equation*}
\nabla \times(\nabla f) \equiv \operatorname{curl}(\operatorname{grad} f)=0 \tag{11.1}
\end{equation*}
$$

- For any vector function $\mathbf{f}(\mathbf{r})$,

$$
\begin{equation*}
\nabla \cdot(\nabla \times \mathbf{f}) \equiv \operatorname{div}(\text { curl } \mathbf{f})=0 . \tag{11.2}
\end{equation*}
$$

(ii) Laplace operator expressed via the curl of a curl:

$$
\begin{equation*}
\nabla^{2} \mathbf{f}=\nabla(\nabla \cdot \mathbf{f})-\nabla \times(\nabla \times \mathbf{f}) \tag{11.3}
\end{equation*}
$$

(iii) Spatial differentiation of a product of a scalar function by a vector function:

- The scalar 3D generalization of Eq. (4.1) is

$$
\begin{equation*}
\nabla \cdot(f \mathbf{g})=(\nabla f) \cdot \mathbf{g}+f(\nabla \cdot \mathbf{g}) . \tag{11.4a}
\end{equation*}
$$

- Its vector generalization is similar:

$$
\begin{equation*}
\nabla \times(f \mathbf{g})=(\nabla f) \times \mathbf{g}+f(\nabla \times \mathbf{g}) . \tag{11.4b}
\end{equation*}
$$

(iv) 3 D spatial differentiation of products of two vector functions:

$$
\begin{gather*}
\nabla \times(\mathbf{f} \times \mathbf{g})=\mathbf{f}(\nabla \cdot \mathbf{g})-(\mathbf{f} \cdot \nabla) \mathbf{g}-(\nabla \cdot \mathbf{f}) \mathbf{g}+(\mathbf{g} \cdot \nabla) \mathbf{f},  \tag{11.5}\\
\nabla(\mathbf{f} \cdot \mathbf{g})=(\mathbf{f} \cdot \nabla) \mathbf{g}+(\mathbf{g} \cdot \nabla) \mathbf{f}+\mathbf{f} \times(\nabla \times \mathbf{g})+\mathbf{g} \times(\nabla \times \mathbf{f}),  \tag{11.6}\\
\nabla \cdot(\mathbf{f} \times \mathbf{g})=\mathbf{g} \cdot(\nabla \times \mathbf{f})-\mathbf{f} \cdot(\nabla \times \mathbf{g}) . \tag{11.7}
\end{gather*}
$$

## 12. Integro-differential relations

(i) For an arbitrary surface $S$ limited by closed contour $C$ :

- The Stokes theorem, valid for any differentiable vector field $\mathbf{f}(\mathbf{r})$ :

$$
\begin{equation*}
\int_{S}(\nabla \times \mathbf{f}) \cdot d^{2} \mathbf{r} \equiv \int_{S}(\nabla \times \mathbf{f})_{n} d^{2} r=\oint_{C} \mathbf{f} \cdot d \mathbf{r} \equiv \oint_{C} f_{\tau} d r, \tag{12.1}
\end{equation*}
$$

where $d^{2} \mathbf{r} \equiv \mathbf{n} d^{2} r$ is the elementary area vector (normal to the surface), and $d \mathbf{r}$ is the elementary contour length vector (tangential to the contour line).
(ii) For an arbitrary volume $V$ limited by closed surface $S$ :

- Divergence (or "Gauss") theorem, valid for any differentiable vector field $\mathbf{f}(\mathbf{r})$ :

$$
\begin{equation*}
\int_{V}(\nabla \cdot \mathbf{f}) d^{3} r=\oint_{S} \mathbf{f} \cdot d^{2} \mathbf{r} \equiv \oint_{S} f_{n} d^{2} r . \tag{12.2}
\end{equation*}
$$

- Green's theorem, valid for two differentiable scalar functions $f(\mathbf{r})$ and $g(\mathbf{r})$ :

$$
\begin{equation*}
\int_{V}\left(f \nabla^{2} g-g \nabla^{2} f\right) d^{3} r=\oint_{S}(f \nabla g-g \nabla f)_{n} d^{2} r \tag{12.3}
\end{equation*}
$$

- An identity valid for any two scalar functions $f$ and $g$, and a vector field $\mathbf{j}$ with $\nabla \cdot \mathbf{j}=0$ (all differentiable):

$$
\begin{equation*}
\int_{V}[f(\mathbf{j} \cdot \nabla g)+g(\mathbf{j} \cdot \nabla f)] d^{3} r=\oint_{S} f g j_{n} d^{2} r \tag{12.3}
\end{equation*}
$$

## 13. The Kronecker delta and Levi-Civita permutation symbols

- The Kronecker delta symbol (defined for integer indices):

$$
\delta_{i j^{\prime}} \equiv\left\{\begin{array}{lc}
1, & \text { if } j^{\prime}=j  \tag{13.1}\\
0, & \text { otherwise } .
\end{array}\right.
$$

- The Levi-Civita permutation symbol (most frequently used for 3 integer indices, each taking one of values 1 , 2 , or 3 ):

$$
\varepsilon_{i j^{\prime} j "} \equiv\left\{\begin{array}{lc}
+1, & \text { if the indices follow in the "correct"("even") order : } 1 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 2 \ldots,  \tag{13.2}\\
-1, & \text { if the indices follow in the "incorrect"("odd") order }: 1 \rightarrow 3 \rightarrow 2 \rightarrow 1 \rightarrow 3 \ldots, \\
0, & \text { if any two indices coincide. }
\end{array}\right.
$$

- Relation between the Levi-Civita and the Kronecker delta products:

$$
\varepsilon_{i j j^{\prime \prime}} \varepsilon_{k k^{\prime} k^{\prime \prime}}=\sum_{l, l^{\prime}, l^{\prime \prime}=1}^{3}\left|\begin{array}{lll}
\delta_{j l} & \delta_{j l^{\prime}} & \delta_{j l^{\prime \prime}}  \tag{13.3a}\\
\delta_{j^{\prime} l} & \delta_{j^{\prime} l^{\prime}} & \delta_{j^{\prime \prime \prime} l^{\prime \prime}} \\
\delta_{j^{\prime \prime} l} & \delta_{j^{\prime \prime \prime} l^{\prime}} & \delta_{j^{\prime \prime} l^{\prime \prime}}
\end{array}\right| ;
$$

summation of this relation, written for 3 different values of $j=k$, over these values yields the so-called contracted epsilon identity:

$$
\begin{equation*}
\sum_{j=1}^{3} \varepsilon_{j j j^{\prime} \xi^{\prime}} \varepsilon_{j k^{\prime} k^{\prime \prime}}=\delta_{j^{\prime} k^{\prime}} \delta_{j^{\prime \prime} k^{\prime \prime}}-\delta_{j^{\prime} k^{\prime \prime}} \delta_{j^{\prime \prime} k^{\prime}} \tag{13.3b}
\end{equation*}
$$

## 14. Dirac's delta-function, sign function, and theta-function

- Definition of 1D delta-function (for real $a<b$ ):

$$
\int_{a}^{b} f(\xi) \delta(\xi) d \xi=\left\{\begin{array}{c}
f(0), \quad \text { if } a<0<b  \tag{14.1}\\
0, \\
\text { otherwise }
\end{array}\right.
$$

where $f(\xi$ ) is any function continuous near $\xi=0$. In particular (if $f(\xi)=1$ near $\xi=0$ ), the definition yields

$$
\int_{a}^{b} \delta(\xi) d \xi=\left\{\begin{array}{cc}
1, & \text { if } a<0<b  \tag{14.2}\\
0, & \text { otherwise }
\end{array}\right.
$$

- Relation to the theta-function $\theta(\xi)$ and sign function $\operatorname{sgn}(\xi)$

$$
\begin{equation*}
\delta(\xi)=\frac{d}{d \xi} \theta(\zeta)=\frac{1}{2} \frac{d}{d \xi} \operatorname{sgn}(\xi), \tag{14.3a}
\end{equation*}
$$

where

$$
\theta(\xi) \equiv \frac{\operatorname{sgn}(\xi)+1}{2}=\left\{\begin{array}{ll}
0, & \text { if } \xi<0,  \tag{14.3b}\\
1, & \text { if } \xi>1,
\end{array} \quad \operatorname{sgn}(\xi) \equiv \frac{\xi}{|\xi|}= \begin{cases}-1, & \text { if } \xi<0 \\
+1, & \text { if } \xi>1\end{cases}\right.
$$

- An important integral: ${ }^{13}$

$$
\begin{equation*}
\int_{-\infty}^{+\infty} e^{i s \xi} d s=2 \pi \delta(\xi) \tag{14.4}
\end{equation*}
$$

- 3D generalization of the delta-function of the radius-vector (the 2D generalization is similar):

$$
\int_{V} f(\mathbf{r}) \delta(\mathbf{r}) d^{3} r=\left\{\begin{array}{c}
f(0), \quad \text { if } 0 \in V  \tag{14.5}\\
0, \quad \text { otherwise }
\end{array}\right.
$$

it may be presented as a product of 1D delta-functions of Cartesian coordinates:

$$
\begin{equation*}
\delta(\mathbf{r})=\delta\left(r_{1}\right) \delta\left(r_{2}\right) \delta\left(r_{3}\right) \tag{14.6}
\end{equation*}
$$

## 15. The Cauchy theorem and integral

Let a complex function $\boldsymbol{f}(\boldsymbol{z})$ be analytic within a part of the complex plane $\boldsymbol{z}$, that is limited by a closed contour $C$ and includes point $\boldsymbol{z}^{\prime}$. Then

$$
\begin{gather*}
\oint_{C} \boldsymbol{f}(\boldsymbol{z}) d \boldsymbol{z}=0,  \tag{15.1}\\
\oint_{C} \boldsymbol{f}(\boldsymbol{z}) \frac{d \boldsymbol{z}}{\boldsymbol{z}-\boldsymbol{z}^{\prime}}=2 \pi i \boldsymbol{f}\left(\boldsymbol{z}^{\prime}\right) . \tag{15.2}
\end{gather*}
$$

The first of these relations is usually called the Cauchy integral theorem (or the "CauchyGoursat theorem"), and the second one - the Cauchy integral (or the "Cauchy integral formula").

## 16. References

(i) Properties of some special functions are briefly discussed at the relevant points of the lecture notes; in the alphabetical order:

- Airy functions: QM Sec. 2.4;
- Bessel functions: EM Sec. 2.5;
- Fresnel integrals: EM Sec. 8.6;

[^962]- Hermite polynomials: QM Sec. 2.10;
- Laguerre polynomials (both simple and associated): QM Sec. 3.6;
- Legendre polynomials, associated Legendre functions: EM Sec. 2.5 and QM Sec. 3.6;
- Spherical harmonics: QM Sec. 3.6;
- Spherical Bessel functions: QM Secs. 3.6.
(ii) For more formulas, and their discussions, I can recommend the following handbooks (in the alphabetical order): ${ }^{14}$
- M. Abramowitz and I. Stegun (eds.), Handbook of Mathematical Formulas, Dover, 1965 (and numerous later printings); ${ }^{15}$
- I. Gradshteyn and I. Ryzhik, Tables of Integrals, Series, and Products, $5^{\text {th }}$ ed., Acad. Press, 1980;
- G. Korn and T. Korn, Mathematical Handbook for Scientists and Engineers, $2^{\text {nd }}$ ed., Dover, 2000;
- A. Prudnikov et al., Integrals and Series, vols. 1 and 2, CRC Press, 1986.

A popular textbook,

- G. Arfken et al., Mathematical Methods for Physicists, $7^{\text {th }}$ ed., Acad. Press, 2012, may be also used as a formula manual.

Many formulas are also available from the symbolic calculation parts of commercially available software packages listed in Sec. (iv) below.
(iii) Probably the most popular collection of numerical calculation codes are the twin manuals

- W. Press et al., Numerical Recipes in Fortran 77, $2^{\text {nd }}$ ed., Cambridge U. Press, 1992;
- W. Press et al., Numerical Recipes [in C++ - KKL], $3^{\text {rd }}$ ed., Cambridge U. Press, 2007.

My lecture notes include very brief introductions into numerical methods of differential equation solution:

- ordinary differential equations: CM Sec. 3.9, and
- partial differential equations: CM Sec. 8.5 and EM Sec. 2.8,
which include references to literature for further reading.
(iv) The most popular software packages for numerical and symbolic calculations, all with plotting capabilities (in the alphabetical order):
- Maple (http://www.maplesoft.com/);
- MathCAD (http://www.ptc.com/products/mathcad/);
- Mathematica (http://www.wolfram.com/products/mathematica/index.html);
- MATLAB (http://www.mathworks.com/products/matlab/).

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## Lecture Notes and Problems

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Appendix CA

## Selected Physical Constants

| Symbol | Quantity | SI value <br> and unit | Gaussian value <br> and unit | Relative r.m.s. <br> uncertainty |
| :---: | :---: | :---: | :---: | :---: |
| $c$ | speed of light <br> in free space | $2.99792458 \times 10^{8}$ <br> $\mathrm{~m} / \mathrm{s}$ | $2.99792458 \times 10^{10}$ <br> $\mathrm{~cm} / \mathrm{s}$ | 0 <br> (defined value) |
| $G$ | gravitation <br> constant | $6.6741 \times 10^{-11}$ <br> $\mathrm{~m}^{3} /{\mathrm{kg} \cdot \mathrm{s}^{2}}^{2}$ | $6.6741 \times 10^{-8}$ <br> $\mathrm{~cm}^{3} / \mathrm{g} \cdot \mathrm{s}^{2}$ | $\sim 5 \times 10^{-5}$ |
| $\hbar$ | Planck <br> constant | $1.05457180 \times 10^{-34}$ <br> $\mathrm{~J} \cdot \mathrm{~s}$ | $1.05457180 \times 10^{-27}$ <br> $\mathrm{erg} \cdot \mathrm{s}$ | $\sim 1 \times 10^{-8}$ |
| $e$ | elementary <br> electric charge | $1.6021762 \times 10^{-19}$ <br> C | $4.803203 \times 10^{-10}$ <br> statcoulomb | $\sim 6 \times 10^{-9}$ |
| $m_{e}$ | electron's rest <br> mass | $0.91093835 \times 10^{-30}$ <br> kg | $0.91093835 \times 10^{-27}$ <br> g | $\sim 1 \times 10^{-8}$ |
| $m_{p}$ | proton's rest <br> mass | $1.67262190 \times 10^{-27}$ <br> kg | $1.67262190 \times 10^{-24}$ <br> g | $\sim 1 \times 10^{-8}$ |
| $\mu_{0}$ | magnetic <br> constant | $4 \pi \times 10^{-7}$ <br> $\mathrm{~N} / \mathrm{A}^{2}$ | - | 0 |
| $\varepsilon_{0}$ | electric <br> constant | $8.854187817 \times 10^{-12}$ <br> $\mathrm{~F} / \mathrm{m}$ | - | 0 <br> $($ defined value) |
| $k_{\mathrm{B}}$ | Boltzmann <br> constant | $1.380649 \times 10^{-23}$ <br> $\mathrm{~J} / \mathrm{K}$ | $1.380649 \times 10^{-16}$ <br> $\mathrm{erg} / \mathrm{K}$ | $($ defined value) |

[^964]
## Comments:

1. The fixed value of $c$ was defined by an international convention in 1983, in order to extend the official definition of a second (as "the duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 atom") to that of a meter. The values are back-compatible with the legacy definitions of the meter (initially, as the $1 / 40,000,000$-th part of the Earth meridian length) and the second (for a long time, as the $1 /(24 \times 60 \times 60)$ $=1 / 86,400-$ th part of the Earth rotation period), within the experimental errors of those measures.
2. $\varepsilon_{0}$ and $\mu_{0}$ are not really the fundamental constants; in the SI system of units one of them (say, $\left.\mu_{0}\right)$ is selected arbitrarily, ${ }^{2}$ while the other one is defined via relation $\varepsilon_{0} \mu_{0}=1 / \mathrm{c}^{2}$.
3. The Boltzmann constant $k_{\mathrm{B}}$ is also not quite fundamental, because its only role is to comply with the independent definition of the kelvin $(\mathrm{K})$, as the temperature unit in which the triple point of water is exactly 273.16 K . If temperature is expressed in energy units $k_{\mathrm{B}} T$ (as is done, for example, in the SM part of this lecture note series), this constant disappears altogether.
4. The dimensionless fine structure ("Sommerfeld' s") constant $\alpha$ is numerically the same in any system of units:

$$
\alpha \equiv\left\{\begin{array}{c}
e^{2} / 4 \pi \varepsilon_{0} \hbar c \quad \text { in SI units } \\
e^{2} / \hbar c \quad \text { in Gaussian units }
\end{array}\right\} \approx 7.297352566 \times 10^{-3} \approx \frac{1}{137.03599914},
$$

and is known with a much smaller r.m.s. uncertainty $\left(\sim 3 \times 10^{-10}\right)$ than that of the component constants.

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(a partial list of textbooks and monographs used at work on the series ${ }^{1}$ )

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[^0]:    ${ }^{1}$ To the best of author's knowledge, the fair use clause of the U.S. copyright law (see, e.g., http://www.copyright.gov/fls/fl102.html) allows viewing, browsing and/or downloading copyrighted materials for temporary, non-commercial, personal purposes, without requesting copyright holder's permission.

[^1]:    ${ }^{2}$ The texts are saved as separate .pdf files of each chapter, optimized for two-page viewing and double-side printing; merged files for each part and the series as a whole, convenient for search purposes, are also provided.
    ${ }^{3}$ To list just a few: statics and dynamics of elastic and fluid continua, basic notions of physical kinetics, turbulence and deterministic chaos, physics of reversible and quantum computation, relaxation and dephasing of open quantum systems, the van der Pol method, a.k.a. the Rotating-Wave Approximation (RWA), in classical and quantum mechanics, physics of electrons and holes in semiconductors, weak-potential and tight-binding approximations in the energy band theory, optical fiber electrodynamics, macroscopic quantum effects in Bose-

[^2]:    Einstein condensates, Bloch oscillations and Landau-Zener tunneling, cavity QED, and the Density Functional Theory (DFT). All these topics are discussed, if only concisely, in these notes.
    ${ }^{4}$ Recently several high-quality, graduate-level teaching materials became freely available online, including R. Fitzpatrick's text on Classical Electromagnetism (farside.ph.utexas.edu/teaching/jk1/Electromagnetism.pdf), B. Simons' "lecture shrunks" on Advanced Quantum Mechanics (www.tcm.phy.cam.ac.uk/~bds10/aqp.html), and D. Tong's lecture notes on several topics (www.damtp.cam.ac.uk/user/tong/teaching.html).
    ${ }^{5}$ The problems that require either more bulky calculations, or more creative approaches (or both :-), are marked by asterisks.
    ${ }^{6}$ For an introduction to the subject, I can recommend either a review by S. Carroll, Spacetime and Geometry, Addison-Wesley, 2003, or a longer text by A. Zee, Einstein Gravity in a Nutshell, Princeton U. Press, 2013.
    ${ }^{7}$ Note added in June 2019: Revised versions of these lecture notes, and of model solutions of the exercise problems, are now published by the IOP - see the references on the title page of each part. However, in the view of possible future editions, the kind request formulated above remains very much valid.

[^3]:    ${ }^{8}$ Yes Virginia, these notes represent only my personal opinions, not necessarily those of the Department of Physics and Astronomy of Stony Brook University, the SBU at large, the SUNY system, the Empire State of New York, the federal agencies and private companies that funded my group's research, etc. No dear, I cannot be hold responsible for any harm, either bodily or mental, their reading may (?) cause.

[^4]:    ${ }^{9}$ I am very much sorry that I have not kept proper records from the beginning of my lectures at Stony Brook, so I cannot list all the numerous students and TAs who had kindly attracted my attention to typos in earlier versions of these notes. Needless to say, I am very grateful to them all as well.

[^5]:    ${ }^{10}$ The same letter, typeset in different fonts, typically denotes different variables.

[^6]:    ${ }^{1}$ The reader is advised to perform a self-check by solving a few problems of the dozen listed in Sec. 1.7. If the results are not satisfactory, it may make sense to start from some remedial reading. For that, I could recommend, for example (in the alphabetical order): G. R. Fowles and G. L. Cassiday, Analytical Mechanics, $7^{\text {th }}$ ed., Brooks Cole, 2004; K. R. Symon, Mechanics, $3^{\text {rd }}$ ed., Addison-Wesley, 1971; or J. B. Marion and S. T. Thornton, Classical Dynamics of Particles and Systems, $4^{\text {th }}$ ed., Saunders, 1995.
    ${ }^{2}$ This series assumes reader's familiarity with the basic calculus and vector algebra. The formulas most important for this series are listed in the Selected Mathematical Formulas appendix, referred below as MA. In particular, a reminder of the definition and the basic properties of the Laplace operator may be found in MA Sec. 9 .

[^7]:    ${ }^{7}$ Following tradition, an introduction to special relativity is included into the Classical Electrodynamics ("EM") part of these notes. The relativistic effects are small if all particles velocities are much lower than the speed of light, $c \approx 3.00 \times 10^{8} \mathrm{~m} / \mathrm{s}$, and all distances are much larger then the system's Schwarzschild radius $r_{s} \equiv 2 \mathrm{Gm} / \mathrm{c}^{2}$, where $G \approx 6.67 \times 10^{-11}$ SI units ( $\mathrm{m}^{3} / \mathrm{kg} \cdot \mathrm{s}$ ) is the Newtonian gravity constant, and $m$ is system's mass. (More exact values of $c, G$, and some other physical constants may be found in appendix CA: Selected Physical Constants.)

[^8]:    ${ }^{8}$ This approximation is legitimate, crudely, when the product of the coordinate and momentum scales of the particle motion is much larger than the Planck's constant $\hbar \approx 1.054 \times 10^{-34} \mathrm{~J}$ •s. A more exact formulation may be found, e.g., in the Quantum Mechanics ("QM") part of these note series.
    ${ }^{9}$ Due to the genius of Sir Isaac Newton, these laws were formulated as early as in 1687, far ahead of the science of that time.
    ${ }^{10}$ Some laws of Nature (including the Newton laws) may be derived from certain more general postulates, such as the Hamilton (or "least action") principle - see Sec. 10.2 below. Note, however, that such derivations are only acceptable because all known corollaries of the postulates comply with all known experimental results.

[^9]:    ${ }^{11}$ Of course, for composite bodies of varying mass (e.g., rockets emitting jets, see Problem 11), momentum's derivative may differ from ma.

[^10]:    12 Note that the fact that the masses participating in Eqs. (14) and (16) are equal, the so-called weak equivalence principle, is highly nontrivial, but has been verified experimentally to the relative accuracy of at least $10^{-13}$. Due to its conceptual significance of the principle, new space experiments, such as MISCROSCOPE (http://smsc.cnes.fr/MICROSCOPE/), are being planned for a substantial, nearly 100 -fold accuracy improvement.
    ${ }^{13}$ Of course, the most important particular case of Eq. (1.16b) is the motion of objects near Earth's surface. In this case, using the fact that (1.16a) remains valid for the gravity field created by a heavy sphere, we get $g=G M_{\mathrm{E}} / R_{\mathrm{E}}^{2}$, where $M_{\mathrm{E}}$ and $R_{\mathrm{E}}$ are the Earth mass and radius. Plugging in their values, $M_{\mathrm{E}} \approx 5.97 \times 10^{24} \mathrm{~kg}, R_{\mathrm{E}} \approx 6.37 \times 10^{6} \mathrm{~m}$, we get $g \approx 9.82 \mathrm{~m} / \mathrm{s}^{2}$. The effective value of $g$ varies from 9.78 to $9.83 \mathrm{~m} / \mathrm{s}^{2}$ at various locations on Earth's surface (due to the deviations of Earth's shape from a sphere, and the location-dependent effect of the centrifugal "inertial force" - see Sec. 6.5 below), with an average value of $g \approx 9.807 \mathrm{~m} / \mathrm{s}^{2}$.

[^11]:    ${ }^{14}$ Symbol a.b denotes the scalar (or "dot-") product of vectors a and b-see, e.g., MA Eq. (7.1).
    ${ }^{15}$ Note that because of its definition via the gradient, the potential energy is only defined to an arbitrary additive constant.
    ${ }^{16}$ Its basic properties are listed in MA Sec. 8.

[^12]:    Total mechanical energy

    Mechanical energy conservation

[^13]:    ${ }^{18}$ Here we imply that the internal motions of the particle, including its rotation about its own axis, are negligible. (Otherwise it could not be represented by a geometrical point, as was postulated in Sec. 1.) For a body with substantial rotation (see Chapter 6 below), vector $\mathbf{L}$ retains its definition (32), but is only a part of the total angular momentum and is called the orbital momentum - even if the particle does not move along a closed orbit. ${ }^{19}$ See, e.g., MA Eq. (7.3).

[^14]:    ${ }^{20}$ Assuming that the additional, non-conservative forces (such as viscosity) responsible for the mechanical energy drain, vanish at equilibrium - as they typically do. (Static friction is one counter-example.)

[^15]:    ${ }^{21}$ Physically, the difference $U_{\mathrm{G}}-U$ specified by Eq. (39) may be considered the r-dependent part of the potential energy $U^{\text {(ext) }}$ of the external system responsible for the force $\mathbf{F}^{(\text {ext })}$, so that $U_{\mathrm{G}}$ is just the total potential energy $U+$ $U^{\text {(ext) }}$, besides the part of $U^{(\text {ext })}$ which does not depend on $\mathbf{r}$ and hence is irrelevant for the fixed point analysis. According to the $3^{\text {rd }}$ Newton law, the force exerted by the particle on the external system equals ( $-\mathbf{F}^{(\mathrm{ext})}$ ), so that its work (and hence the change of $U^{(\text {ext })}$ due to the change of $\mathbf{r}$ ) is given by the second term in the right-hand part of Eq. (39). Thus the condition of equilibrium, $-\nabla U_{\mathrm{G}}=0$, is just the condition of an extremum of the total potential energy, $U+U^{(e x t)}$, of the two interacting systems.
    ${ }^{22}$ Unfortunately, in most physics teaching plans the introduction of $U_{\mathrm{G}}$ is postponed until a course of statistical mechanics and/or thermodynamics - where it is a part of the Gibbs free energy, in contrast to $U$, which is a part of the Helmholtz free energy - see, e.g., Sec. 1.4 of the Statistical Mechanics ("SM") part of my notes. However, the reader should agree that the difference between $U_{\mathrm{G}}$ and $U$, and hence that between the Gibbs and Helmholtz free energies, has nothing to do with statistics or thermal motion, and belongs to the basic mechanics.
    ${ }^{23}$ This is essentially a simplified model of the famous mechanical control device called the centrifugal (or "flyball, or "centrifugal flyball") governor - see, e.g., http://en.wikipedia.org/wiki/Centrifugal governor.

[^16]:    24 It was first stated by R. Clausius in 1870.

[^17]:    ${ }^{1}$ Possibly, the simplest example of a non-holonomic constraint is a set of inequalities describing the hard walls confining the motion of particles in a closed volume. Non-holonomic constraints are better dealt with other methods, e.g., by imposing proper boundary conditions on the (otherwise unconstrained) motion.
    ${ }^{2}$ See, e.g., MA Eq. (10.7).

[^18]:    ${ }^{3}$ For a concise introduction to the field see, e.g., I. Gelfand and S. Fomin, Calculus of Variations, Dover, 2000 or L. Elsgolc, Calculus of Variations, Dover, 2007. An even shorter review may be found in Chapter 17 of Arfken and Weber - see MA Sec. 16. For a more detailed discussion, using many examples from physics, see R. Weinstock, Calculus of Variations, Dover, 2007.
    ${ }^{4}$ See, e.g., MA Eq. (4.2). In all formulas of this section, all summations over index $j$ are from 1 to $J$, while those over the particle number $k$ are from 1 to $N$.

[^19]:    ${ }^{5}$ It had been spelled out in a 1743 work by J.-B. le Rond d'Alembert, though the core of this result has been traced to an earlier work by J. Bernoulli (1667-1748).
    ${ }^{6}$ Note that since the dimensionality of generalized coordinates may be arbitrary, that of generalized forces may also differ from the newton.

[^20]:    ${ }^{7}$ They were derived in 1788 by J.-L. Lagrange who pioneered the whole field of analytical mechanics - not to mention his key contributions to number theory and celestial mechanics.

[^21]:    ${ }^{8}$ Note that due to the possible time dependence of $U$, Eq. (17) does not mean that forces $\mathbf{F}_{k}$ have to be conservative - see the next section for more discussion. With this understanding, I will still use for function $U$ the convenient name of "potential energy".

[^22]:    ${ }^{9}$ This expression for $T \equiv(m / 2)\left(\dot{x}^{2}+\dot{y}^{2}+\dot{z}^{2}\right)$ may be readily obtained either by the formal differentiation of Eq. (2) over time, or just by noticing that the velocity vector has two perpendicular components: one along the ring (with magnitude $R \dot{\theta}$ ) and another one normal to the ring plane (with magnitude $\omega \rho=\omega R \sin \theta$ - see Fig. 1).
    ${ }^{10}$ Let me hope that this traditional notation would not lead to the confusion between the inductance and the Lagrange function.

[^23]:    ${ }^{11}$ See, e.g., EM Sec. 9.8.

[^24]:    ${ }^{13}$ This is just one of many theorems bearing the name of the mathematics genius L. Euler (1707-1783).
    ${ }^{14}$ Such functions are called quadratic-homogeneous.

[^25]:    ${ }^{15}$ Such coordinates are frequently called cyclic, because in some cases (like in the second example considered below) they represent periodic coordinates such as angles. However, this terminology is misleading, because some "cyclic" coordinates (e.g., $x$ in our first example) have nothing to do with rotation.
    ${ }^{16}$ This fact may be considered a particular case of a more general mathematical statement called the Noether theorem (named after its author, A. E. Nöther, sometimes called the "greatest woman mathematician ever lived"). For its discussion see, e.g., Sec. 13.7 in H. Goldstein et al., Classical Mechanics, $3^{\text {rd }}$ ed. Addison Wesley, 2002.
    ${ }^{17}$ Note that here $\dot{r}^{2}$ is just the square of the scalar derivative $\dot{r}$, rather than the square of vector $\dot{\mathbf{r}}=\mathbf{v}$.

[^26]:    ${ }^{18}$ More discussion of the Josephson effect and the physical sense of the variable $\varphi$ may be found, for example, in EM Sec. 6.4 and QM Secs. 2.3 and 2.8 of this lecture note series.

[^27]:    ${ }^{1}$ Those terms may be important only in the very special case then $\kappa_{\text {ef }}$ is exactly zero, i.e. when a fixed point is an inflection point of function $U_{\text {ef }}(q)$.
    ${ }^{2}$ In what follows, I will assume that the effective mass $m_{\text {ef }}$ is positive, which is true in most (but not all!) dynamic systems. The changes necessary if it is negative are obvious.

[^28]:    ${ }^{3}$ Mathematically, the growing part vanishes at some special (exact) initial conditions which give $c_{+}=0$. However, the futility of this argument for real physical systems should be obvious for anybody who had ever tried to balance a pencil on its sharp point.
    ${ }^{4}$ Note that Eq. (19) coincides with Eq. (2.25). This is a good sanity check illustrating that the procedure (5)-(6) of moving of a term from the potential to kinetic energy within the Lagrangian function is indeed legitimate.
    ${ }^{5}$ For this particular problem, the values of $\theta$ that differ by a multiple of $2 \pi$, are physically equivalent.

[^29]:    ${ }^{6}$ See, e.g., MA Eqs. (5.2) and (5.3).

[^30]:    ${ }^{7}$ This terminology comes from quantum mechanics which shows that actually a particle (or rather its wavefunction) can, to a certain extent, penetrate the "classically forbidden range" where $H<U_{\text {ef }}(x)$.

[^31]:    ${ }^{11}$ Here index $z$ stands for the coordinate perpendicular to the motion plane. Since other components of the angular momentum are equal zero, the index is not really necessary, but I will still use it, just to make a clear distinction between the angular momentum $L_{z}$ and the Lagrangian function $L$.
    ${ }^{12}$ One of three laws deduced almost exactly 400 years ago by J. Kepler ( $1571-1630$ ), from the extremely detailed astronomical data collected by T. Brahe (1546-1601). In turn, the set of three Kepler laws were the main basis for Isaac Newton's discovery of the gravity law (1.16). That's how physics marched on...

[^32]:    ${ }^{13}$ One may claim that this fact should have been evident from the very beginning, because the effective particle of mass $m$ moves in a potential field $U(r)$ which conserves energy.
    ${ }^{14}$ Note that this reduction has been done in a way different from that used for our testbed problem (shown in Fig. 2.1) in Sec. 2 above. (The reader is encouraged to analyze this difference.) In order to emphasize this fact, I will keep writing $E$ instead of $H$ here, though for the planetary problem we are discussing now these two notions coincide.

[^33]:    ${ }^{15}$ In the opposite case when the interaction is repulsive, $U(r)>0$, the addition of the positive angular energy term only increases the trend, and only the scattering scenario is possible.

[^34]:    ${ }^{16}$ See, e.g., MA Eq. (6.3a).
    ${ }^{17}$ It may be proved that for the power-law interaction, $U \propto r^{\nu}$, the orbits are closed line only if $v=-1$ (i.e. our current case of the Coulomb potential) or $v=+2$ (the 3D harmonic oscillator) - the so-called Bertrand theorem.

[^35]:    ${ }^{18}$ Mathematicians prefer a more solemn terminology: parameter $2 p$ is called the latus rectum of the elliptic trajectory - see Fig. 7.
    ${ }^{19}$ In this figure, the constant participating in Eqs. (58)-(59) is assumed to be zero. It is evident that a different choice of the constant corresponds just to a constant turn of the ellipse about the origin.

[^36]:    20 The energy conservation law is frequently emphasized by calling this process elastic scattering.
    ${ }^{21}$ Indeed, at $r \gg b$, the definition $\mathbf{L}=\mathbf{r} \times(m \mathbf{v})$ yields $L_{z}=b m v_{\infty}$, where $v_{\infty}=(2 E / m)^{1 / 2}$ is the initial (and hence the final) velocity of the particle.

[^37]:    ${ }^{22}$ Alternatively, this result may be recovered directly from Eq. (59) whose parameters, at $E>0$, may be expressed via the same dimensionless parameter $(2 E b / \alpha): p=b(2 E b / \alpha), e=\left[1+(2 E b / \alpha)^{2}\right]^{1 / 2}>1$.
    ${ }^{23}$ This terminology stems from the fact that an integral of $d \sigma d \Omega$ over the full solid angle, called the full crosssection $\sigma$, has the dimension of area: $\sigma=N / n$, where $N$ is the total number of scattered particles.

[^38]:    ${ }^{24}$ This divergence, which persists at the quantum-mechanical treatment of the problem, is due to particles with large values of $b$, and disappears at an account, for example, of a finite concentration of the scattering centers.

[^39]:    ${ }^{25}$ Solving this problem is a very good preparation for the analysis of symmetric top rotation in Sec. 6.5.

[^40]:    ${ }^{26}$ It was not the first confirmation, though. The first one came 4 years earlier from A. Einstein himself, who showed that his theory may qualitatively explain the difference between the rate of Mercury orbit's precession, known from earlier observations, and the nonrelativistic theory of this effect.

[^41]:    ${ }^{3}$ Here I treat Eq. (5) as a phenomenological model, but in statistical mechanics such dissipative term may be derived as an average force exerted on a body by its environment whose numerous degrees of freedom are in random, though possibly thermodynamically-equilibrium states. Since such environmental force also has a random component, the dissipation is fundamentally related to fluctuations, and the latter effects may be neglected (as they are in this course) only if the oscillation energy is much higher than the energy scale of random fluctuations of the environment - in the thermal equilibrium at temperature $T$, the larger of $k_{\mathrm{B}} T$ and $\hbar \omega_{0} / 2$ - see, e.g., SM Chapter 5 and QM Chapter 7.
    ${ }^{4}$ Systems with very high damping ( $\delta>\omega_{0}$ ) can hardly be called oscillators, and though they are used in engineering and physics experiment (e.g., for the shock, vibration, and sound isolation), for their discussion I have to refer the interested reader to special literature - see, e.g., C. Harris and A. Piersol, Shock and Vibration Handbook, $5^{\text {th }}$ ed., McGraw Hill, 2002. Let me only note that at very high damping, $\delta \gg \omega_{0}$, the system may be adequately described with just one parameter: the relaxation time $1 / \lambda_{+} \approx 2 \delta / \omega_{0}^{2} \gg \omega_{0}$.

[^42]:    ${ }^{5}$ Operator Re, used in Eq. (3), may be dropped here, because for any physical (real) force, the imaginary components of the sum compensate each other. This imposes the following condition on the complex Fourier amplitudes: $f_{-\omega}=f_{\omega}{ }^{*}$, where the star means the complex conjugation.
    ${ }^{6}$ In physics, this mathematical property of linear equations is frequently called the linear superposition principle.

[^43]:    ${ }^{7}$ This is true for all systems in which $f(t)$ represents a cause, and $q(t)$ its effect. Following tradition, I discuss the frequency-domain expression of this causality relation (called the Kramers-Kronig relations) in the Classical Electrodynamics part of this lecture series - see EM Sec. 7.3.

[^44]:    ${ }^{8}$ This is a very unfortunate, but common jargon, meaning "the system described by linear equations of motion".
    ${ }^{9}$ For a reminder of the basic properties of the $\delta$-function, see MA Sec. 14.

[^45]:    ${ }^{10}$ The same result may be obtained from Eq. (28) with the response function $\chi(\omega)$ given by Eq. (19). This, more cumbersome, way is left for reader's exercise.

[^46]:    ${ }^{11}$ See, e.g., EM Sec. 2.7, and QM Sec. 2.2.
    ${ }^{12}$ Again, "nonlinear oscillations" is a generally accepted slang term for oscillations in systems described by nonlinear equations of motion.

[^47]:    ${ }^{13}$ The same flexible approach is necessary to approximations used in quantum mechanics. The method discussed here is close in spirit (but not identical) to the WKB approximation (see, e.g., QM Sec. 2.4) rather to the perturbation theory varieties (QM Ch. 6).
    ${ }^{14}$ In various texts, one can meet references to either the small parameter method or asymptotic methods. The list of scientists credited for the development of this method and its variations notably includes J. Poincaré, B. van der Pol, N. Krylov, N. Bogolyubov, and Yu. Mitroplolsky. Expression (41) itself is frequently called the RotatingWave Approximation - RWA. (The origin of the term will be discussed in Sec. 6 below.) In the view of the pioneering role of B. van der Pol in the development of this approach, in some older textbooks the rotating-wave approximation is called the "van der Pol method".
    ${ }^{15}$ This equation is frequently called the Duffing equation (or the equation of the Duffing oscillator), after G. Duffing who was the first one to carry out its (rather incomplete) analysis in 1918.

[^48]:    ${ }^{16}$ For a mathematically rigorous treatment of the higher approximations, see, e.g., Yu. Mitropolsky and N. Dao, Applied Asymptotic Methods in Nonlinear Oscillations, Springer, 2004. A more laymen (and somewhat verbose) discussion of various oscillatory phenomena may be found in the classical text A. Andronov, A. Vitt, and S. Khaikin, Theory of Oscillators, Dover, 2011.
    ${ }^{17}$ Using the second of Eqs. (44), cos $\omega t$ may be rewritten as $\cos (\Psi+\varphi) \equiv \cos \Psi \cos \varphi-\sin \Psi \sin \varphi$. Then using the trigonometric identity $\cos ^{3} \Psi=(3 / 4) \cos \Psi+(1 / 4) \cos 3 \Psi-$ see, e.g., MA Eq. (3.4) results in Eq. (46).

[^49]:    ${ }^{18}$ One may ask why cannot we stick to the just one, most compact, complex-amplitude form (57b) of the RWA equations. The main reason is that when function $f(q, \dot{q}, t)$ is nonlinear, we cannot replace its real arguments, such as $q=A \cos (\omega t-\varphi)$, with their complex-function representations like $a \exp \{-i \omega t\}$ (as could be done in the linear problems considered in Sec. 4.1), and need to use real variables, such as either $\{A, \varphi\}$ or $\{u, v\}$, anyway.

[^50]:    ${ }^{19}$ For that, one needs to use the trigonometric identity $\sin ^{3} \Psi=(3 / 4) \sin \Psi-(1 / 4) \sin 3 \Psi-$ see, e.g., MA Eq. (3.4).

[^51]:    ${ }^{20}$ Actually, this result should be evident, even without calculations, from the comparison of Eqs. (60) and (63).
    ${ }^{21}$ This equation is ubiquitous in phase locking systems, including even some digital electronic circuits used for that purpose.

[^52]:    22 A modulation of pendulum's mass (say, by periodic pumping water in and out of a suspended bottle) gives a qualitatively similar result. Note, however, that parametric oscillations cannot be excited by modulating any oscillator's parameter - for example, oscillator's damping coefficient (at least if it stays positive at all times), because its does not change system's energy, just the energy drain rate.

[^53]:    ${ }^{23}$ Such calculations may be substantially simplified by the use of the so-called Floquet theorem, which is also the mathematical basis for the discussion of wave propagation in periodic media - see the next chapter.
    ${ }^{24}$ This region describes, for example, the counter-intuitive stability of an inverted pendulum with the periodically modulated length, within a limited range of the modulation depth $\mu$.

[^54]:    ${ }^{25}$ Autonomous systems described by a single second-order differential equation, say $F(q, \dot{q}, \ddot{q})=0$, also belong to this class, because we may treat velocity $\dot{q} \equiv v$ as a new variable, and use this definition as one first-order differential equation, and the initial equation, in the form $F(q, v, \dot{v})=0$, as the second first-order equation.

[^55]:    ${ }^{26}$ In terms of linear algebra, $\lambda_{ \pm}$are the eigenvalues, and the corresponding sets $\left[c_{1}, c_{2}\right]_{ \pm}$, the eigenvectors of matrix M with elements $M_{i j}$.
    ${ }^{27}$ The asymptote direction may be found by plugging the value $\lambda_{+}$back into Eq. (89) and finding the corresponding ratio $c_{1} / c_{2}$.
    ${ }^{28}$ The term "saddle" is due to the fact that system's dynamics in this case is qualitatively similar to those of particle's motion in the 2D potential $U\left(\widetilde{q}_{1}, \widetilde{q}_{2}\right)$ having the shape of a horse saddle (or a mountain pass).

[^56]:    ${ }^{29}$ Named after J. H. Poincaré (1854-1912) who is credited, among many other achievements, for his contributions to special relativity (see, e.g., EM Chapter 9) and the idea of deterministic chaos (to be discussed in Chapter 9 below).
    ${ }^{30}$ This notion of phase plane rotation is the basis for the rotating-wave approximation's name. (Word "wave" has sneaked in from this method's wide application in classical and quantum optics.)

[^57]:    ${ }^{31}$ In addition, the Euler method is not time-reversible - the handicap which may be essential for integration of Hamiltonian systems described by systems of second-order differential equations. However, this drawback may be readily overcome by the so-called leapfrogging - the overlap of time steps $h$ for a generalized coordinate and the corresponding generalized velocity.

[^58]:    ${ }^{32}$ The most popular approaches in such cases are the Richardson extrapolation, the Bulirsch-Stoer algorithm, and a set of prediction-correction techniques, e.g. the Adams-Bashforth-Moulton method - see the literature recommended in MA Sec. 16 (iii).
    ${ }^{33}$ All numerical results shown in this section have been obtained by the $4{ }^{\text {th }}$-order Runge-Kutta method with the automatic step adjustment which guarantees the relative error of the order of $10^{-4}$ - much smaller than the pixel size in the plots.

[^59]:    ${ }^{34}$ In this particular case, the higher harmonic contents is about $0.5 \%$, dominated by the $3^{\text {rd }}$ harmonic whose amplitude and phase are in a very good agreement with Eq. (50).
    ${ }^{35}$ This method is used in practice, for example, for the generation of electromagnetic waves with frequencies in the terahertz range $\left(10^{12}-10^{13} \mathrm{~Hz}\right)$ which still lacks efficient electronic self-oscillators.

[^60]:    ${ }^{36}$ This term had been coined in 1957 by R. Bellman in the context of the optimal control theory (where the dimensionality typically means the number of parameters affecting the system under control), but gradually has spread all over quantitative sciences using numerical methods.
    ${ }^{37}$ In EM Sec. 1.2, I discuss implications of the curse implications for a different case, when both analytical and numerical solutions to the same problem are possible.

[^61]:    ${ }^{38}$ See, e.g., MA Eq. (15.1).

[^62]:    ${ }^{1}$ Here it is assumed that the particles are constrained to move in only one dimension (shown horizontal).

[^63]:    ${ }^{2}$ It is useful to rewrite Eq. (12) as $Z_{1} c_{1}= \pm Z_{2} c_{2}$, where $Z_{1,2} \equiv\left(\kappa_{1,2} m_{1,2}\right)^{1 / 2}$ are of the partial oscillator impedances the notion already mentioned in Chapter 4, and to be discussed in more detail in Sec. 4 below.

[^64]:    ${ }^{3}$ In physics, term "mode" is typically used for a particular type of variable distribution in space (in our current case, a certain set of distribution coefficients $c_{1,2}$ ), that sustains oscillations at a single frequency.
    ${ }^{4}$ One more property of weakly coupled oscillators, a periodic slow transfer of energy from one oscillator to the other and back, is more important for quantum rather than for classical mechanics. This is why I refer the reader to QM Secs. 2.5 and 5.1 for a detailed discussion of this phenomenon.

[^65]:    ${ }^{5}$ Fortunately, very effective algorithms have been developed for this matrix diagonalization task - see, e.g., references in MA Sec. 16(iii)-(iv). For example, the popular MATLAB package was initially created for this purpose. ("MAT" in its name stands for "matrix" rather than "mathematics".)

[^66]:    ${ }^{6}$ Named after P. Debye who developed this theory in 1912, in the context of specific heat of solids at low temperatures (beating nobody else than A. Einstein on the way :-) - see, e.g., SM Sec. 2.6.

[^67]:    ${ }^{7}$ This term is purely historical. Though the usual sound waves in air belong to this class, the waves we are discussing may have frequency both well below and well above human ear's sensitivity range.
    ${ }^{8}$ The waveform deformation due to dispersion (which we are considering now) should be clearly distinguished from its possible change due to attenuation, i.e. energy loss - which is not taken into account is our energyconserving model (23) - cf. Sec. 5 below.

[^68]:    ${ }^{9}$ Taking into account the next term in the Taylor expansion of function $\omega(q)$, proportional to $d^{2} \omega / d q^{2}$, we would find that actually the dispersion leads to a gradual change of the envelope form. Such changes play an important role in quantum mechanics, so that I discuss them in that part of my notes (see QM Sec. 2.1).

[^69]:    ${ }^{10}$ This property has especially important implications for quantum properties of periodic structures, e.g., crystals. It means, in particular, that the product $\hbar k$ cannot present the actual momentum of the particle (which is not conserved in periodic systems), but rather serves as its quasi-momentum (or "crystal momentum") - see, e.g., QM Sec. 2.5.

[^70]:    ${ }^{11}$ The direct calculation of the energy (per unit length) is a simple but useful exercise, left for the reader.

[^71]:    ${ }^{12}$ Sorry, one more traditional usage of letter $T$. I do not think there any chance to confuse it with the kinetic energy.

[^72]:    ${ }^{13}$ This equation could be also obtained using Eq. (42), as the condition of balance of the forces exerted on the interface particle with $j=0$ from the left and right - again, neglecting the inertia of that particle.
    ${ }^{14}$ See, e.g., corresponding parts of my lecture notes: QM Sec. 2.3 and EM Sec. 7.4. In 2D and 3D systems, Eqs. (53) are valid for the normal wave incidence only, otherwise they have to be modified - see, e.g., EM Sec. 7.4.

[^73]:    ${ }^{16}$ Actually, this result may be also obtained from Eq. (60) and hence is valid for an arbitrary ratio $\omega_{n} / \omega_{0}$.
    ${ }^{17}$ Equation (65), as well as its multi-dimensional generalizations, is frequently called the Helmholtz equation, named after H. von Helmholtz (1821-1894).

[^74]:    ${ }^{18}$ In engineering, the attenuation coefficient of wave-carrying systems is most frequently characterized by a logarithmic measure called decibel per meter (or just dB/m): $\alpha_{\mathrm{dB} / \mathrm{m}} \equiv 10 \log _{10} \alpha$.

[^75]:    ${ }^{19}$ In optics, the nonlinearity is implemented using transparent crystals such as lithium niobate $\left(\mathrm{LiNbO}_{3}\right)$, with the cubic-nonlinear dependence of the electric polarization as a function of the applied electric field: $\mathcal{P} \propto \mathcal{\varepsilon}+\alpha \boldsymbol{\mathcal { E }}^{3}$.

[^76]:    ${ }^{20}$ See, e.g., the classical monograph by N. Bloembergen, Nonlinear Optics, $4^{\text {th }}$ ed., World Scientific, 1996, or a more modern treatment by R. W. Boyd, Nonlinear Optics, $3^{\text {rd }}$ ed., Academic Press, 2008.
    ${ }^{21}$ Which is, surprisingly, not much more complex than the classical theory - see, e.g., QM Sec.5.5.
    ${ }^{22}$ See, e.g., QM Secs. 8.5 and 10.1, correspondingly.
    ${ }^{23}$ The classical (and perhaps still the best) monograph on the subject is Ya. Zeldovich, Physics of Shock Waves and High-Temperature Phenomena, Dover, 2002.

[^77]:    ${ }^{24}$ The reader familiar with the WKB approximation in quantum mechanics (see, e.g., QM Sec. 2.4) is welcome to adapt it for this classical application. Another possible starting point is the rotating-wave approximation (RWA), discussed in Sec. 4.3 above, which should be translated from the time domain to the space domain.
    ${ }^{25}$ This is a good model for small oscillations of linear molecules such as $\mathrm{CO}_{2}$ (for which the values of elastic constants $\kappa$ and $\kappa$ ' are well known).

[^78]:    ${ }^{1}$ Actually, all symbols for particle masses, coordinates and velocities should carry the particle index, say $k$, over which the summation is carried out. However, for the sake of notation simplicity, this index is just implied.

[^79]:    ${ }^{2}$ Hopefully, there is a little chance of confusion between the angular momentum $\mathbf{L}$ (a vector) and its Cartesian components $L_{j}$ (scalars with an index) on one hand, and the Lagrange function $L$ (a scalar without an index) on the other hand.
    ${ }^{3}$ See, e.g., MA Eq. (7.5).

[^80]:    ${ }^{4}$ Note that according to Eq. (22), other Cartesian components of the angular momentum, $L_{x}=I_{x z} \omega_{z}$ and $L_{y}=I_{y z} \omega_{z}$ may be different from zero, and even evolve in time. (Indeed, if axes $x$ and $y$ are fixed in lab frame, $I_{x z}$ and $I_{y z}$ may change due to body's rotation.) The corresponding torques $\tau_{x}^{(\mathrm{ext})}$ and $\tau_{y}^{(\text {ext })}$, which obey Eq. (33), are automatically provided by external forces which keep the rotation axis fixed.

[^81]:    ${ }^{5}$ Such beautiful experimental physics does not come cheap: the total Gravity Probe B project budget was about $\$ 750 \mathrm{M}$. Even at this price tag, the declared main goal of the project, an accurate measurement of a more subtle relativistic effect, the so-called frame-dragging drift (or "the Schiff precession"), predicted to be about 0.04 arc seconds per year, has not been achieved.
    ${ }^{6}$ This is also true for an asymmetric top, i.e. an arbitrary body (with, say, $I_{1}<I_{2}<I_{3}$ ), but in this case the alignment of vector $\mathbf{L}$ with axis $\mathbf{n}_{2}$, corresponding to the intermediate moment of inertia, is unstable.

[^82]:    ${ }^{7}$ Much more compact (and much less accurate) gyroscopes used, e.g., in smartphones and tablet computers, are based on the effect of rotation on oscillator frequency, and implemented as micro-electromechanical systems (MEMS) on silicon chip surface - see, e.g., Chapter 22 in V. Kaajakari, Practical MEMS, Small Gear Publishing, 2009.

[^83]:    Free precession frequency

[^84]:    ${ }^{8}$ For Earth, the free precession amplitude it so small (below 10 m of linear displacement on the Earth surface) that this effect is of the same order as other, irregular motions of the rotation axis, resulting from the turbulent fluid flow effects in planet's interior and its atmosphere.
    ${ }^{9}$ It is frequently called the Poinsot ellipsoid, after L. Poinsot (1777-1859) who has made several pioneering contributions to the rigid body mechanics.

[^85]:    ${ }^{10}$ These equations are of course valid in the simplest case of the fixed rotation axis as well. For example, if $\omega=$ $\mathbf{n}_{z} \omega$, i.e. $\omega_{x}=\omega_{y}=0$, Eq. (66) is reduced to Eq. (38).

[^86]:    ${ }^{11}$ Such discussion may be found, e.g. in Sec. 37 of L. Landau and E. Lifshitz, Mechanics, $3{ }^{\text {rd }}$ ed., ButterworthHeinemann, 1976.

[^87]:    ${ }^{12}$ Of the several choices more convenient in the absence of fast rotation, the most common is the set of so-called Tait-Brian angles (called the yaw, pitch, and roll) that are broadly used in airplane and maritime navigation.

[^88]:    ${ }^{13}$ Indeed, since the Lagrangian does not depend on time explicitly, $H=$ const, and since the full kinetic energy $T$ is a quadratic-homogeneous function of the generalized velocities, $E=H$.

[^89]:    ${ }^{14}$ In that simple case the body continues to rotate about the vertical symmetry axis: $\theta(t)=0$. Note, however, that such motion is stable only if the spinning speed is sufficiently high - see below.
    ${ }^{15}$ Indeed, the derivative of the fraction $1 / 2 I_{A} \sin ^{2} \theta$, taken at the point $\cos \theta=L_{z} / L_{3}$, is multiplied by the numerator, $\left(L_{z}-L_{3} \cos \theta\right)^{2}$, which at this point vanishes.

[^90]:    ${ }^{16}$ Details of this calculation may be found, e.g., in Sec. 5.8 of the textbook by H. Goldstein, C. Poole, and J. Safko, Classical Mechanics, $3^{\text {rd }}$ ed., Addison Wesley, 2002.

[^91]:    ${ }^{17}$ For this problem, all other inertial "forces", besides the Coriolis force (see below) vanish, while the latter force is directed perpendicular to the ring and does not affect the bead's motion along it.
    18 Named after G.-G. Coriolis (1792-1843), who is also credited for the first unambiguous definitions of mechanical work and kinetic energy.

[^92]:    19 The same force causes also the counter-clockwise circulation inside our infamous "Nor'easter" storms, in which velocity $\mathbf{v}$, caused by lower atmospheric pressure in the middle of the cyclone, is directed toward its center. ${ }^{20}$ Note again the difference between the negative sign before the (always positive) second term, and the positive sign before the similar positive second term in Eq. (3.44). As was already discussed in Chapter 3, this difference hinges on different background physics: in the planetary problem, the angular momentum (and hence its component $L_{z}$ ) is fixed, while the corresponding angular velocity $\dot{\varphi}$ is not. On the opposite, in our current discussion, the angular velocity $\omega$ (of the reference frame) is fixed, i.e. is independent on particle's motion.

[^93]:    ${ }^{21} \partial L / \partial \mathbf{v}$ is just a shorthand for a vector with Cartesian components $\partial L / \partial v_{j}$. In a different language, this is the gradient of $L$ in the velocity space.
    ${ }^{22}$ A very similar situation arises at the motion of a particle with electric charge $q$ in magnetic field $\mathbf{B}$. In that case the role of the additional term $\boldsymbol{p}-\mathbf{p}=m \omega \times \mathbf{r}$ is played by product $q \mathbf{A}$, where $\mathbf{A}$ is the vector-potential of the field $(\mathbf{B}=\nabla \times \mathbf{A})-$ see, e.g., EM Sec. 9.7, and in particular Eqs. (9.183) and (9.192).
    ${ }^{23}$ Note that by definition (1.36), angular momenta $\mathbf{L}$ of particles merely add up. As a result, Eq. (102) is valid for an arbitrary system of particles.

[^94]:    ${ }^{1}$ Since both $d \mathbf{q}$ and $d \mathbf{r}$ are legitimate physical vectors (whose Cartesian components are properly transformed as the transfer between reference frames), the $3 \times 3$ matrix with elements $\partial q_{j} / \partial r_{j}$; is indeed a legitimate physical tensor - see the discussion in Sec. 6.2.
    ${ }^{2}$ See, e.g., MA Eq. (13.2).

[^95]:    ${ }^{3}$ The traditional European notation for Tr is Sp (from German Spur meaning "trace" or "track").
    ${ }^{4}$ Actually, the tensor theory shows that the trace does not depend on the particular choice of the coordinate axes.

[^96]:    ${ }^{5}$ See, e.g., MA Eqs. (10.1) and (10.7).

[^97]:    ${ }^{6}$ It is frequently called the Cauchy stress tensor, partly to honor A.-L. Cauchy (1789-1857) who introduced it, and partly to distinguish it from and other possible definitions of the stress tensor, including the $1^{\text {st }}$ and $2^{\text {nd }}$ PiolaKirchhoff tensors. (For the infinitesimal deformations discussed in this course, all these notions coincide.)

[^98]:    ${ }^{7}$ Named after R. Hooke (1635-1703) who was first to describe the law in its simplest, 1D version.
    ${ }^{8}$ The inclusion of coefficients 2 and 3 into Eq. (34) is justified by the simplicity of some of its corollaries - see, e.g., Eqs. (38) and (43) below.
    ${ }^{9}$ Since the strain tensor elements, defined by Eq. (5), are dimensionless, while the strain defined by Eq. (18) has the dimensionality of pressure (force by unit area), so do the elastic moduli $K$ and $\mu$.

[^99]:    ${ }^{10}$ It may be proved that such situation may be implemented not only in a fluid with pressure $P$, but also by placing a solid sample of an arbitrary shape into a compressed fluid.

[^100]:    ${ }^{11}$ For the derivation and detailed discussion of Eq. (40) see, e.g., SM Sec. 3.1
    ${ }^{12}$ See, e.g., SM Sec. 1.3.

[^101]:    ${ }^{13}$ Though the analysis of compression in this situation gives similar results, in practical experiments a strong compression may lead to the loss of horizontal stability - the so-called buckling - of the rod.
    ${ }^{14}$ According to Eq. (47), $E$ may be thought of as the force per unit area, which would double sample's length, if only our theory was valid for deformations that large.

[^102]:    ${ }^{15}$ It is probably somewhat higher (up to $2,000 \mathrm{GPa}$ ) in such nanostructures as carbon nanotubes and monoatomic sheets (graphene), though there is still a substantial uncertainty in experimental values of elastic moduli of these structures - see, e.g., C. Lee et al, Science 321, 5887 (2008) and J.-U. Lee et al., Nano Lett. 12, 4444 (2012). ${ }^{16}$ The only known exceptions are certain exotic media with very specific internal microstructure - see, e.g., R. Lakes, Science 235, 1038 (1987) and references therein.

[^103]:    ${ }^{17}$ For clarity, let me reproduce a similar integration for the 1D motion of a particle on a spring. In this case, $\delta U=$ $-\delta W=-F \delta x$, and if spring's force is elastic, $F=-\kappa x$, the integration yields $U=\kappa x^{2} / 2=F x / 2$.
    ${ }^{18}$ As follows from Eqs. (50), the coefficient before the first sum in Eq. (53) is just the shear modulus $\mu$, while that before the second sum is equal to $(K+\mu / 3)$.
    ${ }^{19}$ See, e.g., MA Eq. (11.3).

[^104]:    ${ }^{20}$ If this is not immediately evident, have a look at MA Eq. (10.11) with $\mathbf{f}=f_{r}(r) \mathbf{n}_{r}$.
    ${ }^{21}$ See, e.g., MA Eq. (10.10) with $\mathbf{f}=q(r) \mathbf{n}_{r}$

[^105]:    ${ }^{22}$ Indeed, according to Eq. (50), the material-dependent factor in the second of Eqs. (63) is just $1 / 4 \mu$.

[^106]:    ${ }^{23}$ Strictly speaking, this is only true if the pressure difference is not too small, namely, if $\left|P_{1}-P_{2}\right| \gg P_{1,2} t / R$.

[^107]:    ${ }^{24}$ Strictly speaking, that dashed line is the intersection of the neutral surface (the continuous set of such neutral lines for all cross-sections of the rod) with the plane of drawing.
    ${ }^{25}$ Indeed, for $(d x / d z)^{2} \ll 1$, the general formula MA Eq. (4.3) for curvature (with the appropriate replacements $f$ $\rightarrow x$ and $x \rightarrow z)$ is reduced to $1 / R=d^{2} x / d z^{2}=d(d x / d z) / d z=d\left(\tan \varphi_{y}\right) / d z \approx d \varphi_{y} / d z$.
    ${ }^{26}$ In particular, this is the reason why the usual electric wires are made not of a solid copper core, but rather a twisted set of thinner sub-wires, which may slip relative to each other, increasing the wire flexibility.

[^108]:    ${ }^{27}$ As clear from their derivation, Eqs. (76)-(79) are valid for any distribution of parameters $A, E, I$, and $\rho$ over the rod's length, provided that the rod is quasi-uniform, i.e. its parameters' changes are so slow that the local relation (78) is still valid at any point.

[^109]:    ${ }^{28}$ For this problem, with purely shear deformation, using alternative elastic moduli $E$ and $v$ would be rather unnatural. If needed, we may always use the second of Eqs. (50): $\mu=E / 2(1+v)$.

[^110]:    ${ }^{29}$ I would not be terribly shocked if the reader skipped the balance of this section at the first reading. Though the following calculation is very elegant and instructive, its results will not be used in other parts of these notes.

[^111]:    ${ }^{30}$ In geophysics, the longitudinal waves are known as $P$-waves (with letter $P$ standing for "primary"), because due to their higher velocity (see below) they arrive at the detection site (from a distant earthquake or explosion) before waves of other types.

[^112]:    ${ }^{33}$ However, if the initial wave is an arbitrary mixture (109) of longitudinal and transverse components, these components, propagating with different velocities, will "run from each other".

[^113]:    ${ }^{34}$ Named after N. Umov who introduced this concept in 1874. Ten years later, a similar concept for electromagnetic waves (see, e.g., EM Sec. 6.4) was suggested by J. Poynting, so that some textbooks use the term "Umov-Poynting vector". In a dissipation-free, elastic medium, the Umov vector obeys the following continuity equation, $\partial\left(\rho v^{2} / 2+u\right) / \partial t+\nabla \cdot p=0$, with $u$ given by Eq. (52), which expresses the conservation of the total (kinetic plus potential) energy of elastic deformation.

[^114]:    ${ }^{35}$ See, e.g., EM Sec. 7.5.
    ${ }^{36}$ Their discussion may be also found in EM Sec. 7.5.

[^115]:    ${ }^{37}$ Named, respectively, after Lord Rayleigh (born J. Strutt, 1842-1919) who has theoretically predicted the very existence of surface acoustic waves, and A. Love (1863-1940).
    ${ }^{38}$ See, e.g., Sec. 24 in L. Landau and E. Lifshitz, Theory of Elasticity, $3^{\text {rd }}$ ed., Butterworth-Heinemann, 1986.
    ${ }^{39}$ See, for example, K. Aki and P. G. Richards, Quantitative Seismology, $2^{\text {nd }}$ ed., University Science Books, 2002, and D. Morgan, Surface Acoustic Waves, ${ }^{\text {nd }}$ ed., Academic Press, 2007.

[^116]:    ${ }^{40}$ Due to this reason, the tensile waves can be called longitudinal only in a limited sense: while the stress wave is purely longitudinal $\sigma_{x x}=\sigma_{y y}=0$, the strain wave is not: $s_{x x}=s_{y y}=-\sigma \pi_{z z} \neq 0$, i.e. $\mathbf{q}(\mathbf{r}, t) \neq \mathbf{n}_{z} q_{z}$.

[^117]:    ${ }^{41}$ Note that since the "moment of inertia" $I_{y}$, defined by Eq. (72), may depend on the bending direction (unless the cross-section is sufficiently symmetric), the dispersion relation (138) may give different results for different directions of the bending wave polarization.

[^118]:    ${ }^{42}$ For acoustic waves, such condition is easy to implement. Indeed, from Sec. 7 we already know that the strong inequality of wave impedances $Z$ is sufficient for such reflection. The numbers of Table 1 show that, for example,

[^119]:    ${ }^{1}$ As was discussed in Sec. 7.3 in the context of Table 7.1, this is an excellent approximation, for example, for human-scale experiments with water.
    ${ }^{2}$ The equation, and the SI unit of pressure $1 \mathrm{~Pa}=1 \mathrm{~N} / \mathrm{m}^{2}$, are named after B. Pascal (1623-1662) who has not only pioneered hydrostatics, but also invented the first mechanical calculator and made several other important contributions to mathematics - and Christian philosophy!
    ${ }^{3}$ An example of such a problem is given by fluid equilibrium in coordinate systems rotating with a constant angular velocity. Here the real bulk forces should be complemented by the centrifugal "force" - the only inertial force which does not vanish at constant $\omega$ and $\mathbf{r}-$ see Eq. (6.92).

[^120]:    ${ }^{4}$ If $\gamma$ of the interface of certain two fluids is negative, it self-reconfigures to decrease $U_{s}$ by the interface area, i.e. fragments the system into a solution.
    ${ }^{5}$ This equality readily follows from the general Eq. (7.32), with the stress tensor elements expressed by Eq. (2), but in this simple case of the net stress force $d \mathbf{F}=\left(P_{1}-P_{2}\right) d \mathbf{A}$ parallel to the interface element vector $d \mathbf{A}$, it may be even more simply obtained just from the definition of work $\delta W=d \mathbf{F} \cdot \delta \mathbf{r}$ at the virtual displacement $\delta \mathbf{r}=\mathbf{n} \delta r$. ${ }^{6}$ This general formula may be verified by elementary means for a sphere of radius $r$ (for which $R_{1}=R_{2}=r$ and $d A$ $=r^{2} d \Omega$, so that $\delta(d A) / d A=\delta\left(r^{2}\right) / r^{2}=2 \delta r / r$ ), and a round cylindrical interface of radius $R$ (for which $R_{1}=r, R_{2}=$ $\infty$, and $d A=r d \varphi d z$, so that $\delta(d A) / d A=\delta r / r)$.
    ${ }^{7}$ This formula (not to be confused with Eq. (12), called the Young's equation) was derived in 1806 by P.-S. Laplace (of the Laplace operator/equation fame) on the basis of the first analysis of the surface tension effects by T. Young a year earlier.

[^121]:    ${ }^{8}$ Note that this is not true for tubes with different shapes of their cross-section.
    ${ }^{9}$ One of them is the sound propagation, where particle displacements $\mathbf{q}$ are typically small, so that results of Sec. 7.7 are applicable. As a reminder, they show that in fluids, with $\mu=0$, the transverse sound cannot propagate (formally, has zero velocity and impedance), while the longitudinal sound's velocity is finite - see Eq. (7.116).

[^122]:    ${ }^{10}$ The operator relation $d / d t=\partial / \partial t+(\mathbf{v} \cdot \nabla)$, applicable to an arbitrary (scalar or vector) function, is frequently called the convective derivative. (Alternative adjectives, such as "Lagrangian", "substantial", or "Stokes", are sometimes used for this derivative as well.) The relation has numerous applications well beyond the fluid dynamics - see, e.g., EM Chapter 9 and QM Chapter 1.

[^123]:    ${ }^{11}$ If the reader still needs a reminder, see MA Eq. (12.1).
    ${ }^{12}$ See, e.g., EM Sec. 4.1, QM Sec. 1.4, and SM Sec. 5.6.
    ${ }^{13}$ It was derived in 1755 by the same L. Euler whose name has already been (reverently) mentioned several times in this course.

[^124]:    ${ }^{14}$ It readily follows, for example, from MA Eq. (11.6) with $\mathbf{g}=\mathbf{f}=\mathbf{v}$.
    ${ }^{15}$ Perhaps the most spectacular manifestation of the vorticity conservation are the famous toroidal vortex rings (see, e.g., nice photo and movie at https://en.wikipedia.org/wiki/Vortex ring), predicted in 1858 by H. von Helmholtz, and then demonstrated by P. Tait in a series of spectacular experiments with smoke in air. The persistence of such a ring, once created, is only limited by fluid's viscosity - see the next section.
    ${ }^{16}$ First formulated verbally by H. von Helmholtz.
    ${ }^{17}$ Its proof may be found, e.g., in Sec. 8 of L. Landau and E. Lifshitz, Fluid Mechanics, $2^{\text {nd }}$ ed., ButterworthHeinemann, 1987.

[^125]:    ${ }^{18}$ See, e.g., EM Secs. 2.3 and 2.4.
    ${ }^{19}$ Evidently, motion of the cylinder, with constant velocity $\left(-\mathbf{v}_{0}\right)$, in the otherwise stationary fluid leads to exactly the same problem - in the reference frame bound to the moving body.
    ${ }^{20}$ See, e.g., MA Eq. (10.3).
    ${ }^{21}$ Let me hope that letter $\rho$, used here for the magnitude 2D radius-vector $\rho=\{x, y\}$, will not be confused with fluid's density - which does not participate in this boundary problem.
    ${ }^{22}$ See, e.g., EM Eq. (2.112). Note that the most general solution of Eq. (29) also includes a term proportional to $\varphi$, but this term should be zero for such a single-valued function as the velocity potential.

[^126]:    ${ }^{23}$ They may be found by integration of the evident equation $d y / d x=v_{y}(x, y) / v_{x}(x, y)$. For our simple problem this integration may be done analytically, giving the relation $y\left[1-R^{2} /\left(x^{2}+y^{2}\right)\right]=$ const, where the constant is specific for each streamline.
    ${ }^{24}$ The alternative, historic term "gravity waves" for this phenomenon may nowadays lead to a confusion with the relativistic effect of gravity waves (which may propagate in vacuum), whose direct detection is a focus of so much current experimental effort.
    ${ }^{25}$ Such a wave is "plane" only in direction $x$ (perpendicular to the propagation direction $z$, see Fig. 4).

[^127]:    ${ }^{26}$ Probably the most important effect we miss by neglecting $\zeta$ is the attenuation of (longitudinal) acoustic waves, into which the second viscosity makes a major (and in some cases, the main) contribution.
    ${ }^{27}$ Actually, at even lower temperatures (for $\mathrm{He} 4, T<T_{\lambda} \approx 2.17 \mathrm{~K}$ ), helium becomes a superfluid, i.e. looses viscosity completely, as result of the Bose-Einstein condensation - see, e.g., SM Sec. 3.4.
    ${ }^{28}$ Named after C.-L. Navier (1785-1836) who had suggested the equation, and G. Stokes (1819-1903) who has demonstrated its relevance by solving it for several key situations.

[^128]:    ${ }^{29}$ This is essentially an additional experimental fact, but may be readily understood as follows. A solid may be considered as an ultimate case of a fluid (with infinite viscosity), and the tangential component of velocity should be a continuous an interface between two fluids, in order to avoid infinite stress - see Eq. (50).

[^129]:    ${ }^{30}$ It was solved theoretically by G. Stokes in 1845 in order to explain Eq. (60) that had been formulated by G. Hagen and J. Poiseuille in 1839-1840 on the basis of their experimental results.

[^130]:    ${ }^{31}$ For example, the Green's function method (see, e.g., EM Sec. 2.7).
    ${ }^{32}$ For more details see, e.g., R. J. Leveque, Finite Difference Methods for Ordinary and Partial Differential Equations, SIAM, 2007.

[^131]:    ${ }^{33}$ Note that value (65) is exactly the same as given for $v_{\max }=\left.v\right|_{\rho=0}$ by the analytical formula (58) for the round cross-section with radius $R=a / 2$. This is not an occasional coincidence. The velocity distribution given by (58) is a quadratic function of both $x$ and $y$. For such functions, with all derivatives higher than $\partial^{2} / \partial r_{j}^{2}$ being equal to zero, equation (64) is exact rather than approximate.
    ${ }^{34}$ See, e.g., C. Johnson, Numerical Solution of Partial Differential Equations by the Finite Element Method, Dover, 2009, or T. J. R. Hughes, The Finite Element Method, Dover, 2000.

[^132]:    ${ }^{37}$ The time scale of some problems may be different from $l / v$; for example, for forced oscillations of a fluid flow it is given by the reciprocal oscillation frequency $f$. For such problems, ratio $S \equiv f(l / v)$ serves as another, independent dimensionless constant, commonly called either the Strouhal number or the reduced frequency.
    ${ }^{38}$ For substantially compressible fluids (e.g., gases), the most important additional dimensionless parameter is the Mach number $M \equiv v / v_{l}$, where $v_{l}=(K / \rho)^{1 / 2}$ is the velocity of the longitudinal sound - which is, as we already know, the only wave mode possible in an infinite fluid. Especially significant for practice are supersonic effects (including the shock wave in the form of the famous Mach cone with the half-angle $\theta_{\mathrm{M}}=\sin ^{-1} M^{-1}$ ) which arise at $M>1$. For a more thorough discussion of these issues, I have to refer the reader to more specialized texts e e.g., Chapter IX of the Landau and Lifshitz volume cited above, or Chapter 15 in I. M. Cohen and P. K. Kundu, Fluid Mechanics, $4^{\text {th }}$ ed., Academic Press, 2007 - which is generally a good book on the subject. Another popular, rather simple textbook is R. A. Granger, Fluid Mechanics, Dover, 1995.

[^133]:    ${ }^{39}$ Note that the "dynamic" viscosity $\eta$ participates in this number (and many other problems of fluid dynamics) only in the combination $\eta / \rho$ that thereby has deserved a special name of kinematic viscosity.
    ${ }^{40}$ For example, the values of $\eta$ and $\rho$ for water listed in Table 1 imply that for a few-meter object, $R e>1,000$ at any speed above just $\sim 1 \mathrm{~mm} / \mathrm{s}$.
    ${ }^{41}$ A rare exception is the relatively recent theoretical result by S. Orszag (1971) for the turbulence threshold in a flow of an incompressible fluid through a gap of thickness $t$ between two parallel plane walls: $R e_{t} \approx 5,772$ (for $l=$ $\left.t / 2, v=v_{\max }\right)$. However, this result does not predict the turbulence patterns at $R e>R e_{t}$.
    ${ }^{42}$ The crucial condition of correct modeling is the equality of the Reynolds numbers (74) (and if relevant, also of the Froude numbers and/or the Mach numbers) of the object of interest and its model.
    ${ }^{43}$ See, e.g., P. A. Davidson, Turbulence, Oxford U. Press, 2004.
    ${ }^{44}$ The following famous quote is attributed to W. Heisenberg on his deathbed: "When I meet God, I will ask him two questions: Why relativity? And why turbulence? I think he will have an answer for the first question." Though probably inaccurate, this story reflects rather well the understandable frustration of the fundamental physics community, known for their reductionist mentality, with the enormous complexity of phenomena which obey simple (e.g., Navier-Stokes) equations.

[^134]:    ${ }^{45}$ See, e.g., EM Secs. 2.6, 3.3, and 4.3.

[^135]:    ${ }^{46}$ See, e.g., EM Sec. 2.5(iv) and/or QM Sec. 3.6.

[^136]:    ${ }^{1}$ In this context, this term is understood as "systems described by deterministic differential equations".
    ${ }^{2}$ Actually, the notion of quasi-random dynamics due to the exponential divergence of trajectories may be traced back at least to (apparently independent) works by J. Poincaré in 1892 and by J. Hadamard in 1898. Citing Poincaré, "...it may happen that small differences in the initial conditions produce very great ones in the final phenomena. [...] Prediction becomes impossible."
    ${ }^{3}$ Its chaotic properties were first discussed in 1976 by R. May, though the map itself is one of simple ecological models repeatedly discussed earlier, and may be traced back at least to the 1838 work by P. Verhulst.
    ${ }^{4}$ Since the maximum value of function $f(q)$, achieved at $q=1 / 2$, equals $r / 4$, the mapping may be limited by segment $x=[0,1]$, if parameter $r$ is between 0 and 4 . Since all interesting properties of the map, including chaos, may be found within these limits, I will focus on this range.

[^137]:    ${ }^{5}$ The reader should remember that just as the usual ("nature") experiments, numerical experiments also have limited accuracy, due to unavoidable rounding errors.
    ${ }^{6}$ The geometry of these regions are essentially fractal, i.e. has a dimensionality intermediate between 0 (which any final set of geometric points would have) and 1 (pertinent to a 1D continuum). An extensive discussion of fractal geometries, and their relation to the deterministic chaos may be found, e.g., in the book by B. B. Mandelbrot, The Fractal Geometry of Nature, W. H. Freeman, 1983.
    ${ }^{7}$ This does not mean that the chaos development is a monotonic function of $r$. As Fig. 2 shows, within certain intervals of this parameter chaos suddenly disappears, being replaced, typically, with a few-point limit cycle, just to resume on the other side of the interval. Sometimes (but not always!) the "route to chaos" on the borders of these intervals follows the same Feigenbaum sequence of period-doubling bifurcations.

[^138]:    ${ }^{8}$ After A. Lyapunov (1857-1918), famous for his studies of stability of dynamic systems.
    ${ }^{9} \mathrm{~N}$-dimensions maps, which relate $N$-dimensional vectors rather than scalars, may be characterized by $N$ Lyapunov exponents rather than one. In order to have chaotic behavior, it is sufficient for just one of them to become positive. For such systems, another measure of chaos, the Kolmogorov entropy, may be more relevant. This measure, and its relation with the Lyapunov exponents, are discussed, e.g., in SM Sec. 2.2.
    ${ }^{10}$ See, e.g., Chapters 2-4 in H. G. Schuster and W. Just, Deterministic Chaos, $4^{\text {th }}$ ed., Wiley-VCH, 2005, or Chapters 8-9 in J. M. T. Thompson and H. B. Stewart, Nonlinear Dynamics and Chaos, $2^{\text {nd }}$ ed., Wiley, 2002.

[^139]:    ${ }^{11}$ In the actual simulation, a small term $\varepsilon q$, with $\varepsilon \ll 1$, has been added to the left-hand part of this equation. This term slightly somewhat tames the trend of the solution to spread along $q$ axis, and makes the presentation of results easier, without affecting the system dynamics too much.

[^140]:    ${ }^{12}$ In some cases, it is possible to predict a parameter region where chaos cannot happen, due to lack of any instability-amplification mechanism. Unfortunately, typically the analytically predicted boundaries of such region form a rather loose envelope of the actual (numerically simulated) chaotic regions.

[^141]:    ${ }^{13}$ A mathematically-strict formulation of this statement is called the Poincaré-Bendixon theorem, which was proved by I. Bendixon as early as in 1901.
    ${ }^{14}$ Since a typical dynamic system with one degree of freedom is described by two such equations, the number of the first-order equations describing a dynamic system is sometimes called the number of half-degrees of freedom. This notion is very useful and popular in statistical mechanics - see, e.g., SM Sec. 2.2 and on.

[^142]:    ${ }^{15}$ A more scientific-sounding name for such a reflection is specular (from Latin "speculum" meaning a metallic mirror).
    ${ }^{16}$ Indeed, it is fully described by Lagrangian function $L=m v^{2} / 2-U(\rho)$, with $U(\rho)=0$ for 2D radius-vectors $\rho$ belonging to the table area, and $U(\rho)=+\infty$ outside of the area.

[^143]:    ${ }^{17}$ Superficially, Eq. (17) is also valid for a plane wall, but as was discussed above, a billiard with such walls features a full correlation between sequential reflections, so that angle $\varphi$ always returns to its initial value. In a Sinai billiard, such correlation disappears. Because of that, concave walls may also make a billiard chaotic. A famous example is the stadium billiard, suggested by L. Bunimovich, with two straight, parallel walls connecting two semi-circular, concave walls. Another example, which allows a straightforward analysis, is the Hadamard billiard: an infinite (or rectangular) table with non-horizontal surface of negative curvature.
    18 Billiards are also a convenient platform for a discussion of a conceptually important issue of quantum properties of classically chaotic systems (sometimes improperly named "quantum chaos").
    ${ }^{19}$ Actually, quantitative characterization of the fraction is not trivial, because it may have fractal dimensionality. Unfortunately, due to lack of time I have to refer the reader interested in this issue to special literature, e.g., the monograph by B. Mandelbrot (cited above) and references therein.

[^144]:    ${ }^{20}$ It was first studied in 1964 by M. Hénon and C. Heiles as a simple model of star rotation about a gallactic center. Most studies of this equation have been carried out for the following particular case: $m_{2}=2 m_{1}, m_{1} \omega_{1}{ }^{2}=$ $m_{2} \omega_{2}^{2}$. In this case, introducing new variables $x \equiv \varepsilon q_{1}, y \equiv \varepsilon q_{2}$, and $\tau \equiv \omega_{1} t$, it is possible to rewrite Eqs. (18)-(20) in parameter-free forms. All the results shown in Fig. 9 below are for this case.
    ${ }^{21}$ Generally, it has a trajectory in 4D space, e.g., that of coordinates $q_{1,2}$ and their time derivatives, although the first integral of motion (20) means that for each fixed energy $E$, the motion is limited to a 3D sub-space. Still, this is too much for convenient representation of the motion.

[^145]:    ${ }^{22}$ See, e.g., M. V. Berry, in: S. Jorna (ed.), Topics in Nonlinear Dynamics, AIP Conf. Proc. No. 46, AIP, 1978, pp. 16-120.
    ${ }^{23}$ This fact complies with the necessary condition of chaos, discussed in the end of Sec. 2, because Eqs. (19) may be rewritten as a system of four differential equations of the first order.

[^146]:    ${ }^{24}$ An important milestone on that way was the work by S. Newhouse et al., Comm. Math. Phys. 64, 35 (1978), who proved the existence of a strange attractor in a rather abstract model of fluid flow.
    ${ }^{25}$ See, e.g., U. Frisch, Turbulence: The Legacy of A. N. Kolmogorov, Cambridge U. Press, 1996.
    ${ }^{26}$ The reader interested in the deterministic chaos as such, may also like to have a look at a very popular book by S. Strogatz, Nonlinear Dynamics and Chaos, Westview, 2001.

[^147]:    ${ }^{1}$ Due to not only W. Hamilton (1805-1865), but also and C. Jacobi (1804-1851).
    ${ }^{2}$ Actually, this differential has already been used in Sec. 2.3 to derive Eq. (2.35).

[^148]:    ${ }^{3}$ Of course, the right-hand part of each equation (7) generally can include coordinates and momenta of other degrees of freedom as well, so that the equations of motion for different $j$ are generally coupled.

[^149]:    ${ }^{4}$ Named after S. Poisson - of the Poisson equation and the Poisson statistical distribution fame.

[^150]:    ${ }^{5}$ See, e.g., QM Sec. 2.1.
    ${ }^{6}$ There is of course a conceptual difference between the "usual" products of function derivatives participating in the Poisson brackets, and the operator "products" (meaning their sequential action on a state vector - see, e.g., QM Sec. 4.1) forming the commutator.

[^151]:    ${ }^{7}$ See, e.g., QM Sec. 4.6.
    ${ }^{8}$ Various aspects of this problem and its quantum-mechanical extension were first discussed by L. Le Cornu (1895), Lord Rayleigh (1902), H. Lorentz (1911), P. Ehrenfest (1916), and M. Born and V. Fock (1928).
    ${ }^{9}$ This term has come from thermodynamics and statistical mechanics, where it implies not only a slow parameter variation, but also the thermal insulation of the system - see, e.g., SM Sec. 1.3. Evidently, the latter condition is irrelevant in our current context.
    ${ }^{10}$ In Sec. 4.6, we discussed this plane for the particular case of sinusoidal oscillations - see Fig. 9

[^152]:    ${ }^{11}$ This is the most critical point of this proof, because at any finite rate of parameter change the oscillations are, strictly speaking, non-periodic. Because of the approximate nature of this conjecture (which is very close to the assumptions made at the derivation of the RWA equations in Sec. 4.3), new, more strict (but also much more

[^153]:    ${ }^{12}$ For certain particular oscillators, e.g., a mathematical pendulum, Eq. (42) may be also proved directly - an exercise highly recommended to the reader.
    ${ }^{13}$ This, again, is a plausible argument but not a strict proof. Indeed, though, according to its definition (39), $J$ is nothing more than a sum of several (formally, infinite number of) values of momentum $p$, they are not independent, but have to be selected on the same closed trajectory on the phase plane. For more mathematical vigor, the reader is referred to Sec. 45 of Mechanics by Landau and Lifshitz (which was repeatedly cited above), which discusses the general rules of the so-called canonical transformations from one set of Hamiltonian arguments to another one - say from $\{p, q\}$ to $\{J, \Theta\}$.

[^154]:    ${ }^{14}$ See, e.g., Chapter 6 in J. Jose and E. Saletan, Classical Dynamics, Cambridge U. Press, 1998.

[^155]:    ${ }^{15}$ Please note that despite a close relation between the abbreviated action $S_{0}$ and the action variable $J$ defined by Eq. (39), these notions are not identical. Most importantly, $J$ is an integral over a closed trajectory, while $S_{0}$ in defined for an arbitrary point of a trajectory.
    ${ }^{16}$ See, e.g., QM Sec. 2.3.

[^156]:    ${ }^{17}$ Eq. (58) was the starting point for R. Feynman's development of his path-integral formulation of quantum mechanics - see, e.g., QM Sec. 5.3.
    18 As a reminder, we have run into a similar situation at our discussion of the non-degenerate parametric excitation in Sec. 5.5.

[^157]:    ${ }^{19}$ See, e.g., Chapters 6-9 in I. C. Percival and D. Richards, Introduction to Dynamics, Cambridge U. Press, 1983.
    ${ }^{20}$ See, e.g., T. P. Bertsekas, Dynamic Programming and Optimal Control, vols. 1 and 2, Aetna Scientific, 2005 and 2007. The reader should not be deceived by the unnatural term "dynamic programming" that was invented by the founding father of this field, R. Bellman, to lure government bureaucrats into funding his research, which had been deemed too theoretical at that time, but now has a broad range of important applications.

[^158]:    ${ }^{1}$ For remedial reading, virtually any undergraduate text on electricity and magnetism may be used; I can recommend either the classical text by I. Tamm, Fundamentals of Theory of Electricity, Mir, 1979, or the more readily available textbook by D. Griffiths, Introduction to Electrodynamics, $3^{\text {rd }}$ ed., Prentice-Hall, 1999.
    ${ }^{2}$ Discovered experimentally in the early 1780 s, and formulated in 1785 by C.-A. de Coulomb.
    ${ }^{3}$ On the top of the more general notions of classical Cartesian space, point particles and forces, which are used in classical mechanics - see, e.g., CM Sec. 1.1. (Acronyms CM, SM, and QM refer to other three parts of my lecture note series. In those parts, this Classical Electrodynamics part is referred to as EM.)
    ${ }^{4}$ As in all other parts of my lecture notes, chapter numbers are omitted in references to equations, figures, and sections within the same chapter.

[^159]:    ${ }^{5}$ In the formal metrology, one coulomb is defined as the charge carried over by a constant current of one ampere (see Ch. 5 for its definition) during one second.
    ${ }^{6}$ Constant $\varepsilon_{0}$ is called either the electric constant or the free space permittivity; from Eq. (2) with the free-space speed of light $c \approx 3 \times 10^{8} \mathrm{~m} / \mathrm{c}, \varepsilon_{0} \approx 8.85 \times 10^{-12}$ SI units. For more accurate values of the constants, and their brief discussion, see appendix CA: Selected Physical Constants.
    ${ }^{7}$ Physically this is a very strong statement: it means that Eq. (1) is valid for any pair of charges regardless of presence of other charges, i.e. not only in the free space, but in also placed into an arbitrary medium. The apparent modification of this relation by conductors (Ch. 2) and dielectrics (Ch. 3) is just the result of appearance of additional electric charges within those media.

[^160]:    ${ }^{8}$ Moreover, there are some widely used approximations, e.g., the Kohn-Sham equations in the density functional theory of multiparticle systems, which essentially violate this law, thus limiting the accuracy and applicability of these approximations - see, e.g., QM Sec. 8.4.
    ${ }^{9}$ The 2D (areal) charge density $\sigma$ and 1D (linear) density $\lambda$ may be defined absolutely similarly: $d Q=\sigma d^{2} r, d Q=$ $\lambda d r$. Note that a finite value of $\sigma$ and $\lambda$ means that the volume density $\rho$ is infinite in the charge location points; for example for a plane $z=0$, charged with a constant areal density $\sigma, \rho=\sigma \delta(z)$.

[^161]:    ${ }^{10}$ Note that for a continuous, smooth charge distribution, integral (9) does not diverge at $\mathbf{R} \equiv \mathbf{r}-\mathbf{r}^{\prime} \rightarrow 0$, because in this limit the fraction under the integral increases as $R^{-2}$, i.e. slower than the decrease of the elementary volume $d^{3} r^{\prime}$, proportional to $R^{3}$.
    ${ }^{11}$ See, e.g., Sec. 14 of the Selected Mathematical Formulas appendix, referred below as MA.

[^162]:    ${ }^{12}$ Actually, the term "curse of dimensionality" was coined in the 1950s by R. Bellman in the context of the optimal control theory, and only later spread to other sciences that heavily rely on numerical calculations.

[^163]:    ${ }^{13}$ See, e.g., MA Eq. (12.2). Note that the scalar product under the integral in Eq. (25) is nothing more that the divergence of vector $\mathbf{E}$ - see, e.g., MA Eq. (8.4).
    ${ }^{14}$ See, e.g., MA Secs. 8-10.
    ${ }^{15}$ In the Gaussian units, just as in the initial Eq. (5), $\varepsilon_{0}$ has to be replaced with $1 / 4 \pi$, so that the Maxwell equation (27) looks like $\nabla \cdot \mathbf{E}=4 \pi \rho$, while Eq. (28) stays the same.
    ${ }^{16}$ This follows, for example, from the direct application of MA Eq. (10.11) to the spherically-symmetric vector function $\mathbf{f}=\mathbf{E}(\mathbf{r})=E(r) \mathbf{n}_{r}$ field of a point charge placed at the origin, giving $f_{\theta}=f_{\varphi}=0$ and $\partial f_{r} / \partial \theta=\partial f_{r} / \partial \varphi=0$.
    ${ }^{17}$ See, e.g., MA Eq. (10.10) for this particular case (when $\partial / \partial \theta=\partial / \partial \varphi=0$ ).

[^164]:    ${ }^{18}$ See, e.g., CM Sec. 1.4.
    ${ }^{19}$ Eq. (28) could be also derived from this relation, because according to vector algebra, any gradient field has vanishing curl - see, e.g., MA Eq. (11.1).

[^165]:    ${ }^{20}$ This may be done either by Cartesian components or using the well-known expression $\nabla f=(d f / d r) \mathbf{n}_{r}$ valid for any spherically-symmetric scalar function $f(r)$ - see, e.g., MA Eq. (10.8) for the particular case $\partial / \partial \theta=\partial / \partial \varphi=0$.

[^166]:    ${ }^{21}$ Named after S. D. Poisson (1781-1840), also famous for the Poisson distribution - one of the central results of the probability theory - see, e.g., SM Sec. 5.2.
    ${ }^{22}$ After mathematician (and astronomer) P. S. de Laplace (1749-1827) who, together with A. Clairault, is credited for the development of the very concept of potential.

[^167]:    ${ }^{23}$ See, e.g., MA Eq. (10.8) for $\partial / \partial \theta=\partial / \partial \varphi=0$.

[^168]:    ${ }^{24}$ The nature of this additional factor $1 / 2$ is absolutely the same as in the well-known formula $U=(1 / 2) k x^{2}$ for the potential energy of an elastic spring providing returning force $F=-\kappa x$ proportional to the deviation $x$ from equilibrium.
    ${ }^{25}$ This transformation follows from the divergence theorem MA (12.2) applied to vector function $\mathbf{f}=\phi \nabla \phi$, taking into account the 3D differentiation rule MA Eq. (11.4a): $\nabla \cdot(\phi \nabla \phi)=(\nabla \phi) \cdot(\nabla \phi)+\phi \nabla \cdot(\nabla \phi)=(\nabla \phi)^{2}+\phi \nabla^{2} \phi$.

[^169]:    ${ }^{26}$ In the Gaussian units, the standard replacement $\varepsilon_{0} \rightarrow 1 / 4 \pi$ turns the last of Eqs. (67) into $u(\mathbf{r})=E^{2} / 8 \pi$.
    ${ }^{27}$ Note that $U \rightarrow \infty$ at $R \rightarrow 0$. Such divergence appears at application of Eq. (67) to any point charge. Since it does not affect the force acting on the charge, the divergence does not create any technical difficulty for analysis of charge statics or non-relativistic dynamics, but it points to a conceptual problem of classical electrodynamics as the whole. This issue will be discussed in the very end of the course (Sec. 10.6).

[^170]:    ${ }^{28}$ This is only the simplest one of the whole family of reciprocity theorems in electromagnetism. (Sometimes it is called "Green's reciprocity theorem", but historically it is more fair to reserve the last name for the generalization to surface charges, using Eq. (2.210), to be discussed in Sec. 2. 7 below.)

[^171]:    ${ }^{1}$ More detailed discussions may be found, e.g., in Sec. 13.5 of J. Hook and H. Hall, Solid State Physics, $2^{\text {nd }}$ ed., Wiley, 1991, or the section on electric field screening in Chapter 17 of N. Ashcroft and N. Mermin, Solid State Physics, Brooks Cole, 1976.
    ${ }^{2}$ This term, used for electric field, should not be confused with shielding - the word used for the description of magnetic field reduction by magnetic materials - see Chapter 5 below.

[^172]:    ${ }^{3}$ See, e.g., MA Eq. (12.1).

[^173]:    ${ }^{4}$ This scale originates from the quantum-mechanical effects of electron motion, characterized by the Bohr radius $r_{\mathrm{B}} \approx 0.5 \times 10^{-10} \mathrm{~m}-$ see, e.g., QM Eq. (1.13).
    ${ }^{5}$ Here $e$ denotes the positive fundamental charge, $e \approx 1.6 \times 10^{-19} \mathrm{C}$, so that the electron charge equals $(-e)$.
    ${ }^{6}$ See, e.g., SM Sec. 3.1.
    ${ }^{7}$ This equation and/or its straightforward generalization to the case of charged particles (ions) of several kinds is frequently (especially in the theories of electrolytes and plasmas) called the Debye-Hückel equation.

[^174]:    ${ }^{8}$ There is a good reason for making an estimate of $\lambda_{\mathrm{D}}$ for this case: the electric field created by the gate electrode of a field-effect transistor, penetrating into doped silicon by a depth $\sim \lambda_{\mathrm{D}}$, controls current in this most important electronic device - on whose back all the current information revolution rides. Because of that, $\lambda_{\mathrm{D}}$ establishes the possible scale of semiconductor circuit shrinking which is the basis of the well-known Moore's law. (Practically, the scale is determined by integrated circuit patterning techniques, and Eq. (8) may be used to find the proper charge carrier density $n$ and hence the level of silicon doping.)
    ${ }^{9}$ See, e.g., SM Sec. 2.8. For a more detailed derivation of Eq. (10), see SM Chapter 3.
    ${ }^{10}$ In good metals this equation is valid up to the fields $\sim E_{\mathrm{F}} / e \lambda_{\mathrm{TF}} \sim 10^{9} \mathrm{~V} / \mathrm{m}$, very high by the usual standards. For example, the electric breakdown threshold for vacuum (or air-filled) gaps is $\sim 3 \times 10^{6} \mathrm{~V} / \mathrm{m}$.
    ${ }^{11}$ See, e.g., SM Sec. 3.3.

[^175]:    ${ }^{12}$ In the Gaussian units, using the standard replacement $4 \pi \varepsilon_{0} \rightarrow 1$, this relation takes a remarkably simple form: $C$ $=R$, good to remember. Generally, in the Gaussian units (but not in the SI system!) the capacitance has the dimensionality of length, i.e. is measured in centimeters. Note also that a convenient fractional SI unit, 1 picofarad $\left(10^{-12} \mathrm{~F}\right)$ is very close to the Gaussian unit: $1 \mathrm{pF}=\left(1 \times 10^{-12}\right) /\left(4 \pi \varepsilon_{0} \times 10^{-2}\right) \approx 0.8998 \mathrm{~cm}$.
    ${ }^{13}$ These arguments are somewhat insufficient to say which size should be used for $a$ in the case of narrow, extended conductors, e.g., a thin, long wire of length $L$ and diameter $D \ll L$. In the Very soon we will see that in such cases the electrostatic energy, and hence $C$, should mostly depend on the larger size of the conductor.

[^176]:    ${ }^{14}$ See, e.g., CM Chapter 2.
    ${ }^{15}$ A word of caution: in condensed matter physics, voltage is usually defined differently, as the difference of electrochemical rather than electrostatic potentials - see, e.g., SM Sec. 6.4. These two definitions coincide if the conductors have equal workfunctions (for example, if they are made of the same material), and in this course their difference will be ignored.

[^177]:    $C_{m}$ of planar capacitor

[^178]:    ${ }^{16}$ Frequently referred to "fringe" fields resulting in an additional "stray" capacitance $C_{m}{ }^{\prime} \sim \varepsilon_{0} a$.
    ${ }^{17}$ Just as in Sec. 1, in order for the estimate to be realistic, I took into account the additional factor $\varepsilon_{r}$ (for aluminum oxide, close to 10 ) which should be included into the numerator of Eq. (28) to make it applicable to dielectrics - see Chapter 3 below.

[^179]:    ${ }^{18}$ In electrical engineering, such constant-potential conductor is called the ground. This term stems from the fact that in many cases the Earth surface may be considered a good electric ground, because its potential is unaffected by laboratory-scale electric charges.

[^180]:    ${ }^{19}$ See, e.g. MA Eq. (9.1).

[^181]:    ${ }^{20}$ See, e.g., MA Eq. (10.3).
    ${ }^{21}$ See, e.g., MA Eq. (10.2).

[^182]:    ${ }^{22}$ Alternative names for this surface are "degenerate ellipsoid", "ellipsoid of rotation", and "spheroid".

[^183]:    ${ }^{23}$ I have called disk's potential $V$, to distinguish it from the potential $\phi$ at an arbitrary point of space.

[^184]:    ${ }^{24}$ If you seriously worry about the formal infinity of charge density at $r \rightarrow R$, please remember that this mathematical artifact disappears for any nonvanishing disk thickness.
    ${ }^{25}$ The complex variable $z$ should not be confused with the (real) $3^{\text {rd }}$ spatial coordinate $z$ ! We are considering 2D problems now, with the potential independent of $z$.

[^185]:    ${ }^{26}$ The analytic (or "holomorphic") function may be defined as the one that may be expanded into the complex Taylor series, i.e. is infinitely differentiable in the given point. (Almost all "regular" functions, such as $\boldsymbol{z}^{n}, \boldsymbol{z}^{1 / n}$, $\exp \boldsymbol{z}, \ln \boldsymbol{z}$, etc. and their combinations are analytic at all $\boldsymbol{z}$, maybe besides certain special points.) If the reader needs to brush up his or her background on this subject, I can recommend a popular (and very inexpensive :-) textbook by M. Spiegel et al., Complex Variables, ${ }^{\text {nd }}$ ed., McGraw-Hill, 2009.
    ${ }^{27}$ These relations may be, in particular, to prove the famous Cauchy integral formula - see, e.g., MA Eq. (15.1).
    ${ }^{28}$ Let me remind the reader that in mathematics, term cylindrical describes a surface formed by translation, along a straight line, of an arbitrary curve, and hence more general than the usual circular cylinder. (In this terminology, for example, a prism is also a particular form of cylinder, formed by translating a polygon.)

[^186]:    ${ }^{29}$ See, e.g., textbook by P. Grivet, Electron Optics, $2^{\text {nd }}$ ed., Pergamon, 1972, or the review collection A. Septier (ed.), Focusing Charged Particles, vol. I, Academic Press, 1967, in particular the review by K.-J. Hanszen and R. Lauer, pp. 251-307.

[^187]:    ${ }^{30}$ Integral (70) includes only $(N-1)$ rather than $N$ poles, because polygon's shape is completely determined by $(N$ - 1) positions $\boldsymbol{\omega}_{j}$ of its vertices and $(N-1)$ angles $\pi k_{j}$. In particular, since the algebraic sum of all external angles of a polygon equals $\pi$, the last angle parameter $k_{j}=k_{N}$ is uniquely determined by the set of the previous ones.

[^188]:    ${ }^{31}$ See, e.g., MA Eq. (3.5).

[^189]:    ${ }^{32}$ This result could also be obtained using the so-called elliptical (not ellipsoidal!) coordinates.
    ${ }^{33}$ Another graphical representation of the electric field distribution, by field lines, is much less convenient. As a reminder, the field lines are defined as lines to whom the (in our current case, electrostatic) field vectors are tangential at each point. By this definition, the field lines are always normal to the equipotential surfaces, so that it is always straightforward to sketch them from the equipotential surface pattern - such as shown in Fig. 10.

[^190]:    ${ }^{34}$ Such distributions may be implemented in practice using so-called mosaic electrodes consisting of many electrically-insulated and individually-biased panels.

[^191]:    ${ }^{35}$ Note that according to Eqs. (91)-(92), as the spatial dimensions $a$ and $b$ of the system are increased, the distances between adjacent eigenvalues tend to zero. This fact implies that for spatially-infinite, non-periodic systems, the eigenvalue spectra are continuous, so that the sums of the type (84) become integrals. A few problems of this type are provided in Sec. 9 for reader's exercise.

[^192]:    ${ }^{36}$ See, e.g., MA Eq. (10.3) with $\partial / \partial z=0$.

[^193]:    ${ }^{38}$ This problem does belong to our current topic of electrostatic fields between conductors, because the uniform electric field may be created by a large plane capacitor.

[^194]:    ${ }^{39}$ Exceptions are possible only for highly symmetric configurations when the external field are crafted to make $a_{1}$ $=0$. In this case the solution is led by the first nonvanishing term of the series (121).

[^195]:    ${ }^{40}$ See，e．g．，MA Eq．（10．3）．
    ${ }^{41}$ Please note that this normalization is specific for each value of the variable separation parameter $\gamma$ ．Also，note that the normalization is meaningless for $\gamma=0$ ，i．e．for the case $Z(z)=$ const．However，if we need partial solutions for this value of $\gamma$ ，we can use Eqs．（108）－（109）．

[^196]:    ${ }^{42}$ For a more complete discussion of these functions, see the literature listed in MA Sec. 16, for example, Chapter 9 (written by F. Olver) in the collection compiled and edited by Abramowitz and Stegun.

[^197]:    ${ }^{43}$ These two formulas for the Bessel function peak are strictly valid for $n \gg 1$, but may be used for reasonable estimates starting already from $n=1$; for example, $\max _{\xi}\left[J_{1}(\xi)\right]$ is close to 0.58 and is reached at $\xi \approx 2.4$, just about $30 \%$ away from the values given by the asymptotic formulas.
    ${ }^{44}$ Eq. (135) and Fig. 16 clearly show the close analogy between the Bessel functions and the usual trigonometric functions, sine and cosine. In order to emphasize this similarity, and help the reader to develop more gut feeling of the Bessel functions, let me mention one fact of the elasticity theory: while sine functions describe, in particular, possible modes of standing waves on a guitar string, functions $J_{n}(\xi)$ describe, in particular, possible standing waves on an elastic round membrane, with $J_{0}(\xi)$ describing their lowest (fundamental) mode.

[^198]:    ${ }^{48}$ See, e.g., MA Eq. (6.7a). I used word "almost" because the gamma-function tends to infinity at all non-positive integer values of its argument $(s=0,-1 .-2, \ldots)$.
    ${ }^{49}$ They are also sometimes called the Neumann functions, and denoted as $N_{\wedge}(\xi)$.

[^199]:    ${ }^{50}$ A pair of independent linear functions，used for presentation of the general solution of the Bessel equation，may be also chosen in a different way，using the so－called Hankel functions

    $$
    H_{n}^{(1,2)}(\xi) \equiv J_{n}(\xi) \pm i Y_{n}(\xi) .
    $$

    For representing the general solution of Eq．（130），this alternative is completely similar to using the pair of complex functions $\exp \{ \pm i \alpha x\}=\cos \alpha x \pm i \sin \alpha x$ instead of the pair of real functions $\{\cos \alpha x, \sin \alpha x\}$ for representing the general solution of Eq．（89）for $X(x)$ ．

[^200]:    ${ }^{51}$ These complex functions still obey the general relations (143) and (146), with $\xi$ replaced with $\boldsymbol{z}$.

[^201]:    ${ }^{52}$ Later in the course we will also run into the so-called spherical Bessel functions $j_{n}(\xi)$ and $y_{n}(\xi)$, which may be expressed via the Bessel functions of a semi-integer order. Surprisingly enough, the spherical Bessel functions turn out to be much simpler than $J_{n}(\xi)$ and $Y_{n}(\xi)$.
    ${ }^{53}$ See, e.g., MA Eq. (10.9).

[^202]:    ${ }^{54}$ Just for reader's reference: if $l$ is not integer, the general solution of Eq. (2.168) may be represented as a linear combination of the so-called Legendre functions (not polynomials!) of the first and second kind, $\mathcal{P}_{1}(\xi)$ and $Q_{l}(\xi)$.

[^203]:    ${ }^{55}$ As a result, there is not practical sense, at least for the purposes of this course, in pursuing (more complex) solutions to Eq. (168) for non-integer values of $l$.

[^204]:    ${ }^{56}$ In quantum mechanics, letter $n$ is typically reserved used for the "main quantum number", while the azimuthal functions are numbered by index $m$. However, I will keep using $n$ as their index, because for this course's purposes, this seems more logical in the view of the similarity of the spherical and cylindrical functions.

[^205]:    ${ }^{57}$ In quantum mechanics, it is more convenient to use a slightly different set of basic functions, namely complex functions called spherical harmonics,

    $$
    Y_{l}^{n}(\theta, \varphi) \equiv\left[\frac{2 l+1}{4 \pi} \frac{(l-n)!}{(l+n)!}\right]^{1 / 2} P_{l}^{n}(\cos \theta) e^{i n \varphi},
    $$

    which are defined for both positive and negative $n$ (within the limits $-l \leq n \leq+l$ ), because they form a full set of orthonormal eigenfunctions of angular momentum operators $L^{2}$ and $L_{z}-$ see, e.g., QM Secs. 3.6 and 5.6.

[^206]:    ${ }^{58}$ According to Eq. (179), these functions involve only the Legendre polynomials $\mathcal{P}_{l} \equiv \mathcal{P}_{l}^{0}$.

[^207]:    59 Actually, this term (for which the author of these notes should be blamed :-) is misleading: operation of the "single-electron transistor" is based on the interplay of discrete charges (multiples of $e$ ) transferred between conductors, and sub-single-electron polarization charges - see, e.g., K. K. Likharev, Proc. IEEE 87, 606 (1999).

[^208]:    ${ }^{60}$ For more discussion of workfunction, and its effect on electron kinetics, see, e.g., SM Sec. 6.4.

[^209]:    ${ }^{61}$ The practical development of such "cold" cathodes is strongly affected by the fact that any nanoscale surface irregularity (a protrusion, an atomic cluster, or even a single "adatom" stuck to the surface) may cause a strong increase of the local field well above the average applied field $E_{0}$ (see, for example our discussion in Sec. 4 above), making the emission reproducibility an issue.

[^210]:    ${ }^{62}$ In geometry, such points, with $d d^{\prime}=R^{2}$, are referred to as the result of mutual inversion in a sphere of radius $R$.

[^211]:    ${ }^{63}$ See, e.g., CM Sec. 4.1, QM Secs. 2.2, 7.2 and 7.4, and SM Sec. 5.5.
    ${ }^{64} G$ so defined is sometimes called the Dirichlet function.

[^212]:    ${ }^{65}$ See, e.g., MA Eq. (12.3). Actually, this theorem is a ready corollary of the divergence theorem, MA Eq. (12.2).
    ${ }^{66}$ This symmetry, virtually evident from Eq. (204), may be formally proved by applying Eq. (207) to functions $f$ $(\mathbf{r}) \equiv G\left(\mathbf{r}, \mathbf{r}^{\prime}\right)$ and $g(\mathbf{r}) \equiv G\left(\mathbf{r}, \mathbf{r}^{\prime \prime}\right)$. With this substitution, the left-hand part becomes equal to $-4 \pi\left[G\left(\mathbf{r}^{\prime \prime}, \mathbf{r}^{\prime}\right)-G\left(\mathbf{r}^{\prime}\right.\right.$, $\left.\mathbf{r}^{\prime \prime}\right)$, while the right-hand part is zero, due to Eq. (205).

[^213]:    ${ }^{67}$ In some textbooks, the sign before the surface integral is negative, because their authors use the outer normal of the free-space region $V$ rather than that occupied by conductors - as I do.
    ${ }^{68}$ Indeed, if all parts of the cut plane are grounded, a narrow cut does not change the field distribution, and hence the Green's function, significantly.

[^214]:    ${ }^{69}$ See, for example, MA Secs. 16 (iii) and (iv).
    ${ }^{70}$ For more details see, e.g., R. Leveque, Finite Difference Methods for Ordinary and Partial Differential Equations, SIAM, 2007.

[^215]:    ${ }^{71}$ See, e.g., C. Johnson, Numerical Solution of Partial Differential Equations by the Finite Element Method, Dover, 2009, or T. J. R. Hughes, The Finite Element Method, Dover, 2000.

[^216]:    ${ }^{72}$ This fact should not be surprising, because Eq. $\left(^{*}\right)$ is essentially the conformal map $\boldsymbol{z}=c \cosh \boldsymbol{\omega}$, where $\boldsymbol{z}=x+$ $i y$, and $\boldsymbol{\mu}=\alpha+i \beta$ - see the discussion in Sec. 4 .

[^217]:    ${ }^{73}$ As a reminder, the double factorial (also called "semifactorial") operator (!!) is similar to the usual factorial operator (!), but with the product limited to numbers of the same parity as its argument (in our particular case, of the odd numbers in the numerator, and even numbers in the denominator).

[^218]:    ${ }^{74}$ In this context, weak junction means a tunnel junction with transparency so low that the tunneling electron's wavefunction looses its quantum-mechanical coherence before the electron has time to tunnel back. In a typical junction of a macroscopic area this condition is fulfilled if the effective tunnel resistance of the junction is much higher than the quantum unit of resistance (see, e.g., QM Sec. 3.2), $R_{Q} \equiv \pi \hbar / 2 e^{2} \approx 6.5 \mathrm{k} \Omega$.

[^219]:    ${ }^{75}$ Here the notation $\tan ^{-1}$ is used for the multi-valued function (alternatively called Arctan) which is reciprocal to $\tan$. (Due to the $\pi$-periodicity of the tan, function $\tan ^{-1}$ is defined to an arbitrary additive multiple of $\pi$.) At the value interval $[-\pi / 2,+\pi / 2], \tan ^{-1}$ is usually called arctan.

[^220]:    ${ }^{1}$ See, e.g., MA Eq. (2.11b).
    ${ }^{2}$ The third term (responsible for quadrupole effects), as well as all the following, multipole terms would require a tensor (rather then vector) representation.

[^221]:    ${ }^{3}$ Accordingly, a localized system of charges with $Q=0$, but $\mathbf{p} \neq 0$, is called an (electric) dipole.

[^222]:    ${ }^{4}$ Other examples of dipole fields are given by two more systems discussed in Chapter 2 - see Eqs. (2.215) and (2.219). Those systems, however, do have higher-order multipole moments, so that for them, Eq. (7) gives only the long-distance approximation.
    ${ }^{5}$ See, e.g., MA Eq. (10.8) with $\partial / \partial \varphi=0$.

[^223]:    ${ }^{6}$ See, e.g., SM Sec. 3.5.
    ${ }^{7}$ The equivalence may be proved, for example, by using MA Eq. (11.6) with $\mathbf{f}=\mathbf{p}=$ const and $\mathbf{g}=\mathbf{E}_{\text {ext }}$, taking into account that according to the general Eq. (1.28), $\nabla \times \mathbf{E}_{\text {ext }}=0$.

[^224]:    ${ }^{8}$ See, e.g., the end of Sec. 4.1 in the textbook by J. Jackson, Classical Electrodynamics, $3^{\text {rd }}$ ed., Wiley, 1999.

[^225]:    ${ }^{9}$ To prove this (almost evident) formula strictly, it is sufficient to apply the divergence theorem given by MA Eq. (12.2), to vector function $\mathbf{f}=\mathbf{P}\left(\mathbf{r}^{\prime}\right) /\left|\mathbf{r}-\mathbf{r}^{\prime}\right|$, in the "source space" of radius-vectors $\mathbf{r}$ '.

[^226]:    ${ }^{10}$ Note that the dimensionality of $\mathbf{D}$ in SI units is different from that of $\mathbf{E}$. In contrast, in the Gaussian units the electric displacement is defined as $\mathbf{D}=\mathbf{E}+4 \pi \mathbf{P}$, so that $\nabla \cdot \mathbf{D}=4 \pi \rho$ (the relation $\rho_{\mathrm{ef}}=-\nabla \cdot \mathbf{P}$ remains the same as in SI units), and the dimensionalities of $\mathbf{D}$ and $\mathbf{E}$ coincide. Philosophically, this coincidence is a certain handicap, because it is frequently convenient to consider Cartesian components of $\mathbf{E}$ as a generalized force, and those of $\mathbf{D}$ as a generalized coordinate (see Sec. 6 below), and it is comforting to have their dimensionality different.

[^227]:    ${ }^{11}$ Note, however, that such averaging does not include the inner-dipole fields which is (approximately) described by the second term of Eq. (25).
    ${ }^{12}$ In anisotropic materials, such as crystals, a susceptibility tensor may be necessary to give an adequate description of the linear relation of vectors $\mathbf{P}$ and $\mathbf{E}$. Fortunately, in most important crystals (such as silicon) the anisotropy of polarization is small, so that they may be reasonably well characterized by scalar susceptibility.

[^228]:    ${ }^{13}$ Note that in electrical engineering literature, the dielectric constant is often denoted by letters $\kappa$ or $K$.
    ${ }^{14}$ In Gaussian units, $\chi_{e}$ is defined by relation $\mathbf{P}=\chi_{e} \mathbf{E}$, while $\varepsilon$ is still defined as $\mathbf{D}=\varepsilon \mathbf{E}$. Because of that, $\varepsilon$ is dimensionless and equals $\left(1+4 \pi \chi_{e}\right)$. Note that $(\varepsilon)_{\text {Gaussian }}=\left(\varepsilon / \varepsilon_{0}\right)_{\mathrm{SI}}=\varepsilon_{\mathrm{r}}$, and $\left(\chi_{e}\right)_{\mathrm{SI}}=4 \pi\left(\chi_{e}\right)_{\text {Gaussian }}$, sometimes creating a confusion with the numerical values of the latter parameter.

[^229]:    ${ }^{15}$ Note that for all materials listed in Table $1, \varepsilon_{r}>1$, i.e. $\alpha_{\text {mol }}>0$. Actually, this is true for all stable dielectrics. Let me postpone a discussion of this fact until Sec. 5.5 where I will compare physical mechanisms of the electric and magnetic polarization.
    ${ }^{16}$ A more accurate model of atomic polarization is discussed in QM Chapter 6.
    ${ }^{17}$ See, e.g., SM Secs. 1.4 and 3.1.
    ${ }^{18}$ Such radius is defined by the requirement that the volume of the corresponding sphere, used in the van-derWaals equation (see, e. g., SM Sec. 4.1) gives the best fit to the experimental equation of state $n=n(P, T)$.

[^230]:    ${ }^{19}$ Actually, selecting the slit size $d$ much less that the characteristic scale of the field change, we can apply the following arguments to any external field distribution.

[^231]:    ${ }^{20}$ This is true for any ellipsoid, at arbitrary external field orientation.

[^232]:    ${ }^{21}$ The reader may wonder how have we managed to proof Eq. (24), at least for this particular case, using only the relations based on the dipole approximation (7) for the field, which does not cover the inter-dipole fields responsible for Eq. (24) - see Fig. 3 and its discussion. The reason is that according to Eq. (30), the additional field $\mathbf{E}_{\text {self }}$ inside the sphere may be considered as been created by effective charges, of density $\rho_{\text {ef }}$, distributed on sphere's surface. For these charges, field $\mathbf{E}_{\text {ef }}$ is internal, similar to the field between two charges, shown in Fig. 3.

[^233]:    ${ }^{22}$ This qualifier is important: $\mathbf{E}$ is the long-range (dipole field) average participating in the macroscopic Maxwell equations, rather than the exact average that would include the inner-dipole fields, for which Eq. (24) would be valid.
    ${ }^{23}$ This geometry, due to its isotropy, most fairly represents the relation between $\mathbf{E}$ and $\mathbf{E}_{0}$.

[^234]:    ${ }^{24}$ It was derived by in 1869 by L. Lorenz and then (in 1878) independently by H. Lorentz. Actually, they discussed optical frequencies at which $\varepsilon_{r}$ should be understood as the square of the refraction coefficient at the wave frequency (see Chapter 7), but since the optical wavelengths $\sim 10^{-4} \mathrm{~m}$ are much longer than interatomic distances $a \sim 10^{-9} \mathrm{~m}$, the derivation remains absolutely the same in electrostatics.
    ${ }^{25}$ Any quantitative description of this transition should account of for thermal fluctuations of the molecular dipoles, which reduce the dipole-dipole ordering and hence suppress the transition to the ferroelectric phase until temperature has been lowered to a certain Curie temperature $T_{\mathrm{C}}$ - named after P. Curie (1859-1906). Right above that temperature, the dielectric remains linear, but has a high, temperature-dependent dielectric constant that diverges at $T \rightarrow T_{\mathrm{C}}$. Such materials are frequently called paraelectric, and the paraelectric-to-ferroelectric transition at $T_{\mathrm{C}}$ in crystals is a typical example of a continuous (or "second-order") phase transition - see, e.g., SM Sec. 4.4. (As will be discussed in Sec. 5.5 below, some magnetic materials exhibit a very similar phase transition between their ferromagnetic and paramagnetic phases.) Moreover, in non-crystalline materials, such as bulk ceramics and thin films, the ferroelectric behavior is further complicated by different, field-dependent

[^235]:    directions of polarization $\mathbf{P}$ in individual "domains" of the sample, making the average hysteresis more smooth (Fig. 11a) and dependent on sample's polarization history - for example the amplitude of the applied ac electric field (Fig. 11b).
    ${ }^{26}$ See, e.g., J. F. Scott, Ferroelectric Memories, Springer, 2000.
    ${ }^{27}$ For a detailed coverage of ferroelectrics, I can recommend an encyclopedic monograph by M. Lines and A. Glass, Principles and Applications of Ferroelectrics and Related Materials, Oxford U. Press, 2001, and a recent collection of reviews by K. Rabe, C. Ahn, and J.-M. Triscone (eds.), Physics of Ferroelectrics: A Modern Perspective, Springer, 2010.

[^236]:    ${ }^{28}$ See, e.g., MA Eq. (11.4a).
    ${ }^{29}$ Again, in Gaussian units this expression should be divided by $4 \pi$.

[^237]:    ${ }^{30}$ This is the point where the SI units, prescribing fields $\mathbf{E}$ and $\mathbf{D}$ different dimensionalities, are more revealing than the Gaussian units.
    ${ }^{31}$ See, e.g., CM Sec. 1.5. Note that as Eq. (84) clearly illustrates, once again, that the difference between potential energies $g$ and $U$, usually discussed in courses of statistical physics and/or thermodynamics as the difference between the Gibbs and Helmholtz free energies (see, e.g., SM 1.6), exists regardless of statistics or thermal motion.

[^238]:    ${ }^{32}$ In electrical engineering, such materials (typically, synthetic polymers) are frequently called electrets. As an approximation, this condition may be applied to hard ferroelectrics, if the external or self-induced electric fields are not too high.

[^239]:    ${ }^{1}$ Just as a (hopefully, unnecessary :-) reminder, in the SI units the current is measured in amperes (A). In the legal metrology, the ampere (rather than the coulomb, which is defined as $1 \mathrm{C}=1 \mathrm{~A} \times 1 \mathrm{~s}$ ) is a primary unit. I will mention its formal definition in the next chapter. In the Gaussian units, Eq. (1) remains the same, so that the current's unit is the so-called statampere - defined as statcoulomb per second.

[^240]:    ${ }^{2}$ Similar differential relations are valid for the density of any conserved quantity, for example for mass in classical fluid dynamics (see, e.g., CM Sec. 8.2), and for the probability in statistical physics (SM Sec. 5.6) and quantum mechanics (QM Sec. 1.4).

[^241]:    ${ }^{3}$ In SI units, the conductivity is measured in siemens per meter, where one siemens $(S)$ is the reciprocal of one ohm: $1 \mathrm{~S} \equiv(1 \Omega)^{-1} \equiv 1 \mathrm{~A} / 1 \mathrm{~V}$. The constant reciprocal to conductivity, $1 / \sigma$, is called resistivity, and is commonly denoted by letter $\rho$. I will, however, try to avoid using this notion, because I am already overusing this letter.

[^242]:    ${ }^{4}$ As will be discussed in Chapter 6, such simple analysis is only valid if $\sigma$ is not too high.
    ${ }^{5}$ It was suggested by P. Drude in 1900.

[^243]:    ${ }^{6}$ For such a discussion see, e.g., SM Sec. 6.3.
    ${ }^{7}$ Electrodynamic properties of superconductors are so interesting (and important) that I will discuss them in more detail in Chapter 6.

[^244]:    ${ }^{8}$ Unfortunately, these notes are not an appropriate platform to discuss details of the floating-gate memory technology. However, I think that every educated physicist should know its basics, because such memories are presently the driver of all semiconductor integrated circuit technology development, and hence of the whole information technology progress. Perhaps the best available book is J. Brewer and M. Gill (eds.), Nonvolatile Memory Technologies with Emphasis on Flash, IEEE, 2008.

[^245]:    ${ }^{9}$ The first of Eqs. (21) is essentially the integral form of the Ohm law (8), and is valid not only for a uniform wire, but for any Ohmic conductor with a geometry in which $I$ and $V$ may be clearly defined.

[^246]:    ${ }^{10}$ Such situations are even more natural in 2D situations, for example, think about a wire soldered, in a small spot, to a thin metallic foil. (Note that here the current density distribution law is different, $j \propto 1 / r$ rather than $1 / r^{2}$.)

[^247]:    ${ }^{11}$ In practice, the current injection may be produced, due to electrochemical reactions, by an ore mass itself, so that one need only measure (and interpret :-) the resulting potential distribution - the so-called self-potential method - see, e.g., Sec. 6.1 in monograph by W. Telford et al., Applied Geophysics, $2^{\text {nd }}$ ed., Cambridge U. Press, 1990.
    ${ }^{12}$ Since the electric field and hence the electrostatic energy are time-independent, this means that the energy is replenished at the same rate from the current source(s).

[^248]:    ${ }^{13}$ As was mentioned in Sec. 4.2 of the lecture notes, the assumption of constant (charge-density-independent) mobility is most suitable for semiconductors.

[^249]:    ${ }^{1}$ The most important case when the electroneutrality does not hold is the motion of electrons in vacuum. In this case, magnetic forces coexist with (typically, stronger) electrostatic forces - see Eq. (3) below and its discussion. In some semiconductor devices, local violations of electroneutrality also play an important role.
    ${ }^{2}$ Most notably, by H. C. Ørsted, J.-B. Biot and F. Savart, and A.-M. Ampère.
    ${ }^{3}$ In the Gaussian units, coefficient $\mu_{0} / 4 \pi$ is replaced with $1 / c^{2}$ (i.e., implicitly with $\mu_{0} \varepsilon_{0}$ ) where $c$ is the speed of light, in modern metrology considered exactly known - see, e.g., appendix CA: Selected Physical Constants.

[^250]:    ${ }^{4}$ The discovery and initial studies of such a subtle, relativistic phenomenon as magnetism in the early 19th century was much facilitated by the relative abundance of natural ferromagnets, materials with spontaneous magnetic polarization, whose strong magnetic field may be traced back to relativistic effects (such as spin) in atoms. (The electrostatic analogs of such materials, electrets, are much more rare.) I will briefly discuss the ferromagnetism in Sec. 5 below.

[^251]:    ${ }^{5}$ In particular, Eq. (7) is used for the legal definition of the SI unit of current, one ampere (A), via the SI unit of force (the newton, N ), with coefficient $\mu_{0}$ fixed as listed above.

[^252]:    ${ }^{6}$ The SI unit of the magnetic field is called tesla, T - after N. Tesla, an electrical engineering pioneer. In the Gaussian units, the already discussed constant $1 / c^{2}$ in Eq. (1) is equally divided between Eqs. (8) and (9), so that in them both, the constant before the integral is $1 / c$. The resulting Gaussian unit of field $\mathbf{B}$ is called gauss (G); taking into account the difference of units of electric charge and length, and hence current density, 1 G equals exactly $10^{-4} \mathrm{~T}$. Note also that in some textbooks, especially old ones, $\mathbf{B}$ is called either the magnetic induction, or the magnetic flux density, while the term "magnetic field" is reserved for vector $\mathbf{H}$ that will be introduced Sec. 5 below.
    Named after H. Lorentz, who received a Nobel prize for his explanation of the Zeeman effect, but is more famous for his numerous contributions to the development of special relativity - see Chapter 9. To be fair, the magnetic part of the Lorentz force was correctly calculated first by O. Heaviside.

[^253]:    ${ }^{8}$ See, e.g., MA Eq. (7.5).
    ${ }^{9}$ Just in electrostatics, one needs to exercise due caution at transfer from these expressions to the limit of discrete classical particles, and extended wavefunctions in quantum mechanics, in order to avoid the (non-existing) magnetic interaction of a charged particle upon itself.

[^254]:    ${ }^{10}$ In the Gaussian units, Eq. (27) remains the same, and hence in Eq. (28), coefficient $\mu_{0} / 4 \pi$ is replaced with $1 / c$.
    ${ }^{11}$ See, e.g., MA Eq. (11.2).
    ${ }^{12}$ See, e.g., MA Eq. (11.3).

[^255]:    ${ }^{13}$ As in all earlier formulas for the magnetic field, in the Gaussian units the coefficient $\mu_{0}$ in this relation has to be replaced with $4 \pi / c$.
    ${ }^{14}$ See, e.g., MA Eq. (12.1) with $\mathbf{f}=\mathbf{B}$.

[^256]:    ${ }^{15}$ Applying the Ampère law to a circular contour of radius $\rho$, coaxial with the solenoid, we see that the field outside (but not inside!) it has an azimuthal component $B_{\varphi}$, similar to that of the straight wire (see Eq. (38) above) and hence (at $N \gg 1$ ) much weaker than the longitudinal field inside the solenoid - see Eq. (40).

[^257]:    ${ }^{16}$ See, e.g., MA Eq. (11.1).
    ${ }^{17}$ The use of term "gauge" (originally meaning "a measure" or "a scale") in this context is purely historic, so the reader should not try to find too much hidden sense in it.
    ${ }^{18}$ See, e.g., MA Eq. (10.3).

[^258]:    ${ }^{19}$ See, e.g., MA Eq. (10.5) with $\partial / \partial \varphi=\partial / \partial z=0$.
    ${ }^{20}$ Since the magnetic field at the wire axis has to be zero (otherwise, being perpendicular to the axis, where would it be directed?), the integration constant in Eq. (50) should be zero.
    ${ }^{21}$ See, e.g., MA Eq. (10.6).
    ${ }^{22}$ See, e.g., MA Eq. (8.5).
    ${ }^{23}$ See, e.g., QM Sec. 3.2.

[^259]:    ${ }^{24}$ This relation remains the same in the Gaussian units, because in those units both Eq. (28) and Eq. (54) should be stripped of their $\mu_{0} / 4 \pi$ coefficients.
    ${ }^{25}$ For that, we may use MA Eq. (11.7) with $\mathbf{f}=\mathbf{A}$ and $\mathbf{g}=\mathbf{B}$, giving $\mathbf{A} \cdot(\nabla \times \mathbf{B})=\mathbf{B} \cdot(\nabla \times \mathbf{A})-\nabla \cdot(\mathbf{A} \times \mathbf{B})$.

[^260]:    ${ }^{26}$ The transfer to the Gaussian units in Eqs. (77)-(78) may be accomplished by the usual replacement $\mu_{0} \rightarrow 4 \pi$, thus giving, in particular, $u=B^{2} / 8 \pi$.
    ${ }^{27}$ As evident from Eq. (60), these coefficients depend only on the geometry of the system. Moreover, in the Gaussian units, in which Eq. (60) is valid without the factor $\mu_{0} / 4 \pi$, the inductance coefficients have the dimension of length (centimeters). The SI unit of inductance is called the henry, abbreviated H-after J. Henry, 1797-1878, who in particular discovered the effect of electromagnetic induction (see Sec. 6.1) independently of M. Faraday. ${ }^{28}$ Note that the matrix of the mutual inductances $L_{i j}$, is very much similar to the matrix of reciprocal capacitance coefficients $p_{k k^{\prime}}$ - for example, compare Eq. (62) with Eq. (2.21).

[^261]:    ${ }^{29}$ The SI unit of magnetic flux is called weber, abbreviated Wb - after W. Weber, who in particular co-invented (with C. Gauss) the electromagnetic telegraph, and in 1856 was first, together with R. Kohlrausch, to notice that the value of (in modern terms) $1 /\left(\varepsilon_{0} \mu_{0}\right)^{1 / 2}$, derived from electrostatic and magnetostatic measurements, coincides with the independently measured speed of light $c$, giving an important motivation for Maxwell's theory.

[^262]:    ${ }^{30}$ Numerous applications of this Neumann formula to electrical engineering problems may be found, for example, in the classical text F. Grover, Inductance Calculations, Dover, 1946.

[^263]:    ${ }^{31}$ As a reminder, the mutual capacitance $C$ between the conductors of such a system was calculated in Sec. 2.3. As will be discussed in Chapter 7 below, the pair of parameters $L$ and $C$ define the propagation of the most important, TEM mode of electromagnetic waves along the cable.

[^264]:    ${ }^{32}$ See, e.g., MA Eq. (6.13) for $a=1$.

[^265]:    ${ }^{33}$ Its solution may be found, for example, just after Sec. 34 of L. Landau et al., Electrodynamics of Continuous Media, $2^{\text {nd }}$ ed., Butterwort Heinemann, 1984.
    ${ }^{34}$ See, e.g., MA Eq. (12.3) with additional condition $\left.j_{n}\right|_{S}=0$, pertinent for space-restricted currents.

[^266]:    ${ }^{35}$ In the Gaussian units, definition (91) is kept valid, so that Eq. (90) is stripped of the factor $\mu_{0} / 4 \pi$.

[^267]:    ${ }^{36}$ In SI units, $m_{e} \approx 0.91 \times 10^{-30} \mathrm{~kg}$, so that $\mu_{\mathrm{B}} \approx 0.93 \times 10^{-23} \mathrm{~J} / \mathrm{T}$.
    ${ }^{37}$ See, e.g., QM Sec. 4.1 and beyond.
    ${ }^{38}$ Another way to arrive at the same estimate is to take $I \sim e f=e \omega / 2 \pi$ with $\omega \sim 10^{16} \mathrm{~s}^{-1}$ being the typical frequency of radiation due to atomic interlevel quantum transitions.

[^268]:    ${ }^{39}$ Similarly to the situation with the electric dipoles (see Eq. (3.24) and its discussion), it may be shown that the magnetic field of any closed current loop (or any system of such loops) satisfies the following equality:

    $$
    \int_{r<R} \mathbf{B}(\mathbf{r}) d^{3} r=(2 / 3) \mu_{0} \mathbf{m}
    $$

    where the integral is over any sphere confining all the currents. On the other hand, for field (99), derived from the asymptotic approximation (90), such integral vanishes. In order to get a course-grain description of the magnetic field of a small system located at $r=0$, which would be valid everywhere (though at $r \sim a$, only approximately), Eq. (99) should be modified as follows:

    $$
    \mathbf{B}_{c g}(\mathbf{r})=\frac{\mu_{0}}{4 \pi}\left(\frac{3 \mathbf{r}(\mathbf{r} \cdot \mathbf{m})-\mathbf{m} r^{2}}{r^{5}}+\frac{8 \pi}{3} \mathbf{m} \delta(\mathbf{r})\right) .
    $$

    Hence, strictly speaking, the macroscopic field $\mathbf{B}$ participating in Eq. (106) and beyond is the average long-range field of the magnetic dipoles (plus of the stand-alone currents $\mathbf{j}$ ) rather than the genuine average magnetic field.
    ${ }^{40}$ This confusion is exacerbated by the fact that in Gaussian units, Eq. (108) has the form $\mathbf{H}=\mathbf{B}-4 \pi \mathbf{M}$, and hence fields $\mathbf{B}$ and $\mathbf{H}$ has one dimensionality (and are equal in free space!) - though the unit of $\mathbf{H}$ has a different name (oersted, abbreviated as Oe). Mercifully, in the SI units, the dimensionality of $\mathbf{B}$ and $\mathbf{H}$ is different, with the unit of $\mathbf{H}$ being called ampere per meter.

[^269]:    ${ }^{41}$ According to Eq. (110) (i.e. in SI units), $\chi_{m}$ is dimensionless, while $\mu$ has the same the same dimensionality as $\mu_{0}$. In the Gaussian units, $\mu$ is dimensionless, $(\mu)_{\text {Gaussian }}=(\mu)_{\mathrm{SI}} / \mu_{0}$, and $\chi_{m}$ is also introduced differently, as $\mu=1+$ $4 \pi \chi_{m}$, Hence, just as for the electric susceptibilities, these dimensionless coefficients are different in the two systems: $\left(\chi_{m}\right)_{\mathrm{SI}}=4 \pi\left(\chi_{m}\right)_{\text {Gaussian }}$. Note also that $\chi_{m}$ is formally called the volume magnetic susceptibility, in order to distinguish it from the molecular susceptibility $\chi$ defined by a similar relation, $\mathbf{m} \equiv \chi \mathbf{H}$, where $\mathbf{m}$ is the average induced magnetic moment of a single dipole - e.g., a molecule. Evidently, in a dilute medium, i.e. in the absence of substantial dipole-dipole interaction, $\chi_{m}=n \chi$, where $n$ is the dipole density.

[^270]:    ${ }^{42}$ The proportionality of $\left|\left\langle p_{0}\right\rangle\right|$ (and hence $P$ ) to $E$ is a result of a dynamic balance between the dipole-orienting torque (101) and disordering thermal fluctuations. A qualitative description of such balances is one of the main tasks of statistical mechanics - see, e.g., SM Chapters 2 and 4. However, the very fact of proportionality $P \propto E$ in low fields may be readily understood as the result of the Taylor expansion of function $P(E)$ at $E \rightarrow 0$.
    ${ }^{43}$ After J. Larmor (1857-1947) who first described the torque-induced precession mathematically.

[^271]:    ${ }^{44}$ For a detailed discussion of the effect see, e.g., CM Sec. 6.5.
    ${ }^{45}$ The quantum-mechanical treatment (see, e.g., QM Sec. 6.4) confirms this qualitative picture, while giving quantitative corrections to the classical result for $\chi_{m}$.

[^272]:    ${ }^{46}$ See, e.g., D. J. Jiles, Introduction to Magnetism and Magnetic Materials, $2^{\text {nd }}$ ed., CRC Press, 1998, or R. C. O'Handley, Modern Magnetic Materials, Wiley, 1999.
    ${ }^{47}$ Materials with very high coercivity $H_{C}$ are frequently called hard ferromagnets or permanent magnets.

[^273]:    ${ }^{48}$ A discussion of such transitions may be found, in particular, in SM Chapter 4.
    49 "A magnetic head slider [the read/write head - KKL] flying over a [rather uneven - KKL] disk surface with a flying height of 25 nm with a relative speed of 20 meters/second is equivalent to an aircraft flying at a physical spacing of $0.2 \mu \mathrm{~m}$ at 900 kilometers/hour." B. Bhushan, as quoted in a (generally good) book by G. Hadjipanayis, Magnetic Storage Systems Beyond 2000, Springer, 2001.

[^274]:    ${ }^{50}$ The reader is highly encouraged to carry out a similar analysis of fields inside narrow gaps cut in a linear magnetic, similar to that carried out for linear dielectrics in Sec. 3.3 - see Fig. 3.6 and its discussion.

[^275]:    ${ }^{51}$ This similarity may seem strange, because earlier we have seen that parameter $\mu$ is physically more similar to $1 / \varepsilon$. The reason for this paradox is that in magnetostatics, the introduced potential $\phi_{m}$ is traditionally used to describe the "would-be field" $\mathbf{H}$, while in electrostatics, potential $\phi$ describes the real (average) electric field $\mathbf{E}$. (This tradition persists from the old days when $\mathbf{H}$ was perceived as a genuine magnetic field.)
    ${ }^{52}$ Instead of differentiating the $\phi_{m}$ given by Eq. (125a), we may use the absolute similarity of Eqs. (3.13) and (99), to derive from Eq. (3.17) a similar expression for the magnetic potential of an arbitrary magnetic dipole:

    $$
    \phi_{m}=\frac{1}{4 \pi} \frac{m \cos \theta}{r^{2}} .
    $$

    Now comparing this formula with the second term of Eq. (125a), we immediately get Eq. (125b).

[^276]:    ${ }^{53}$ From the standpoint of mathematics, this happens because the solution to a boundary problem is determined by not only the differential equation inside the system (in our case, the Laplace equation for potential $\phi_{m}$ ), but also by boundary conditions - which are affected by magnetics - see Eqs. (118)-(119).
    ${ }^{54}$ Note that in this respect, the analogy with electrostatics is incomplete. Indeed, according to Eq. (3.82), in electrostatics the role of a generalized coordinate is played by would-be field $\mathbf{D}$, and that of the generalized force, by the real (average) electric field $\mathbf{E}$. This difference may be traced back to the fact that electric field $\mathbf{E}$ may perform work on a moving charged particle, while the magnetic part of the Lorentz force (10), $\mathbf{v} \times \mathbf{B}$, is always perpendicular to particle's velocity, and its work equals zero. However, this difference does not affect the full analogy of expressions (3.79) and (127) for field energy density in linear media.

[^277]:    ${ }^{57}$ Such system, producing a highly uniform field near its center, is called the Helmholtz coils, and is broadly used in physics experiment.

[^278]:    ${ }^{58}$ It was invented by M. Faraday in 1821, i.e. well before his celebrated work on electromagnetic induction. The adjective "homopolar" refers to the constant "polarity" (sign) of the current; the alternative term is "unipolar".

[^279]:    ${ }^{59}$ See, e.g., MA (6.13).

[^280]:    ${ }^{60}$ This problem is of an evident relevance for the perpendicular magnetic recording (PMR) technology, which presently dominates the high-density digital magnetic recording, with the density already approaching $1 \mathrm{~Tb} / \mathrm{in}^{2}$.

[^281]:    ${ }^{1}$ The induction e.m.f. was discovered independently by J. Henry and M. Faraday, but is was a brilliant experiment series of the latter physicist, carried out in 1831, which resulted in this general formulation of the law.
    ${ }^{2}$ In Gaussian units, the right-hand part of this formula has the additional coefficient $1 / c$.
    ${ }^{3}$ If necessary, see MA Eq. (12.1) again.

[^282]:    ${ }^{4}$ Let me admit that from the beginning of the course, I was carefully sweeping under the rug a very important question: in what exactly reference frame(s) all the equations of electrodynamics are valid? I promise to discuss this issue in detail later in the course (in Chapter 9), and for now would like to get away with a very short answer: all the formulas discussed so far are valid any inertial reference frame, as defined in classical kinematics - see, e.g., CM Chapter 1. It is crucial, however, to have fields $\mathbf{E}$ and $\mathbf{B}$ measured in the same reference frame.
    ${ }^{5}$ See, e.g., MA Eq. (11.1).

[^283]:    ${ }^{6}$ See, e.g., MA Eq. (7.6).

[^284]:    ${ }^{7}$ Actually, Eq. (14) is just an integral version of Eq. (5.128).
    ${ }^{8}$ Actually, the absence of time-dependent corrections to other Maxwell equations in the quasistatic approximation should be considered as an additional experimental fact.

[^285]:    ${ }^{9}$ Due to the simple linear relation between fields $\mathbf{B}$ and $\mathbf{H}$, it does not matter too much which of them is used for the solution of this problem. A slight preference is for $\mathbf{H}$, due to the simplicity of the boundary condition (5.118).

[^286]:    ${ }^{10}$ Another important opportunity to exploit the linearity of Eq. (6.20) (as well as any linear, homogeneous differential equation) is to use the spatial-temporal Green's function approach to explore the dependence of its solutions on various initial conditions. Unfortunately, because of lack of time, I have to leave such exploration for reader's exercise.
    ${ }^{11}$ This common name is awkward, because Eq. (26) results from macroscopic Maxwell equations (16), but is justified as the counterpart to the "macroscopic" boundary condition (30), to be discussed in a minute.

[^287]:    ${ }^{12}$ They are frequently called eddy currents, because of the loop form of their lines. (In the 1D geometry explored above these loops are implicit, closing at infinity.)
    ${ }^{13}$ Notice that vectors $\mathbf{j}$ and $\mathbf{E}$ are parallel, and have the same time dependence. This means that the time average of the power dissipation $\mathbf{j} \cdot \mathbf{E}$ is finite. We will return to its discussion later in this chapter.

[^288]:    ${ }^{14}$ A brief discussion of the mean free path may be found, for example, in SM Chapter 6. In very clean metals at low temperatures, $\delta_{\mathrm{s}}$ may approach $l$ at frequencies as low as $\sim 1 \mathrm{GHz}$, though at room temperature the crossover from the normal to the anomalous skin affect takes place at $\sim 100 \mathrm{GHz}$.
    ${ }^{15}$ See, e.g., A. Abrikosov, Introduction to the Theory of Normal Metals, Academic Press, 1972.
    ${ }^{16}$ Discovered experimentally in 1911 by H. Kamerlingh Onnes.

[^289]:    ${ }^{17}$ Named to acknowledge the pioneering theoretical work of brothers F. and H. London - see below.
    ${ }^{18}$ It is hardly fair to shorten the name to just the "Meissner effect", as it is frequently done, because of the reportedly crucial contribution made by R. Ochsenfeld, then W. Meissner's student, into the discovery.

[^290]:    ${ }^{19}$ A qualitative discussion of the Bose-Einstein condensation of bosons may be found in SM Sec. 3.4, though the full theory of superconductivity is more complex, because it describes the condensation taking place simultaneously with the formation of effective bosons (Cooper pairs). For a more detailed coverage of physics of superconductors, the reader may be referred, for example, to the already cited monograph by M. Tinkham, Introduction to Superconductivity, $2^{\text {nd }}$ ed., McGraw-Hill, 1996.
    ${ }^{20}$ See, e.g., QM Sec. 1.4, in particular Eq. (1.47).
    ${ }^{21}$ I am sorry to use traditional notations $\mathbf{p}$ and $\mathbf{P}$ for the momenta - the same symbols which were used for the electric dipole moment and polarization in Chapter 3. I hope there will be no confusion, because the latter notions are not used in this section.
    ${ }^{22}$ See, e.g., CM Sec. 10.1, in particular Eq. (10.26).

[^291]:    ${ }^{23}$ This is the so-called London gauge which, for our geometry, is also the Coulomb gauge.
    ${ }^{24}$ Since not all electrons of a superconductor form Cooper pairs, at any frequency $\omega \neq 0$ they provide Joule losses which are not described by Eq. (48). These losses become very substantial when frequency $\omega$ becomes so high that the skin-effect length $\delta_{s}$ of the material (as measured with superconductivity suppressed, say by high magnetic field) becomes less than $\delta_{\mathrm{L}}$. For typical metallic superconductors, this happens at frequencies of a few hundred GHz , so that even for microwaves, Eq. (51) gives a fairly good description of the field penetration.

[^292]:    ${ }^{25}$ Of course, this analogy sweeps under the rug the real physics of the Meissner-Ochsenfeld effect. In particular, in superconductors the role of the surface "magnetization currents" with effective density $\mathbf{j}_{\text {ef }}=\nabla \times \mathbf{M}$ (see Fig. 5.11 and its discussion) is played by the real, persistent surface supercurrents (48).
    ${ }^{26}$ The interested reader may be referred, e.g., to Chapter 5 of M. Tinkham's monograph cited above.

[^293]:    ${ }^{27}$ Independently and virtually simultaneously by two groups: B. Deaver and W. Fairbank, and R. Doll and M. Näbauer, so that their reports were published back-to-back in Phys. Rev. Lett.
    ${ }_{28}$ Actually, the ring is not entirely necessary. In 1957, A. Abricosov used the Ginzburg-Landau equations (see below) to explain the counter-intuitive behavior of the so-called type-II superconductors, known experimentally as the Shubnikov phase since the 1930s. He showed that high magnetic field may penetrate into such

[^294]:    ${ }^{31}$ This derivation belongs to L. Aslamazov and A. Larkin, JETP Lett. 9, 87 (1969). If the reader is not interested in this topic, he or she may safely skip it, jumping directly to the text following Eq. (68).
    ${ }^{32}$ At $T \rightarrow T_{\mathrm{c}}$, where $n_{s} \rightarrow 0$, the Taylor expansion of the nonlinear function in Eq. (60) may be limited to just one term proportional to $|\psi|^{2} \propto n_{s}$. In this limit, Eq. (60) is called the Ginzburg-Landau equation - see SM (4.58). Derived by V. Ginzburg and L. Landau in 1950 from phenomenological arguments (see, e.g., SM Sec. 4.3) , i.e. before the advent of the BSC theory, this simple equation, solved together with Eq. (48) and the Maxwell equations, may describe a very broad range of macroscopic quantum effects including the Abrikosov vortices, critical fields and currents, etc. - see, e.g., M. Tinkham' monograph cited above.

[^295]:    ${ }^{33}$ The name is due to the deep analogy between this phenomenon and the interference between two waves, to be discussed in detail in Sec. 8.4.

[^296]:    ${ }^{34}$ For a more detailed discussion of the AB effect, which also takes place for single quantum particles, see, e.g., QM Sec. 3.2.
    ${ }^{35}$ Later, similar experiments were carried out with electron beams, and then even with "normal" (meaning nonsuperconducting) solid-state conducting rings. In this case, the effect is due to interference of the wavefunction of a single charged particle (an electron) with itself, and if of course is much harder to observe that in SQUIDs. In particular, the ring size has to be very small, and temperature low, to avoid "dephasing" effects due to unavoidable interactions of the particles with environment.
    ${ }^{36}$ The sign before $L I$ would be positive, as in Eq. (5.61), if $I$ was the current flowing into the inductance. However, in order to keep the sign in Eq. (69) intact, I should mean the current flowing into the Josephson junction, i.e. from the inductance, thus changing the sign of the term.

[^297]:    ${ }^{37}$ For more on that technology, see, e.g., the review paper by P. Bunyk et al., Int. J. High Speed Electron. Syst. 11, 257 (2001) and references therein.
    ${ }^{38}$ Since the induced e.m.f. $V_{\text {ind }}$ cannot drop on the superconducting path between the Josephson junction electrodes 1 and 2 (Fig. 3), it should equal to $(-V)$, where $V$ is the voltage across the junction.
    ${ }^{39}$ It may be also obtained from simple Schrödinger equation arguments - see, e.g., QM Sec. 2.2.

[^298]:    ${ }^{40}$ In experiment, this condition is hard to implement, due to relatively high inductance of the current leads providing de voltage supply. However, these complications do not change the main conclusion of the analysis.
    ${ }^{41}$ This 1962 prediction by B. Josephson was confirmed experimentally - implicitly (by phase locking of the oscillations with an external oscillator) in 1963, and explicitly (by the detection of microwave radiation) in 1967.
    ${ }^{42}$ For more on the Josephson effect and other macroscopic quantum phenomena in superconductivity, see, e.g., Chapters 6 and 7 in the monograph by M. Tinkham, which was cited above.

[^299]:    ${ }^{43}$ If the resistance is substantial, it may be represented, in calculations, by a separate lumped circuit element (resistor) connected in series with the coil.
    ${ }^{44}$ Starting from the pioneering experiments by M. Faraday - who invented such devices.

[^300]:    ${ }^{45}$ Interestingly, these effects include the wave propagation in periodic $L C$ circuits, despite still staying within the quasistatic approximation! However, within this approximation, speed $1 /(L C)^{1 / 2}$ of these waves is much lower than speed $1 /(\varepsilon \mu)^{1 / 2}$ of electromagnetic waves in the surrounding medium - see the next chapter.

[^301]:    ${ }^{46}$ Again, see MA Eq. (11.2) if you need.
    ${ }^{47}$ No physicist should be ashamed of doing this. J. C. Maxwell himself has arrived at his equations with a heavy use of mechanical engineering arguments. (His main book, A Treatise of Electricity and Magnetism, is full of drawings of gears and levers.) More generally, the whole history of science teaches us that snobbishness toward engineering and other "not-a-real-physics" disciplines is a sure way toward producing nothing of either practical value or fundamental importance. In real science, any method leading to novel, correct results should be welcome. ${ }^{48}$ This is of course just the integral form of the continuity equation (85).

[^302]:    ${ }^{49}$ This vector form of the equations, magnificent it its symmetry and simplicity, was developed in 1884-85 by O . Heaviside, with substantial contributions by H. Lorentz. (The original Maxwell's result, circa 1861, looked like a system of 20 equations for Cartesian components of the vector and scalar potentials.)
    ${ }^{50}$ Despite numerous efforts, no other corrections (e.g., additional terms) to Maxwell equations have been ever found, and these equations are still considered exact within the range of their validity, i.e. while the electric and magnetic fields may be considered classically. Moreover, even in quantum case, these equations are believed to be strictly valid as relations between the Heisenberg operators of the electric and magnetic field.
    ${ }^{51}$ Let me emphasize that this is only possible due to the "displacement current" term $\partial \mathbf{D} / \partial t$.
    ${ }^{52}$ The fact that $T$ cancels shows (or rather hints) that these estimates are valid for waves of arbitrary frequency.

[^303]:    ${ }^{53}$ See, e.g., MA Eq. (11.7) with $\mathbf{f}=\mathbf{E}$ and $\mathbf{g}=\mathbf{H}$.

[^304]:    ${ }^{54}$ Called after J. Poynting, though this fact was independently discovered by O. Heaviside, while a similar expression for the intensity of mechanical elastic waves had been derived earlier by N. Umov.
    ${ }^{55}$ Actually, an addition to $\mathbf{S}$ of the curl of an arbitrary vector function $\mathbf{f}(\mathbf{r}, t)$ does not change Eq. (103). Indeed, we may use the divergence theorem to transform the corresponding change of the surface integral in Eq. (103) to a volume integral of scalar function $\nabla \cdot(\nabla \times \mathbf{f})$ that equals zero at any point - see, e.g., MA Eq. (11.2).
    ${ }^{56}$ Later in the course we will show that the Poynting vector is also directly related to the density of momentum of the electromagnetic field.

[^305]:    ${ }^{62}$ See, e.g., CM Sec. 5.3.

[^306]:    ${ }^{1}$ Though B rather then $\mathbf{H}$ is the actual (microscopically-averaged) magnetic field, it is mathematically more convenient (just as in Sec. 6.2) to use the latter vector in our current discussion, because at sharp media boundaries, $\mathbf{H}$ obeys the boundary condition (5.118) similar to that for $\mathbf{E}-$ see Eq. (3.47).

[^307]:    ${ }^{2}$ In Gaussian units, $E$ and $H$ have the same dimensionality (in particular, in a free-space wave, $E=H$ ), making the (very useful) notion of the wave impedance less manifestly exposed - and in some textbooks not mentioned at all.

[^308]:    ${ }^{3}$ Due to the linearity of Eqs (2), operator Re in Eq. (11) may be ignored until the end of almost any calculation. Because of that, the exponential presentation of monochromatic variables is more convenient than manipulation with sine and cosine functions. (See also CM Sec. 4.1.)

[^309]:    ${ }^{4}$ In the convention that dominates research and engineering literature (but unfortunately is not universal), the wave is called right-polarized (RP) if it is described by the lower sign in Eqs. (18)-(20), and left-polarized (LP) in the opposite case. Another popular term for these cases is the "waves of negative / positive helicity".

[^310]:    ${ }^{5}$ For further reading about the Stokes parameters, as well as about many optics topics I will not have time to cover (especially the geometrical optics and the diffraction-imposed limits on optical imaging resolution), I can recommend the classical text by M. Born et al., Principles of Optics, $7^{\text {th }}$ ed., Cambridge U. Press, 1999.
    ${ }^{6}$ In an isotropic media, vectors $\mathbf{E}, \mathbf{P}$, and hence $\mathbf{D}=\varepsilon_{0} \mathbf{E}+\mathbf{P}$, are all parallel, and for the notation simplicity I will drop the vector sign. I am also assuming that $\mathbf{P}$ at any point $\mathbf{r}$ is only dependent on the electric field at the same point, and hence drop term $i k z$ from the exponent's argument. This assumption is valid if wavelength $\lambda$ is much larger than the elementary media dipole size $a$. In most systems of interest, the scale of $a$ is atomic ( $\sim 10^{-10} \mathrm{~m}$ ), so that the last approximation is valid up to very high frequencies, $\omega \sim c / a \sim 10^{18} \mathrm{~s}^{-1}$, corresponding to hard X-rays. ${ }^{7}$ Note that this condition (which excludes, in particular, the molecular-field effects discussed in Sec. 3.5) is not mentioned in most E\&M textbooks. If the molecular fields are important, Eq. (21) and its corollaries are only valid for the relation between $\mathbf{P}$ and the effective local electric field $\mathbf{E}_{\text {ef }}$.

[^311]:    ${ }^{8}$ A discussion of the temporal Green's functions in application to classical oscillations may be also found in CM Sec. 4.1.

[^312]:    ${ }^{9}$ It may be tempting to attribute this effect to wave absorption, i.e. the dissipation of the wave's energy, but we will see very soon that wave attenuation may be also due to effects different from absorption.
    ${ }^{10}$ The reader is probably familiar with the most noticeable effect of the dispersion, namely the difference between that group velocity $v_{\mathrm{gr}} \equiv d \omega / d k^{\prime}$, giving the speed of the envelope of a wave packet with a narrow frequency spectrum, and the phase velocity $v_{\mathrm{ph}} \equiv \omega / k^{\prime}$ of the component waves. The second-order dispersion effect, proportional to $d^{2} \omega / d^{2} k^{\prime}$, leads to the deformation (gradual broadening) of the envelope itself. Following tradition,

[^313]:    ${ }^{14}$ See, e.g., QM Chapters 5 and 9.

[^314]:    ${ }^{15}$ For an arbitrary plane wave the total average power flow may be calculated as an integral of Eq. (42) over all frequencies. By the way, combining this integral and the Poynting theorem (6.103), one can also prove the following interesting expression for the average electromagnetic energy density in an arbitrary dispersive (but linear and isotropic) medium:

    $$
    \bar{u}=\frac{1}{2} \int_{\omega}\left[\frac{d(\omega \varepsilon)}{d \omega} E_{\omega} E_{\omega}^{*}+\frac{d(\omega \mu)}{d \omega} H_{\omega} H_{\omega}^{*}\right] d \omega .
    $$

[^315]:    16 Alternatively, according to Eq. (45), it is possible (and in infrared spectroscopy, conventional) to attribute the ac response of a medium at all frequencies to effective complex conductivity $\sigma_{\text {ef }}(\omega)=\sigma(\omega)-i \omega \varepsilon(\omega)=-i \omega \varepsilon_{\mathrm{ef}}(\omega)$.

[^316]:    ${ }^{17}$ It may be also derived from the Boltzmann kinetic equation in the so-called relaxation-time approximation (RTA) - see, e.g., SM Sec. 6.2.
    ${ }^{18}$ See, e.g., MA Eq. (15.2).

[^317]:    ${ }^{19}$ Strictly speaking, this also requires $|f(\Omega)|$ to decrease faster than $\Omega^{-1}$ at the real axis (at $\Omega{ }^{\prime \prime}=0$ ), but due to nonvanishing inertia of charged particles, this requirement is fulfilled for all realistic models of dispersion - see, e.g., Eq. (36).
    ${ }^{20}$ I am typesetting this symbol in a Roman font, to exclude any possibility of its confusion with media's polarization.

[^318]:    ${ }^{21}$ For example, the function $\varphi(\omega) \equiv E_{\omega} d P_{\omega}$, in the Lorentz oscillator model, does not obey the Kramers-Kronig relations. This is evident not only from the fact that $E(t)$ is not a causal function of $P(t)$, but even mathematically. Indeed, the Green's function describing a causal relationship has to tend to zero at small time delays $\theta \equiv t-t^{\prime}$, so that its Fourier image has to tend to zero at $\omega \rightarrow \pm \infty$. This is certainly true for the function $f(\omega)$ given by Eq. (32), but not for the reciprocal function $\varphi(\omega) \equiv 1 / f(\omega) \propto\left(\omega^{2}-\omega_{0}^{2}\right)-2 i \delta \omega$, which diverges at large frequencies.

[^319]:    ${ }^{22}$ For example, the first of conditions (66) may be obtained by integrating the full (time-dependent) Maxwell equation $\nabla \times \mathbf{E}+\partial \mathbf{B} / \partial t=0$ over a narrow and long rectangular contour with dimensions $l$ and $d(d \ll l)$ stretched along the interface. In the Stokes theorem, the first term gives $\Delta E_{l} l$, which the contribution of the second term is proportional to product $d l$ and vanishes as $d / l \rightarrow 0$. The proof of the second boundary condition is similar - as was already discussed in Sec. 6.2.

[^320]:    ${ }^{23}$ Please note that only the media impedances (rather than wave velocities) are important for the reflection in this case! Unfortunately, this fact is not clearly emphasized in some textbooks that discuss only the case $\mu_{ \pm}=\mu_{0}$, when $Z=\left(\mu_{0} / \varepsilon\right)^{1 / 2}$ and $v=1 /\left(\mu_{0} \varepsilon\right)^{1 / 2}$ are proportional to each other.
    ${ }^{24}$ See, e.g., the discussion of elastic waves of mechanical deformations in CM Secs. 5.3, 5.4, 7.7, and 7.8.
    ${ }^{25}$ Before the advent of computers, specially lined paper (called the Smith chart) was commercially available for performing this recalculation graphically; it is occasionally used even nowadays for result presentation.

[^321]:    ${ }^{26}$ This ratio is sometimes also called the transmission coefficient, but in order to avoid its confusion with $T$, it is better to call it the power transmission coefficient.

[^322]:    ${ }^{27}$ See, e.g., QM Sec. 2.3.
    ${ }^{28}$ In a typical metal, $\tau \sim 10^{-13} \mathrm{~s}$, so that this approximation work well all the way up to $\omega \sim 10^{13} \mathrm{~s}^{-1}$, i.e. up to the far-infrared frequencies.

[^323]:    ${ }^{29}$ This relation is traditionally called the Snell law, after a $17^{\text {th }}$ century's author W. Snellius, though it has been traced back to a circa 984 manuscript by Abu Saad al-Ala ibn Sahl.

[^324]:    ${ }^{30}$ Note that we may calculate the reflection and transmission coefficients $R$ ' and $T^{\prime}$ for the wave traveling in the opposite direction just by making parameter swaps $Z_{+} \leftrightarrow Z_{-}$and $\theta \leftrightarrow r$, and that the resulting coefficients satisfy the following Stokes relations: $R^{\prime}=-R$, and $R^{2}+T T^{\prime}=1$, for any $\mathrm{Z}_{ \pm}$.

[^325]:    ${ }^{31}$ After A.-J. Fresnel (1788-1827), one of the pioneers of the wave optics, who is credited, among many other contributions (see in particular Ch. 8), for the concept of light as a purely transverse wave.
    ${ }^{32}$ A very simple interpretation of Eq. (93) is based on the fact that, together with the Snell law (82), it gives $r+\theta$ $=\pi / 2$. As a result, vector $\mathbf{E}_{+}$is parallel to vector $\mathbf{k}$.', and hence oscillating dipoles of medium at $z>0$ do not have the component which could induce the transverse electric field $\mathbf{E}$.' of the reflected wave.
    ${ }^{33}$ This effect is used in practice to obtain linearly polarized light, with the electric field vector perpendicular to the plane of incidence, from the natural light with its random polarization. An even more practical application of the effect is a partial reduction of undesirable glare from wet surfaces (for the water/air interface, $n_{+} / n_{-} \approx 1.33$, giving $\theta_{\mathrm{B}} \approx 50^{\circ}$ ) by making car light covers and sunglasses of vertically-polarizing materials.
    ${ }^{34}$ Despite some important background theoretical work by A. Schuster (1904), L. Mandelstam (1945), D. Sivikhin (1957), and especially V. Veselago (1966-67), the negative refractivity effects have only recently become a subject of intensive scientific research and engineering development.

[^326]:    ${ }^{35}$ Inspired by this fact, in some publications the left-hand materials are prescribed a negative index of refraction $n$. However, this prescription should be treated with care (for example, it complies with the first form of Eq. (84), but not its second form), and the sign of $n$, in contrast to that of wave vector $\mathbf{k}$, is the matter of convention.

[^327]:    ${ }^{36}$ For a recent review, see, e.g., B. Wood, Comptes Rendus Physique 10, 379 (2009).

[^328]:    ${ }^{37}$ Note that for the notation simplicity, I am dropping index $\omega$ in the complex amplitudes of the field components, and later will drop argument $\omega$ in $k_{z}$ and $Z$, though they may depend on the wave frequency rather substantially see below.

[^329]:    ${ }^{38}$ The wave equation presented in the form (101) is called the (in our particular case, 2D) Helmholtz equation, after H. von Helmholtz (1821-1894) - the mentor of H. Hertz and M. Planck, among many others.

[^330]:    ${ }^{39}$ The alternative is to have a virtually plane wave, which propagates along the transmission line conductors, and whose fields are just slightly deformed in their vicinity. Such a wave cannot be "guided" by the conductors, and hardly deserves the name of a "wave in the waveguide".

[^331]:    ${ }^{40}$ The coaxial cable was first patented by O. Heaviside in 1880.

[^332]:    ${ }^{41}$ The twisting reduces mutual induction ("crosstalk") between the lines, and parasitic radiation at their bends.
    ${ }^{42}$ For that, one of these two linear equations should be first vector-multiplied by $\mathbf{n}_{z}$. Note that this approach could not be used to analyze TEM waves, because for them $k_{t}=0, E_{z}=0, H_{z}=0$, and Eqs. (121) yield uncertainty.

[^333]:    ${ }^{43}$ An interesting recent twist in the ideas of electromagnetic metamaterials (mentioned in Sec. 5 above) is the socalled $\varepsilon$-near-zero materials, designed to have the effective product $\varepsilon \mu$ much lower than $\varepsilon_{0} \mu_{0}$ within certain frequency ranges. Since at these frequencies the speed $v(4)$ becomes much lower than $c$, the cutoff frequency (123) virtually vanishes. As a result, waves may "tunnel" through very narrow sections of metallic waveguides filled with such materials - see, e.g., M. Silveirinha and N. Engheta, Phys. Rev. Lett. 97, 157403 (2006).

[^334]:    ${ }^{44}$ Let me hope that the solution of equations of the type $d^{2} X / d x^{2}+k_{x}^{2} X=0$ does not present a problem for the reader, due to his or her prior experience with problems such as standing waves on a guitar string, wavefunctions in a flat 1D quantum well, or (with the replacement $x \rightarrow t$ ) a classical harmonic oscillator.

[^335]:    ${ }^{45}$ The reader is encouraged to find a simple interpretation of this equality．

[^336]:    ${ }^{46}$ In Chapter 2, it was natural to take the angular dependence in the sin-cos form, which is equivalent to adding a similar term with $n \rightarrow-n$ to the right-hand part of Eq. (141). However, since the functions $f$ we are discussing now are already complex, it is easier to do calculations in the exponential form - though it is vital to restore real fields before calculating any of their nonlinear forms, e.g., the wave power.
    ${ }^{47}$ The lowest root of Eq. (142) with $n=0$, i.e. $\xi^{\prime}{ }_{00}$, equals 0 , and would yield $k=0$ and hence a constant field $H_{z}$, which, according to the first of Eqs. (121), would give vanishing electric field.

[^337]:    ${ }^{48}$ Actually, Eq. (144) does describe a circularly polarized wave, while the real and imaginary parts of this expression describing two mutually perpendicular quasi-linearly-polarized waves.
    ${ }^{49}$ Electric field lines in the $H_{01}$ mode (as well as all higher $H_{0 m}$ modes) are directed straight from the axis to the walls, reminding those of TEM waves in the coaxial cable. Due to this property, these modes provide, at $\omega \gg \omega_{c}$, much lower power losses (see Sec. 10 below) than the fundamental $H_{11}$ mode, and are sometimes used in practice, despite all inconveniences of working in the multimode frequency range.

[^338]:    ${ }^{50}$ This formula ignores the fact that, according to our analysis, some modes (with $n=0$ and $m=0$ for $H$ modes, and $n=0$ or $m=0$ for $E$ modes, are forbidden. However, for $N \gg 1$, the associated corrections of Eq. (147) are negligible.
    ${ }^{51}$ For a comprehensive description of this vital technology see, e.g., A. Yariv and P. Yeh, Photonics, $6^{\text {th }}$ ed., Oxford U. Press, 2007.

[^339]:    ${ }^{52}$ Each frequency band shown in Fig. 26a, at a typical signal-to-noise ratio $S / N>10^{5}(50 \mathrm{db})$, corresponds to the Shannon bandwidth $\Delta f \log _{2}(S / N)$ exceeding $10^{14}$ bits per second, five orders of magnitude (!) higher than that of a modern Ethernet cable. And this is only per one fiber; an optical cable may have hundreds of them.
    ${ }^{53}$ The silica-based fibers were suggested in 1966 by C. Kao (the 2009 Nobel Prize in physics), but the very idea of using optical fibers for communications may be traced back to at least the 1963 work by J. Nishizawa.

[^340]:    ${ }^{54}$ I believe that the following calculation is important - both for practice, and as a good example of Maxwell theory application. However, its results will not be used in the following sections/chapters of the course, so that if the reader is not interested in this topic, he or she may safely jump to the beginning Sec. 9 .

[^341]:    ${ }^{55}$ This fact becomes less surprising if we recall that in the circular metallic waveguide, discussed in Sec. 7, the lowest mode ( $H_{11}$, Fig. 23) also corresponded to $n=1$ rather than $n=0$.

[^342]:    ${ }^{56}$ This is the core assumption of this approximate theory which accounts only for the most important effect of the difference of dielectric constants $\varepsilon_{+}$and $\varepsilon_{-}$: the opposite signs of the differences $\left(k_{+}^{2}-k_{z}^{2}\right)=k_{t}^{2}$ and $\left(k_{-}^{2}-k_{z}^{2}\right)=-$ $\kappa_{t}^{2}$. For more discussion of accuracy of this approximation and some exact results, let me refer the interested reader either to the monograph by A. Snyder and D. Love, Optical Waveguide Theory, Chapman and Hill, 1983, or to Chapter 3 and Appendix B in the monograph by Yariv and Yeh, which was cited above.

[^343]:    ${ }^{57}$ For an axially-symmetric fiber with a smooth function $\varepsilon(\rho)$, the first derivative $d \varepsilon / d \rho$ should vanish at $\rho=0$.
    ${ }^{58}$ Such approach is invalid at arbitrary (large) $\zeta$. Indeed, in the macroscopic Maxwell equations, $\varepsilon(\mathbf{r})$ is under the differentiation sign, and the exact Helmholtz-type equations for fields have additional terms containing $\nabla \varepsilon$.

[^344]:    ${ }^{59}$ See, e.g., QM Sec. 2.6.

[^345]:    ${ }^{60}$ This task should be easier after reviewing results of field's momentum analysis in Sec. 9.8, in particular Eqs. (9.235) and (9.237).
    ${ }^{61}$ Theoretically, the possibility of separating of the angular momentum of an electromagnetic wave to the "spin" and "orbital" parts may be traced back to at least the 1943 work by J. Humblet; however, this issue had not been discussed in literature too much until the spectacular 1992 experiments by L. Allen et al. who demonstrated a simple way of generating such helical optical beams. (For reviews of this and later work see, e.g., G. MolinaTerriza et al., Nature Physics 3, 305 (2007) and/or L. Marrucchi et al., J. Opt. 13, 064001 (2011), and references therein.) Presently there are efforts to use this approach for so-called "orbital angular moment (OAM) multiplexing" of waves for high-rate information transmission - see, e.g., J. Wang et al., Nature Photonics 6, 488 (2012).
    ${ }^{62}$ The device is named after its inventors, M. Fabry and A. Pérot; and is also called the Fabry-Pérot etalon (meaning "gauge"), because of its initial usage for the light wavelength measurement.
    ${ }^{63}$ The resonators formed by well conducting (usually, metallic) walls are frequently called the resonant cavities.

[^346]:    ${ }^{64}$ In this form, the equations are valid even in the presence of dispersion, but with the frequency-dependent wave speed: $v^{2}=1 / \varepsilon(\omega) \mu(\omega)$.
    ${ }^{65}$ This is of course the expression of the first of the general boundary conditions (104). The second if these conditions (for the magnetic field) is satisfied automatically for the transverse waves we are considering.

[^347]:    ${ }^{66}$ In most electrical engineering handbooks, the index corresponding to the shortest side of the resonator is listed last, so that the fundamental mode is nominated as $H_{110}$ and its eigenfrequency as $\omega_{110}$.

[^348]:    Oscillation mode density

[^349]:    ${ }^{67}$ This fact becomes evident from plugging Eq. (196) into the Maxwell equation $\nabla \cdot \mathbf{E}=0$. The resulting equation, $k_{x} E_{1}+k_{y} E_{2}+k_{z} E_{3}=0$, with the discrete, equidistant spectrum (197) for each wave vector component, may be satisfied by two linearly independent sets of constants $E_{1,2,3}$.
    ${ }^{68}$ See, e.g., QM Sec. 1.1 and SM Sec. 2.6.

[^350]:    Energy
    in filling dielectric

[^351]:    ${ }^{70}$ As follows from Eq. (78), which may be used for estimates even in cases of arbitrary incidence, this condition is necessary for low attenuation: $\alpha \ll k$ only if $F \ll 1$.

[^352]:    ${ }^{71}$ For a normally-incident plane wave, this formula would bring us back to Eq. (78).

[^353]:    ${ }^{72}$ As losses grow, the oscillation waveform deviates from sinusoidal one, and the very notion of "oscillation frequency" becomes vague. As a result, parameter $Q$ is well defined only if it is much higher than 1 .
    ${ }^{73}$ See, e.g., CM Sec. 4.1.

[^354]:    ${ }^{74}$ This is the acronym for "Full Width at Half-Maximum".
    ${ }^{75}$ See, e.g., MA Eq. (15.2).

[^355]:    ${ }^{76}$ This function $E(t)$ is of course proportional to the well-known step function $\theta$ - see, e.g., MA Eq. (14.3). I am not using this notion just to avoid a possible confusion between two different uses of the Greek letter $\theta$. ${ }^{77}$ And in more detail in CM Sec. 5.3, and especially in QM Sec. 2.1.

[^356]:    ${ }^{1}$ When necessary (e.g., at the discussion of the Cherenkov radiation in Sec. 10.4), it will be not too hard to generalize these results to dispersive media.
    ${ }^{2}$ Such thinking would not prevent the results from being valid for the case when $\rho(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$ should be calculated self-consistently.

[^357]:    ${ }^{3}$ Admittedly, this expression does not satisfy the continuity equation (4.5), but we will correct this deficiency imminently, at the linear superposition stage - see Eq. (17) below.
    ${ }^{4}$ Let me emphasize that this is not the general solution to Eq. (6). For example, it does nor describe the fields created by other sources, that pass by the considered charge $q(t)$. However, such fields are irrelevant for our current task: to calculate the field created by the charge $q(t)$ itself.
    ${ }^{5}$ See, e.g., MA Eq. (10.9).
    ${ }^{6}$ See also CM Sec. 5.3.

[^358]:    ${ }^{7}$ For relativistic particles, moving with velocities of the order of speed of light, one has to be more careful. As the result, I will postpone the discussion of their radiation until Chapter 10, i.e. until after the discussion of special relativity in Chapter 9.
    ${ }^{8}$ From the first of Eqs. (1), for the electric field, in the first approximation (23), we would get $-\partial \mathbf{A} / \partial t=-(1 / 4 \pi \varepsilon v r)$ $\ddot{\mathbf{p}}(t-r / v)=-(Z / 4 \pi r) \ddot{\mathbf{p}}(t-r / v)$. The transverse component of this vector (see Fig. 2) is the proper wave field $\mathbf{E}=$ $Z \mathbf{H} \times \mathbf{n}$, while its longitudinal component is exactly compensated by $(-\nabla \phi)$ in the next term of expansion of Eq. (17a) with respect to small parameter $r / \lambda \ll 1$.

[^359]:    Full instant power

[^360]:    ${ }^{9}$ In the Gaussian units, for free space $(v=c)$, this important formula reads $P=\left(2 / 3 c^{3}\right) \ddot{p}^{2}$. It was first derived in 1897 by J. Larmor for the particular case of a single point charge $q$ moving with acceleration $\ddot{\mathbf{r}}$, when $\ddot{\mathbf{p}}=q \ddot{\mathbf{r}}$ and hence $\mathcal{P}=\left(2 q^{2} / 3 c^{3}\right) \dot{r}^{2}$. As a result, Eq. (27) is sometimes referred to as the Larmor formula.

[^361]:    ${ }^{10}$ Actually, the formula needs a numerical coefficient adjustment to account for electron's orbital (rather than linear) motion - the task left for reader's exercise. However, this adjustment does not affect the order-ofmagnitude estimate given above.

[^362]:    ${ }^{11}$ A partial list of popular software packages of this kind includes both publicly available codes such as NEC - 2 (whose various versions are available online, e.g., at http://alioth.debian.org/projects/necpp/ and http://www.qsl.net/4nec2/), and proprietary packages - such as Momentum from Aglient Technologies (now owned by Hewlett-Packard), FEKO from EM Software \& Systems, and XFdtd from Remcom.
    ${ }^{12}$ Named after M. Born, one of the founding fathers of quantum mechanics. Note, however, the basic idea of this approach was developed much earlier (in 1881) by Lord Rayleigh - see below.

[^363]:    ${ }^{13} \mathrm{As}$ Eq. (7.30) shows, this calculation is also valid for an oscillator with eigenfrequency $\omega_{0} \ll \omega$.

[^364]:    ${ }^{14}$ Named after Sir J. J. Thomson (1856-1940), the discoverer of the electron - and isotopes as well! He is not to be confused with his son, G. P. Thomson, who discovered (simultaneously with C. Davisson and L. Germer) quantum-mechanical wave properties of the same electron.
    ${ }^{15}$ In the Gaussian units, this formula looks like $r_{c}=q^{2} / m c^{2}$ (giving, of course, the same numerical value: for the electron, $r_{c} \approx 2.82 \times 10^{-13} \mathrm{~cm}$ ). This classical quantity should not be confused with particle's Compton wavelength $\lambda_{c} \equiv h / m c$ (for the electron, close to $2.24 \times 10^{-12} \mathrm{~cm}$ ), which naturally arises in quantum electrodynamics - see a brief discussion in the next chapter, and QM Chapter 9 for more detail.
    ${ }^{16}$ It is fascinating how smartly has the relativistic expression $m c^{2}$ sneaked into the result (40), which was obtained using a non-relativistic equation of particle motion. This was possible because the calculation engaged electromagnetic waves that propagate with the speed of light, and whose quanta (photons), as a result, may be frequently treated as relativistic (moreover, ultra-relativistic) particles - see the next chapter.

[^365]:    ${ }^{17}$ Named after Lord Rayleigh (born J. Strutt, 1842-1919), whose numerous contributions to science include the discovery of argon. He has also pioneered (for the special case we are considering now) the basic idea of what is presently called the Born approximation.
    ${ }^{18}$ These values are approximate because both $n$ and $\left(\varepsilon_{r}-1\right)$ vary through the atmosphere.

[^366]:    ${ }^{19}$ In quantum electrodynamics, $\hbar \mathbf{q}$ has the sense of the momentum transferred from the scattering object to the scattered photon, and this terminology sometimes creeps even into the classical electrodynamic texts.

[^367]:    ${ }^{20}$ Named after Sir William Bragg and his son, Sir William Lawrence Bragg, who in 1912 demonstrated X-ray diffraction by atoms in crystals. The Braggs' experiments have made the existence of atoms (before that, a hypothetical notion ignored by many physicists) indisputable.

[^368]:    ${ }^{21}$ This experiment was described as early as in 1803 by T. Young - one more universal genius of science, who has also introduced the Young modulus in the elasticity theory (see, e.g., CM Chapter 7), besides numerous other achievements - including deciphering Egyptian hieroglyphs! The two-slit experiment has firmly established the wave picture of light, to be replaced by the dualistic photon-vs-wave picture, formalized by quantum electrodynamics, only $100+$ years later.
    ${ }^{22}$ Since the observation point's position $\mathbf{r}$ does not participate in this formula explicitly, the prime sign in $\mathbf{r}$ ' could be dropped, but I keep it as a reminder that the integral is taken over points $\mathbf{r}$ ' of the scattering object.

[^369]:    ${ }^{23}$ Named after C. Huygens (1629-1695) who had conjectured the wave theory of light (that remained controversial for more than a century, until T. Young's experiments), and A.-J. Fresnel (1788-1827) who has developed the mathematical theory of diffraction.

[^370]:    ${ }^{24}$ The fact that the Huygens principle is valid for any field component should not too surprising. Due to condition $a \gg \lambda$, the real boundary conditions at the orifice edges are not important; what is only important that the screen, that limits the orifice, is opaque. Because of this, the Huygens principle's expression (71) is a part of the so-called scalar theory of diffraction. (In this course I will not have time to go beyond this approximation.)

[^371]:    ${ }^{25}$ See, e.g., MA Eq. (6.10).
    ${ }^{26}$ This result very is natural, because $\exp \{i k R\}$ oscillates fast with the change of $\mathbf{r}$ ', so that the contributions from various front point are averaged out. Indeed, the only reason why the central part of plane [ $x^{\prime}, y^{\prime}$ ] gives a nonvanishing contribution (76) to $f_{\omega}(z)$ is that the phase exponents stops oscillating at $\left(x^{, 2}+y^{, 2}\right)$ below $\sim z / k-$ see Eq. (73).
    ${ }^{27}$ This proof was given in 1882 by G. Kirchhoff.

[^372]:    ${ }^{28}$ Actually, this is a somewhat nontrivial point of the proof. Indeed, it may be shown that the solution of Eq. (79) identically equals to zero if $f\left(\mathbf{r}^{\prime}\right)$ and $\partial f\left(\mathbf{r}^{\prime}\right) / \partial n^{\prime}$ vanish together at any part of the boundary. As a result, building the solution with the account of exact boundary conditions (which is the task of the vector theory of diffraction) is possible but cumbersome. Here we base our solution on the physical intuition.
    ${ }^{29}$ It follows, e.g., from Eq. (16) with a monochromatic source $q(t)=q_{\omega} \exp \{-i \omega t\}$, at the value $q_{\omega}=4 \pi \varepsilon$ that fits the right-hand part of Eq. (80).
    ${ }^{30}$ With the integration extended over all boundaries of volume $V$, this would be an exact result.

[^373]:    ${ }^{31}$ The phase shift $\varphi$ vanishes at the normal incidence of a plane wave on the holes. Note, however, that the spatial shift of the interference pattern following from Eq. (90), $\Delta x=-(z / k a) \varphi$, is extremely convenient for the experimental measurement of the phase shift between two waves, especially if it is induced by some factor (such as insertion of a transparent object into one of interferometer's arms, etc.) that may be turned on/off at will.

[^374]:    ${ }^{32}$ Note also that since in this limit $k a^{2} \ll z$, Eq. (97) shows that even the maximum value $S(0, z)$ of the diffracted wave intensity is much less than intensity $S_{0}$ of the incident wave. This is natural, because the incident power $S_{0} a$ per unit length of the slit is now distributed over a much larger width $\delta x \gg a$, so that $S(0, z) \sim S_{0}(a / \delta x) \ll S_{0}$. ${ }^{33}$ Slightly different definitions of these functions, mostly affecting constant factors, may also be met in literature.

[^375]:    ${ }^{34}$ Note that this condition may be also rewritten as $a \sim \delta x$, i.e. $z / a \sim a / \lambda$.

[^376]:    ${ }^{39}$ The rudimentary diffraction grating effect, produced by parallel fibers of bird feathers, was discovered as early as in 1673 by J. Gregory - who has also invented the reflecting ("Gregorian") telescope.

[^377]:    ${ }^{40}$ If you need, see, e.g., MA Eq. (7.5).

[^378]:    ${ }^{41}$ In electrostatics, the symmetric, zero-trace tensor $Q$ determines the next term in the potential expansion (3.5):

    $$
    \phi(\mathbf{r})=\frac{1}{4 \pi \varepsilon_{0}}\left(\frac{1}{r} Q+\frac{1}{r^{2}} \sum_{j=1}^{3} n_{j} p_{j}+\frac{1}{2 r^{3}} \sum_{j, j^{\prime}=1}^{3} n_{j} n_{j^{\prime}} Q_{i j^{\prime}}+\ldots\right) .
    $$

[^379]:    ${ }^{42}$ As a math reminder, tensor is a matrix describing a physical reality independent of the reference frame choice, so that the Cartesian elements of the tensor have to change according to certain geometric rules if the reference frame is changed - e.g., rotated. This notion is very similar to a physical vector, that may be described by an ordered set of its Cartesian components, which change according to certain rules as the result of the reference frame' change. We may be confident that a matrix represents a tensor if it provides a linear relation between components of two physical vectors - such a $\mathbf{Q}$ and $\mathbf{n}$ in Eq. (128).

[^380]:    ${ }^{43}$ As was emphasized in Sec. 2, this is a reasonable guess rather than a controllable approximation. The exact (rather involved!) theory shows that this assumption gives errors $\sim 5 \%$.

[^381]:    ${ }^{1}$ Let me hope that the reader does not need a reminder that in order for Eq. (1) to be valid, the reference frames 0 and 0 ' have to be inertial - see, e.g., CM Sec. 1.3.
    ${ }^{2}$ It had been first formulated by G. Galilei as early as in 1638 - four years before I. Newton was born!
    ${ }^{3}$ Note a very unfortunate term "boost", used sometimes for the transform between the reference frames. (It is especially unnatural in the special relativity, not describing any accelerations.) In these notes, this term is avoided.

[^382]:    ${ }^{4}$ Discussions in this chapter and most of the next chapter will be restricted to the free-space (and hence dispersion-free) case; some media effects on radiation by relativistic particles will be discussed in Sec.10.4.
    ${ }^{5}$ It is interesting that the Schrödinger equation, whose fundamental solution for a free particle is a similar monochromatic wave (albeit with a different dispersion law), is Galilean-invariant, with a certain addition to the wavefunction's phase - see, e.g., QM Chapter 1.
    ${ }^{6}$ See, e.g., CM Secs. 5.5 and 7.7.
    ${ }^{7}$ In the ancient Greek mythology, aether is the clear upper air breathed by the gods residing on Mount Olympus.

[^383]:    ${ }^{8}$ Through the $20^{\text {th }}$ century, the Michelson-Morley-type experiments were repeated using more and more refined experimental techniques, always with the zero result for the apparent ether motion speed. For example, recent experiments, using cryogenically cooled optical resonators, have reduced the upper limit for such speed to just $3 \times 10^{-15} \mathrm{c}$-see H. Müller et al., Phys. Rev. Lett. 91, 020401 (2003).
    ${ }^{9}$ The zero result of a slightly later experiment, namely precise measurements of the torque which should be exerted by the moving ether on a charged capacitor, carried out in 1903 by F. Trouton and H. Noble (following G. FitzGerald's suggestion), seconded the Michelson and Morley's conclusions.
    ${ }^{10}$ The theoretical work toward this goal (which I do not have time to review in detail) included important contributions by W. Voigt (in 1887), H. Lorentz (1892-1904), J. Larmor (1897 and 1900), and H. Poincaré (1900 and 1905).

[^384]:    ${ }^{11}$ Note that though the relativity principle excludes the notion of the special ("absolute") spatial reference frame, its verbal formulation still leaves the possibility of the Galilean "absolute time" open. The quantitative relativity theory kills this option - see Eqs. (6) and their discussion below.

[^385]:    ${ }^{12}$ One more function of $\beta$, the rapidity defined as $\beta \equiv \tanh \varphi$ (so that $\psi=i \varphi$ ), is also useful for some calculations. ${ }^{13}$ Still, in some cases below, it will be more convenient to use Eqs. (6) rather than Eqs. (19).
    ${ }^{14}$ All attempts to rationally conjecture particles moving with $v>c$, called tachyons, have failed (so far, at least :-). Possibly the strongest objection against their existence is the notice that tachyons could be used to communicate back in time, thus violating the causality principle - see, e.g., G. Benford et al., Phys. Rev. D 2, 263 (1970).

[^386]:    ${ }^{15}$ A posteriori, the Lorenz transform may be used to show that consensus-creating procedures (such as clock synchronization) are indeed possible. The basic idea of the proof is that at $v \ll c$ the relativistic corrections to space and time intervals are of the order of $(v / c)^{2}$, they have negligible effects on clocks being brought together into the same point for synchronization very slowly, with velocity $v \ll c$. The reader interested in detailed discussion of this and other fine points of special relativity may be referred to, e.g., either H. Arzeliès, Relativistic Kinematics, Pergamon, 1966, or W. Rindler, Introduction to Special Relativity, $2^{\text {nd }}$ ed., Oxford U. Press, 1991.

[^387]:    ${ }^{16}$ See, e.g., J. Hafele and R. Keating, Science 177, 166 (1972).

[^388]:    ${ }^{17}$ With an account of the well-known trigonometric identity $\tan (a+b)=(\tan a+\tan b) /(1-\tan a \tan b)$ and Eq. (15), Eq. (25) shows that that rapidities $\varphi$ add up exactly as longitudinal velocities at non-relativistic motion, making that notion very convenient for the analysis of transfer between several frames.

[^389]:    ${ }^{18}$ Strictly speaking, in order to reconcile the geometries shown in Fig. 1 (for which all our formulas, including Eq. (27), are valid) and Fig. 8 (giving the traditional scheme of the aberration), it is necessary to invert signs of $\mathbf{u}$ (and hence $\sin \theta^{\prime}$ and $\cos \theta^{\prime}$ ) and $\mathbf{v}$, but as evident from Eq. (27), all the minus signs cancel, and the formula is valid as is.
    ${ }^{19}$ See, e.g., CM Secs. 6.4-6.5.

[^390]:    ${ }^{20}$ Strictly speaking, Eq. (32) is valid to an additive constant, but for notation simplicity, it may be always made equal to zero by selecting (at it has already been done in all relations of Sec. 1) the reference frame origins and/or clock turn-on times so that at $t=0$ and $x=0, t^{\prime}=0$ and $x^{\prime}=0$ as well.

[^391]:    ${ }^{21}$ The same fact, ignored by crackpots, is also valid for other favorite points of their attacks, including the Universe expansion and quantum mechanics in physics, and the evolution theory in biology.

[^392]:    ${ }^{22}$ After H. Minkowski who was first to recast (in 1907) the special relativity relations in a form in which space coordinates and time (or rather $c t$ ) are treated on an equal footing.

[^393]:    ${ }^{23}$ I have opted against using special indices (e.g., $\boldsymbol{\beta}_{u}, \gamma_{u}$ ) to distinguish Eqs. (17) and (61) here and below, in a hope that the suitable velocity (of a reference frame or of a particle) will be always clear from the context.

[^394]:    ${ }^{24}$ I am sorry for using, as in Sec. 6.3, for particle's momentum, the same traditional notation (p) as had been used for the dipole electric moment. However, since the latter notion will be virtually unused in the balance of the notes, this may hardly lead to confusion.
    ${ }^{25}$ Indeed, such a derivation uses additional assumptions, however natural (such as the Lorentz-invariance of $\Omega$ ), so it can hardly be considered as a real proof of the final results, so that they require experimental confirmation. Fortunately, such confirmations have been numerous - see below.
    ${ }^{26}$ See, e.g., CM Sec. 10.3.
    ${ }^{27}$ See, e.g., CM Sec. 2.1.

[^395]:    ${ }^{28}$ See, e.g., CM Sec. 2.3.
    ${ }^{29}$ Let me hope that the reader understands that all the layman talk about the "mass to energy conversion" is only valid in a very limited sense of the word. While the Einstein relation (73) does allow the conversion of "massive" particles (with $m \neq 0$ ) into massless particles such as photons, each of the latter particles also has a nonvanishing relativistic mass $M$, and simultaneously the energy $\mathcal{E}$ related to $M$ by Eq. (73).

[^396]:    ${ }^{30}$ Please note one more useful relation following from Eqs. (70) and (73): $\mathbf{p}=\left(\mathrm{E} / \mathrm{c}^{2}\right) \mathbf{u}$.
    ${ }^{31}$ It may be tempting to interpret this relation as the perpendicular-vector-like addition of the rest energy $m c^{2}$ and the "kinetic energy" $p c$, but from the point of view of the total energy conservation (see below), a better definition of the kinetic energy is $T(u) \equiv \mathcal{E}(u)-\mathcal{E}(0)$.
    ${ }^{32}$ Briefly reviewed in QM Chapter 9.

[^397]:    ${ }^{33}$ Note that according to this definition, the c.o.m.'s radius-vector is $\mathbf{R}=\Sigma_{k} M_{k} \mathbf{r}_{k} / \Sigma_{k} M_{k}=\Sigma_{k} \gamma_{k} m_{k} \mathbf{r}_{k} / \Sigma_{k} \gamma_{k} m_{k}$, generally different from the well-known expression $\Sigma_{k} m_{k} \mathbf{r}_{k} / \Sigma_{k} m_{k}$ of the non-relativistic mechanics.

[^398]:    ${ }^{34}$ This compact notation may take some time to be accustomed to, but can hardly lead to any confusion, due to the following rule: the summation is implied always (and only) when an index is repeated twice, once on the top and another at the bottom. In these notes, this shorthand notation will be used only for 4 -vectors, but not for the usual (spatial) vectors.
    ${ }^{35}$ Note also that, by definition, for any two 4-vectors, $A_{\alpha} B^{\alpha}=B^{\alpha} A_{\alpha}$.

[^399]:    ${ }^{36}$ These forms are 4 -vector extensions of the notions of contravariance and covariance introduced in the 1850s by J. Sylvester for the description of 3D vector change at transfer between different reference frames - e.g., axes rotation - cf. Fig. 3. In this case, the contravariance or covariance of a vector is uniquely determined by its nature: if Cartesian coordinates of a vector (such as the non-relativistic velocity $\mathbf{v}=d \mathbf{r} / d t$ ) are transformed similarly to the radius-vector $\mathbf{r}$, it is called contravariant, while the vectors (such as $\partial f / \partial \mathbf{r} \equiv \nabla f$ ) that require the reciprocal transform, are called covariant. In the Minkowski space, both forms may be used for any 4 -vector.
    ${ }^{37}$ Just as 4 -vectors, 4 -tensors with two top indices are called contravariant, and those with two bottom indices, covariant. Tensors with one top and one bottom index are called mixed.

[^400]:    ${ }^{39}$ As was mentioned above, this is also a property of the "usual" transform of 3D vectors.

[^401]:    ${ }^{40}$ It is straightforward to check that transfer between the contravariant and covariant forms of the same tensor may be readily achieved using the same metric tensor $g$ : $T_{\alpha \beta}=g_{\alpha \gamma} T^{\gamma \delta} g_{\delta \beta}, T^{\alpha \beta}=g^{\alpha \gamma} T_{\gamma \delta} g^{\delta \beta}$.
    ${ }^{41}$ Note that in some texts, the equations preserving their form at a transform are called "covariant", creating a possibility for confusion with covariant vectors and tensors. On the other hand, calling such equations "invariant" does not distinguish them properly from invariant quantities, such as scalar products of 4 -vectors.

[^402]:    ${ }^{42}$ In the Gaussian units, the scalar potential should not be divided by $c$.
    ${ }^{43}$ In the Gaussian units, coefficient $\mu_{0}$ in the right-hand part of Eq. (119) should be replaced, as usual, with $4 \pi / c$.
    ${ }^{44}$ Named after J.-B. d'Alembert (1717-1783). Note that in older textbooks, notation $\square^{2}$ may be met for this operator.

[^403]:    ${ }^{46}$ To be fair, note that just as Eq. (127), Eq. (129) this is also a set of four scalar equations - in the latter case with indices $\alpha, \beta$, and $\gamma$ taking any three different values of the set $\{0,1,2,3\}$.

[^404]:    ${ }^{47}$ This term is very popular in the of particle scattering - see, e.g., CM Sec. 3.7.

[^405]:    ${ }^{48}$ In the next chapter, we will re-derive them in a different way.
    ${ }^{49}$ It is straightforward to use Eq. (140) and the linear superposition principle to calculate, for example, the magnetic field of a string of charges moving along the same line, and separated by equal distances $\Delta x=a$ (so that the average current, as measured in frame 0 , is $q u / a$ ), and to show that the time-average of the magnetic field is given by Eq. (5.20) of magnetostatics, with $b$ instead of $\rho$.

[^406]:    ${ }^{50}$ See, e.g., CM Eq. (1.20) with $d \mathbf{p} / d t=\mathbf{F}=q \mathbf{E}$. (As a reminder, the magnetic field cannot affect particle's energy, because the magnetic component of the Lorentz force is perpendicular to its velocity.)
    51 As was emphasized earlier in this course, in statics this contribution has to be ignored. In dynamics, this is generally not true; these self-action effects will be discussed in Sec. 10.6.

[^407]:    ${ }^{52}$ For more on this topic, I have to refer the interested reader to special literature, for example either S. Lee, Accelerator Physics, $2^{\text {nd }}$ ed., World Scientific, 2004, or E. Wilson, An Introduction to Particle Accelerators, Oxford U. Press, 2001.

[^408]:    ${ }^{53}$ As a reminder, a trochoid may be described as the trajectory of a point on a rigid disk rolled along a straight line. Its canonical parametric presentation is $x=\Theta+a \cos \Theta, y=a \sin \Theta$. (For $a>1$, the trochoid is prolate, if $a<$ 1 , it is curtate, and if $a=1$, it is called the cycloid.) Note, however, that for our problem, the trajectory in the lab frame is exactly trochoidal only in the non-relativistic limit $v \ll c$ (i.e. $E / c \ll B$ ), because otherwise the Lorentz contraction in the drift direction squeezes the cyclotron orbit from a circle into an ellipse.

[^409]:    ${ }^{54}$ See, e.g., CM Sec. 4.4.

[^410]:    ${ }^{55}$ See, e.g., Sec. 12.4 in J. D. Jackson, Classical Electrodynamics, $3{ }^{\text {rd }}$ ed., Wiley, 1999.
    ${ }^{56}$ See, e.g., CM Sec. 2.2 and beyond.

[^411]:    ${ }^{57}$ See, e.g., CM Sec. 2.1.
    ${ }^{58}$ Alternatively called the "Lagrangian derivative"; for its (rather simple) derivation see, e.g., CM Sec. 8.3.

[^412]:    ${ }^{59}$ With regrets, I have to use the same (common) notation as was used earlier for the electric polarization - which is not discussed below.
    ${ }^{60}$ In Gaussian units, Eq. (192) has the form $\mathbf{P}=\mathbf{p}+q \mathbf{A} / c$.

[^413]:    ${ }^{64}$ See, e.g., CM Sec. 10.2.

[^414]:    ${ }^{65}$ For the further reading on this technology, the reader may be referred, for example, to a simple monograph by F. C. Chen, Introduction to Plasma Physics and Controllable Fusion, vol. 1, $2^{\text {nd }}$ ed., Springer, 1984, and/or a graduate-level theoretical treatment by R. D. Hazeltine and J. D. Meiss, Plasma Confinement, Dover, 2003.

[^415]:    ${ }^{66}$ See, e.g., CM Sec. 10.1.
    ${ }^{67}$ Equation (209) is also the basis for discussion of numerous other magnetic field phenomena, including the Aharonov-Bohm and quantum Hall effects - see, e.g., QM Secs. 3.1-3.2.

[^416]:    ${ }^{68}$ As a reminder, the homogeneous Maxwell equations (129) are satisfied by the very structure (125) of the field strength tensor.
    ${ }^{69}$ Here the implicit summation over index $\alpha$ plays the role similar to the convective derivative (188) in replacing the full derivative over time, in a way that reflects the symmetry of time and space in special relativity. I do not want to spend more time to justify Eq. (214) because of the reasons that will be clear very soon.
    ${ }^{70}$ In the Gaussian units, the coefficient is $(-1 / 16 \pi)$.

[^417]:    ${ }^{71}$ Since the Lagrange equations of motion are homogeneous, the simultaneous change of sign of $T$ and $U$ does not change them. Thus, it is not important which of two energy densities, $u_{e}$ or $u_{m}$, we count as the potential energy.

[^418]:    ${ }^{72}$ In this way, we are using Eqs. (214) and (221) just as a useful guesses, leading to the definition of $\theta^{\alpha \beta}$, and may leave their strict justification for more serious field theory courses.

[^419]:    Electric field's

[^420]:    ${ }^{74}$ This impulse is sometimes called the hidden momentum; this term makes sense if the field sources have finite masses, so that their velocity change at the field variation is measurable.
    ${ }^{75}$ See, e.g., CM Sec. 7.2.
    ${ }^{76}$ Note that the field-to-particle interaction gives a vanishing contribution into the net integral, as it should for any internal interaction between internal parts of a system.

[^421]:    ${ }^{77}$ By the way, repeating these arguments for a plane capacitor filled with a linear dielectric, we may readily see that Eq. (239) may be generalized for this case by replacing $\varepsilon_{0}$ for $\varepsilon$. The similar replacement ( $\mu_{0} \rightarrow \mu$ ) is valid for Eq. (241) in a linear magnetic medium.
    ${ }^{78}$ The causal relation is not important here. Especially in the case of a superconductor, the magnetic field may be induced by another source, with the surface supercurrent $\mathbf{j}$ just shielding the superconductor's bulk from its penetration - see Sec. 6.

[^422]:    ${ }^{79}$ Of course, this condition may hold "forever" only for solenoids with superconducting wiring, but even in normal-metal solenoids with practicable inductances, the flux relaxation constants $L / R$ may be rather large (practically, up to a few minutes), quite sufficient to carry out the force measurement.

[^423]:    ${ }^{80}$ Such a decay may happen, for example, with a neutral pion.
    ${ }^{81}$ This the famous Compton scattering problem.

[^424]:    ${ }^{1}$ As Fig. 1 shows, there is always another point $\left\{\mathbf{r} ", t^{\prime \prime}\right\}$, with $t^{\prime \prime}>t$, that is formally also a solution of Eq. (4), but it does not fit Eqs. (1), because the field induced at that point would violate the causality principle.

[^425]:    ${ }^{2}$ Note the following identities: $\gamma^{2}=1 /\left(1-\beta^{2}\right)$ and $\left(\gamma^{2}-1\right)=\beta^{2} /\left(1-\beta^{2}\right)=\gamma^{2} \beta^{2}$, which may be very handy for the relativity-related algebra.
    ${ }^{3}$ They were derived in 1898 by A.-M. Liénard and (apparently, independently) in 1900 by E. Wiechert.

[^426]:    ${ }^{4}$ Note that this time compression effect (linear in $\beta$ ) has nothing to do with the Lorentz time dilation (9.21), which is quadratic in $\beta$. (Indeed, all our arguments above are referred to the same, lab frame.) Rather, it is close in nature to the Doppler effect.

[^427]:    ${ }^{7}$ A similar calculation of magnetic field components from Eq. (20b) gives the results identical to Eqs. (9.140).
    ${ }^{8}$ If the direction of radiation, $\mathbf{n}$, does not change in time, this formula does not contain the observation point $\mathbf{r}$. Hence, from this point on, index $r$ may be safely dropped for brevity, though we should always remember that $\beta$ in Eq. (30) is the reduced velocity of the particle at the instant of radiation's emission, not detection.

[^428]:    ${ }^{9}$ The second form of Eq. (10.37), frequently more convenient for applications, may be readily obtained from the first one by applying MA Eq. (7.7a) to the vector product.

[^429]:    ${ }^{10}$ See, e.g., https://www6.slac.stanford.edu/.

[^430]:    ${ }^{11}$ For proton accelerators, such energy loss is much less of a problem, because $\gamma$ of an ultra-relativistic particle (at fixed $\mathcal{E}$ ) is proportional to $1 / m$, so that the estimates, at the same $R$, should be scaled back by $\left(m_{p} / m_{e}\right)^{4} \sim 10^{13}$. Nevertheless, in the giant modern accelerators such as the LHC (with $R \approx 4.3 \mathrm{~km}$ and $\varepsilon \approx 7 \mathrm{TeV}$ ), the synchrotron radiation loss per revolution is rather noticeable ( $\mathcal{P} \Delta t^{\prime} \sim 6 \mathrm{keV}$ ), leading not as much to particle deceleration as to substantial photoelectron emission from the beam tube walls, creating harmful defocusing effects.

[^431]:    ${ }^{12}$ If the observation point is off-plane, or if the rotation speed is much less than $c$, the radiation is virtually monochromatic, with frequency $\omega_{c}$.

[^432]:    ${ }^{13}$ In contrast to the single-frequency case (i.e. a monochromatic wave), we may avoid taking real part of the complex function $\left(\mathbf{E}_{\omega} e^{-i \omega}\right)$ if we require that $\mathbf{E}_{-\omega}=\mathbf{E}_{\omega}{ }^{*}$. However, it is important to remember the factor $1 / 2$ required for the transition to a monochromatic wave of frequency $\omega_{0}$ : $\mathbf{E}_{\omega}=\mathbf{E}_{0}\left[\delta\left(\omega-\omega_{0}\right)+\delta\left(\omega+\omega_{0}\right)\right] / 2$.
    ${ }^{14}$ Note that the expression under the integral differs from $d \mathcal{P} / d \Omega$ defined by Eq. (29) by the absence of term (1$\beta \cdot \mathbf{n})=\partial t^{\prime} / \partial t$. This is natural, because this is the wave energy arriving at the observation point $\mathbf{r}$ during time interval $d t$ rather than $d t$ '.

[^433]:    ${ }^{15}$ See, e.g. MA Eq. (14.3a).
    16 The notion of spectral density may be readily generalized to random processes - see, e.g., SM Sec. 5.4.
    17 Note that for our current purposes of calculation of spectral density of radiation by a single particle, factor $\exp \{i \omega r / c\}$ has got cancelled. However, as we have seen in Chapter 8, this factor plays the central role at

[^434]:    interference of radiation from several (many) sources. In the context of synchrotron radiation, such interference becomes important in undulators and free-electron lasers - the devices to be (qualitatively) discussed below.
    ${ }^{18}$ Actually, this simplification is not occasional. According to Eq. (10b), the expression under the derivative is just the transverse component of the vector-potential $\mathbf{A}$ (give or take a constant factor), and from the discussion in Sec. 8.2 we know that this component determines the electric dipole radiation of the particle (which dominates the radiation field in our current case of uncompensated electric charge).

[^435]:    ${ }^{19}$ By the way, this expression shows that the in-plane ( $x$ ) component of the electric field is an odd function of $t$ ' (and hence $t$-see its sketch in Fig. 7), while the perpendicular component is an even function of time. Also notice that for an observer exactly in the rotation plane $\left(\theta_{0}=0\right)$ the latter component vanishes.

[^436]:    ${ }^{20}$ The law of the spectral density decrease at large $v$ may be readily obtained from the second of Eqs. (2.158) which is valid even for any (even non-integer) Bessel function index $n: a_{x} \propto a_{y} \propto v^{-1 / 2} \exp \{-v\}$. Here the exponential factor is certainly most important.
    ${ }^{21}$ For that, and many other details, the interested reader may be referred, for example, to the fundamental review collection by E. E. Koch et al. (eds.) Handbook on Synchrotron Radiation (in 5 vols.), North-Holland, 1983-1991, or a more concise monograph by A. Hofmann, The Physics of Synchrotron Radiation, Cambridge U. Press, 2007.

[^437]:    ${ }^{22}$ By modern standards, this energy is not too high. The distinguished feature of NSLS-II is its unprecedented electron beam intensity (planned average beam current up to 500 mA ) which should allow an extremely high synchrotron "brightness" $I(\omega)$.

[^438]:    ${ }^{23}$ A small problem for the reader: use Eqs. (20) and (63) to explain the difference between the shapes of pulses generated at opposite magnetic poles of the wiggler, which is schematically shown in Fig. 12a.

[^439]:    ${ }^{24}$ This important formula may be also interpreted in the following way. Due to the relativistic length contraction (9.20), the undulator structure period as perceived by beam electrons is $\lambda^{\prime}=\lambda / \gamma$, so that the central frequency of radiation is $\omega_{0}{ }^{\prime}=2 \pi c / \lambda^{\prime}=2 \pi c / / \lambda$. For the lab-frame observer, this frequency is Doppler-upshifted according to Eq. (9.44): $\omega_{0}=\omega_{0}{ }^{\prime}[(1+\beta) /(1-\beta)]^{1 / 2} \approx 2 \gamma \omega_{0}{ }^{\prime}$, giving the same result as Eq. (74).
    ${ }^{25}$ Much of the difference is due to the fact that that those plots show the spectral density of the number of photons $n=\varepsilon / \hbar \omega$ per second, which peaks above the density of power, i.e. energy $\varepsilon$ per second.
    ${ }^{26}$ This name is somewhat misleading, because in contrast to the usual ("quantum") lasers, the free-electron laser operation is essentially classical and very similar to that of vacuum-tube microwave generators (such as magnetrons briefly discussed in Sec. 9.6) - see, e.g., E. Salin et al., The Physics of Free Electron Lasers, Springer, 2000.
    ${ }^{27}$ Such X-ray radiation had been observed experimentally, though not correctly interpreted by N. Tesla in 1887, i.e. before the radiation was studied in detail (and much publicized) by W. Röntgen.

[^440]:    ${ }^{28}$ In publications on this topic (whose development peak was in the 1920s and 1930s), Gaussian units are more common, and letter $Z$ is usually reserved for expressing charges as multiples the fundamental charge $e$, rather than for the wave impedance. This is why, in order to avoid confusion, in this section I will use $1 / \varepsilon_{0} c \equiv Z_{0}$ for the free-space wave impedance and, still sticking to the same SI units as used through my lecture notes, will write the coefficients in a form that makes the transfer to the Gaussian units trivial: it is sufficient to replace all $\left(q q^{\prime} / 4 \pi \varepsilon_{0}\right)_{\text {SI }}$ with $\left(q q^{\prime}\right)_{\text {Gaussian. }}$. In the (rare) cases when I spell out the charge values, I will use a different font: $q \equiv \mathcal{Z}^{e}, q^{\prime} \equiv \mathcal{\xi}^{\prime} e$.
    ${ }^{29}$ A more careful analysis shows that this approximation is actually quite reasonable up to much higher frequencies of the order of $\gamma^{2} / \tau$.
    ${ }^{30}$ Evidently, this result (but not the general Eq. (76)!) may be derived from Eq. (8.27) as well.
    ${ }^{31}$ Please note the font-marked difference between this variable $(\boldsymbol{q})$ and particle's electric charge $(q)$.

[^441]:    ${ }^{32}$ See, e.g., CM Sec. 3.7.
    ${ }^{33}$ See, e.g., CM Eq. (3.72) with constant $\alpha=q q$ ' $/ 4 \pi \varepsilon_{0}$. In the form used in Eq. (80), the Rutherford formula is also valid for small-angle scattering of relativistic particles, the criterion being $|\Delta \boldsymbol{\beta}| \ll 2 / \gamma$.
    ${ }^{34}$ Angle $\theta$ ' and differential $d \Omega$ ', describing the direction of scattered particles, should not be confused with $\theta$ and $d \Omega$ describing directions of the radiation emitted at the scattering event.

[^442]:    ${ }^{35}$ The modifications of this formula necessary for the relativistic case description are surprisingly minor - see, e.g., Chapter 15 of J. D. Jackson, Classical Electrodynamics, $3^{\text {rd }}$ ed., Wiley 1999. For more detail, the standard reference monograph on bremsstrahlung is W. Heitler, The Quantum Theory of Radiation, $3^{\text {rd }}$ ed., Oxford U. Press 1954 (reprinted in 2010 by Dover).
    ${ }^{36}$ See, e.g., QM Secs. 6.3, 9.3, 9.5, and 9.7.
    ${ }^{37}$ See, e.g., MA Eq. (6.14).
    ${ }^{38}$ According to Eq. (9.139), $E_{z}=0$, and the net impulse of the longitudinal force $q^{\prime} E_{x}$ is zero.

[^443]:    39 A quantum analysis (carried out by H. Bethe in 1940) replaces, in Eq. (95), $\ln B$ with $\ln \left(2 \gamma^{2} m u^{2} / \hbar\langle\omega\rangle\right)-\beta^{2}$, where $\langle\omega\rangle$ is the average frequency of the atomic quantum transitions weight by their oscillator strength. This refinement does not change the estimate given below. Note that both the classical and quantum formulas describe, a fast increase (as $1 / \beta$ ) of the energy loss rate $(-d \varepsilon / d x)$ at $\gamma \rightarrow 1$ and its slow increase (as $\ln \gamma$ ) at $\gamma \rightarrow \infty$, so that the losses have a minimum at $(\gamma-1) \sim 1$.

[^444]:    ${ }^{40}$ Actually, the above analysis has neglected the change of momentum of the incident particle. This is legitimate at $m^{\prime} \ll m$, but for $m=m$ ' the change approximately doubles the energy losses. Still, this does not change the order of magnitude of the estimate.
    ${ }^{41}$ All integrals here and below are in infinite limits, unless specified otherwise.
    ${ }^{42}$ As was discussed in Sec. 7.2, the Ohmic conductivity of the medium (generally, also a function of frequency) may be readily incorporated into the dielectric permittivity: $\varepsilon(\omega) \rightarrow \varepsilon_{\mathrm{ef}}(\omega)+i \sigma(\omega) / \omega$. In this section, I will assume that such incorporation, which is especially natural for high frequencies, has been performed, so that the current density $\mathbf{j}(\mathbf{r}, \mathrm{t})$ describes only stand-alone currents - for example, the current (105) of the incident particle.

[^445]:    ${ }^{43}$ See, e.g., MA Eq. (6.5a).
    ${ }^{44}$ As a reminder, the main properties of these functions are listed in Sec. 2.5 of these notes - see, in particular, Fig. 2.20b and Eqs. (2.157)-(2.158).

[^446]:    ${ }^{45}$ Strictly speaking, inequality $\kappa^{2}<0$ does not make sense for a medium with complex $\varepsilon(\omega) \mu(\omega)$ and hence complex $\kappa^{2}(\omega)$. However, in a typical medium where particles can propagate over substantial distances, the imaginary part of product $\delta(\omega) \mu(\omega)$ does not vanish only in very limited frequency intervals, much more narrow that the intervals which we are now discussing - please have one more look at Fig. 7.5.
    ${ }^{46}$ This radiation was observed experimentally by P. Cherenkov (in older Western texts, "Čerenkov") in 1934, with the observations explained by I. Frank and E. Tamm in 1937. Note, however, that the effect had been predicted theoretically as early as in 1889 by the same O. Heaviside whose name was mentioned so many times above - and whose genius I believe is still underappreciated.

[^447]:    ${ }^{47}$ See, e.g., a brief discussion in CM Sec. 8.6.

[^448]:    48 See, e.g., http://delphiwww.cern.ch/offline/physics/delphi-detector.html. For a broader view at radiation detectors (including Cherenkov ones), the reader may be referred to the classical text by G. F. Knoll, Radiation Detection and Measurement, $4^{\text {th }}$ ed., Wiley, 2010, and a newer treatment by K. Kleinknecht, Detectors for Particle Radiation, Cambridge U. Press, 1999.
    ${ }^{49}$ The effect was predicted theoretically in 1946 by V. Ginzburg and I. Frank, and only later observed experimentally.

[^449]:    ${ }^{50}$ See, e.g., Sec. 5.3 in K. Kleinknecht's monograph cited above.

[^450]:    ${ }^{51}$ This formula may be readily generalized to the relativistic case:

    $$
    F_{\text {self }}^{\alpha}=\frac{2}{3 m c^{3}} \frac{q^{2}}{4 \pi \varepsilon_{0}}\left[\frac{d^{2} p^{\alpha}}{d \tau^{2}}+\frac{p^{\alpha}}{(m c)^{2}}\left(\frac{d p_{\beta}}{d \tau} \frac{d p^{\beta}}{d \tau}\right)\right],
    $$

[^451]:    ${ }^{52}$ Note: this operation cannot be interpreted as describing a quantum spread due to the finite extent of point particle's wavefunction. In quantum mechanics, parts of wavefunction of the same charged particle do not interact with each other!

[^452]:    ${ }^{53}$ See, e.g., CM Sec. 6.6.
    ${ }^{54}$ See, e.g., QM Chapter 9 and references therein.

[^453]:    ${ }^{55}$ See, e.g., EM Sec. 9.3, in particular Eq. (9.53) and its discussion.
    ${ }^{56}$ As the Maxwell equation for $\nabla \times \mathbf{H}$ shows, such field distribution cannot be created in any nonvanishing volume of free space. However, it may be created on a line - e.g., on particle's straight trajectory.

[^454]:    ${ }^{1}$ For remedial reading, I can recommend, for example, D. Griffith, Quantum Mechanics, $2^{\text {nd }}$ ed., Cambridge U. Press, 2016.
    ${ }^{2}$ This expression was used in a 1900 talk by Lord Kelvin (born W. Thomson) in reference to the blackbody radiation measurements and Michelson-Morley experiment results, i.e. the precursors of the quantum mechanics and relativity theory.
    ${ }^{3}$ See, e.g., EM Sec. 7.9. The degeneracy factor 2 in Eq. (1) is due to two possible polarizations of transverse electromagnetic waves. For waves of other physical nature, which obey with the linear ("acoustic") dispersion law, similar relations are also valid, though possibly with a different degeneracy factor - see, e.g., CM Sec. 7.7. ${ }^{4}$ See, e.g., SM Sec. 2.2.
    ${ }^{5}$ In the SI units, used through these notes, $k_{\mathrm{B}} \approx 1.38 \times 10^{-23} \mathrm{~J} / \mathrm{K}$. Note that in many theoretical papers (and in the SM part of my notes), $k_{\mathrm{B}}$ is taken for 1 , i.e. temperature is measured in energy units.

[^455]:    ${ }^{6}$ M. Planck himself wrote $\hbar \omega$ as $h v$, where $v=\omega / 2 \pi$ is the "cyclic" frequency, measured in Hz (periods per second), so that in early texts the term "Planck's constant" referred to $h \equiv 2 \pi \hbar$, while $\hbar$ was called "the Dirac constant" for a while.

[^456]:    ${ }^{7}$ As a reminder, A. Einstein received his only Nobel Prize (in 1922) for exactly this work, which essentially started quantum mechanics, rather than for his relativity theory.
    ${ }^{8}$ For most metals, $W$ is between 4 and 5 electron-volts (eV), so that the threshold corresponds to $\lambda_{\max }=2 \pi c / \omega_{\min }=$ $c h / W \approx 300 \mathrm{~nm}$ - approximately at the border between the visible light and ultraviolet radiation.
    ${ }^{9}$ See, e.g., SM Sec. 2.5.
    ${ }^{10}$ See, e.g., EM Sec. 8.2.

[^457]:    ${ }^{11}$ Besides very small corrections due to the finite ratio of the electron mass $m_{e}$ to that of the nuclei, and minor spin-orbital and relativistic effects - see Secs. 6.3 and 9.7 below.
    ${ }^{12}$ Unfortunately, another mane, "Rydberg constant" is also frequently used for either this atomic energy unit or its half, $E_{H} / 2 \approx 13.6 \mathrm{eV}$. To add to the confusion, the same term "Rydberg constant" is sometimes used for the reciprocal free-space wavelength $\left(1 / \lambda_{0}=\omega_{0} / 2 \pi c\right)$ corresponding to frequency $\omega_{0}=E_{\mathrm{H}} / 2 \hbar$.

[^458]:    ${ }^{13}$ This fact was noticed and discussed in detail in 1923 by L. de Broglie, so that instead of discussing wavefunctions, especially of free particles, we are still frequently speaking of de Broglie waves.
    ${ }^{14}$ This effect was observed (in 1922) and explained a year later by A. Compton.
    ${ }^{15}$ See, e.g., EM Sec. 9.3.

[^459]:    ${ }^{19}$ Actually, in wave mechanics, the spin of the described particle has not to be equal zero. Rather, it is assumed that the spin effects are negligible - as they are, for example, for a non-relativistic electron moving in a region without an appreciable magnetic field.
    ${ }^{20}$ As a reminder, for many systems (including those whose kinetic energy is a quadratic-homogeneous function of generalized velocities, like $m v^{2} / 2$ ), $H$ coincides with the total energy $E-$ see, e.g., CM Sec. 2.3.
    ${ }^{21}$ Note that this restriction is very important. In particular, it excludes from our current discussion the particles whose interaction with environment is irreversible, for example it is the viscosity leading to particle's energy decay. Such systems need a more general quantum-mechanical description that will be discussed in Chapter 7 .
    ${ }^{22}$ Generally, quantum mechanics, as any theory, may be built on different sets of postulates ("axioms") leading to the same conclusions. In this text, I will not try to beat down the number of postulates to the absolute minimum, not only because this would require longer argumentation, but chiefly because such attempts typically result in making certain implicit assumptions hidden from the reader - the practice as common as regrettable.
    ${ }^{23}$ I will imply such perfect conditions until the discussion of particle's interaction with environment, and realistic ("physical") measurements in Chapter 7.

[^460]:    ${ }^{24}$ This is one more important caveat. As we will see in Chapter 7, in many cases even the Hamiltonian particles cannot be described by a certain wavefunction, and allow only a more general (and less precise) description, e.g., by the density matrix.
    ${ }^{25}$ This key measurement postulate is sometimes called the Born rule.

[^461]:    ${ }^{26}$ For an electrically charged particle in magnetic field, this relation is valid for its canonical momentum - see Sec. 3.1 below.
    ${ }^{27}$ See, e.g., Secs. 8-10 of the Selected Mathematical Formulas appendix (below, referred to as MA). Note that according to these formulas, the del operator follows all the geometric rules of the usual ( $c$-number) vectors. This is, by definition, true for other vector operators of quantum mechanics to be discussed below.
    ${ }^{28}$ See, e.g., CM Sec. 10.3.
    ${ }^{29}$ See, e.g., CM Sec. 7.7 and/or EM Sec. 7.1.

[^462]:    ${ }^{30}$ For infinite space ( $V \rightarrow \infty$ ), Eq. (31) yields $a \rightarrow 0$, i.e. wavefunction (29) vanishes. This formal problem may be readily resolved considering sufficiently long wave packets - see Sec. 2.2 below.

[^463]:    ${ }^{31}$ See, e.g., SM Secs. 5.8 and 6.2, respectively.

[^464]:    ${ }^{32}$ Note that this requirement is not extended to the relativistic quantum theory - see Chapter 9 below.

[^465]:    ${ }^{33}$ As a reminder, such description is valid not only for potential forces (in that case $U$ has to be timeindependent), but also for any force $\mathbf{F}(\mathbf{r}, t)$ which may be presented via the gradient of $U(\mathbf{r}, t)$ - see, e.g., CM Chapters 2 and 10. (A good example when such a description is impossible is given by the magnetic component of the Lorentz force - see, e.g., EM Sec. 9.7, and also Sec. 3.1 of this course.)
    ${ }^{34}$ Historically, this was the main step made (in 1926) by E. Schrödinger on the background of L. de Broglie's idea. The probabilistic interpretation of the wavefunction was put forward, almost simultaneously, by M. Born. ${ }^{35}$ In Chapter 4, we will discuss a more general family of Hermitian operators, which have this property.
    ${ }^{36}$ See, e.g., MA Eq. (11.4a), combined with the del operator's definition $\nabla^{2} \equiv \nabla \cdot \nabla$.
    ${ }^{37}$ See, e.g., MA Eq. (12.2).

[^466]:    ${ }^{38}$ See, e.g., respectively, CM 7.2 and EM Sec. 4.1.
    ${ }^{39}$ By the way, if any equality involving operators is valid for an arbitrary wavefunction, the latter is frequently dropped from notation, resulting in an operator equality. In particular, Eq. (53) may be readily used to prove that the operators are commutative: $\hat{A}_{2}+\hat{A}_{1}=\hat{A}_{1}+\hat{A}_{2}$, and associative: $\left(\hat{A}_{1}+\hat{A}_{2}\right)+\hat{A}_{3}=\hat{A}_{1}+\left(\hat{A}_{2}+\hat{A}_{3}\right)$.

[^467]:    ${ }^{40}$ It may seem strange that the linear Schrödinger equation correctly describes quantum properties of systems whose classical dynamics is described by nonlinear equations of motion (e.g., an anharmonic oscillator - see, e.g., CM Sec. 4.2). Note, however, that equations of classical physical kinetics (see, e.g., SM Chapter 6) also have this property, so it is not specific to quantum mechanics.
    ${ }^{41}$ This argumentation, leading to variable separation, is very common in mathematical physics - see, e.g., its discussion in EM Sec. 2.5.

[^468]:    ${ }^{42}$ In contrast, the initial Eq. (24) is frequently called the time-dependent or nonstationary Schrödinger equation.
    ${ }^{43}$ From German root eigen meaning "particular" or "characteristic".
    ${ }^{44}$ Eigenvalues of energy are frequently called eigenenergies, and it is often said that eigenfunction $\psi_{n}$ and eigenenergy $E_{n}$ together characterize $n$-th stationary eigenstate of the system.

[^469]:    ${ }^{45}$ By using the term "quantum well" for what is essentially a potential well I bow to a common, but a very unfortunate convention. Indeed, this term seems to imply that the particle's confinement in such a "quantum well" is a phenomenon specific for quantum mechanics, while as we will repeatedly see in this course, that the opposite is true: quantum effects do as much as they only can to overcome particle's confinement in a potential well, letting the particle to partly penetrate the "classically forbidden" regions.
    ${ }^{46}$ Rewritten as $\nabla^{2} f+k^{2} f=0$, this is the Helmholtz equation, which describes scalar waves of any nature (with wave vector $\mathbf{k}$ ) in a uniform, linear media - see, e.g., CM Sec. 5.5 and/or EM Secs. 7.7-7.9.

[^470]:    ${ }^{47}$ The front coefficient is selected in a way that ensures the (ortho)normality condition (64).

[^471]:    ${ }^{48}$ In some systems (e.g., a particle interacting with a finite-depth quantum well), a discrete energy spectrum within a certain interval of energies may coexist with a continuous spectrum in a complementary interval. However, the conceptual philosophy of eigenfunctions and eigenvalues remains the same in this case as well.

[^472]:    ${ }^{49}$ For a more detailed discussion of this point, the reader may be referred, e.g., to CM Secs. 5.4 (in the context of 1D mechanical waves), because it is valid for waves of any nature.

[^473]:    ${ }^{50}$ Many textbooks on quantum mechanics jump to solution of 1D without such discussion, and most of my beginning graduate students did not understand that in realistic physical systems, such dimensionality restriction is only possible under very specific conditions.
    ${ }^{51}$ The term "quantum confinement", sometimes used to describe this phenomenon, is as unfortunate as the "quantum well", because of the same reason: the confinement is a purely classical effect, and as we will repeatedly see in this course, quantum mechanics reduces it, allowing a partial penetration of the particle into the classically forbidden regions with $E>U(\mathbf{r})$.
    ${ }^{52}$ The last term in Eq. (86) is frequently referred to as the (partial) confinement energy; despite its inclusion to $U_{\text {ef }}$, it is important to remember about the kinetic-energy origin of this contribution.

[^474]:    ${ }^{53}$ In the frequent case when motion in the $[x, y]$ plane is free (or almost free), the set of quantum states with the same quantum number $n_{z}$ is frequently called a subband, because their energies form a (quasi-) continuum of eigenenergies $E_{x, y}$.
    ${ }^{54}$ To be discussed in Sec. 3.2.
    ${ }^{55}$ See, e.g., P. Harrison, Quantum Wells, Wires, and Dots, $3^{\text {rd }}$ ed., Wiley, 2010.
    ${ }^{56}$ This is a reasonable first approximation, for example, for electron motion potential in so-called quantum wires, for example in the now-famous carbon nanotubes - see, e.g., the same monograph by P. Harrison.

[^475]:    1D number

[^476]:    ${ }^{57}$ Despite the theorem's name, H. Hellmann (in 1937) and R. Feynman (in 1939) were not the first in the long list of physicists who have (apparently, independently) discovered this fact. Indeed, it may be traced back at least to a 1922 paper by W. Pauli, and was carefully proved by P. Güttinger in 1931.

[^477]:    ${ }^{58}$ You may like to start from reading about the finite-difference method - see, e.g., CM Sec. 8.5 or EM Sec. 2.8.

[^478]:    ${ }^{1}$ Eq. (13) may be proved even if $\langle x\rangle$ and $\left\langle p_{x}\right\rangle$ are not equal to zero, by making the following replacements, $x \rightarrow x$ $\langle x\rangle, \partial / \partial x \rightarrow \partial / \partial x+i\langle p\rangle / \hbar$, in Eq. (7), and then repeating all the calculations - which become rather bulky. We will re-derive the uncertainty relations, in a more efficient way, in Chapter 4.

[^479]:    ${ }^{2}$ From this point on, in this chapter I will drop index $x$ in notation for $x$-component of vectors $\mathbf{k}$ and $\mathbf{p}$.
    ${ }^{3}$ This may be readily proven using the well-known integral of the Gaussian function ("bell curve") given by Eq. (17) - see, e.g., MA Eq. (6.9b). It is also straightforward to use MA Eq. (6.9c) to prove that for wave packet (16), parameter $\delta x$ is indeed the r.m.s. uncertainty (1.34) of coordinate $x$, thus justifying its notation.

[^480]:    ${ }^{4}$ For notation's brevity, from this point on the infinite limit signs will be dropped in all 1D integrals.
    ${ }^{5}$ The fact that the argument shift is imaginary is not important, because function under the integral is analytical, and tends to zero at $\operatorname{Re} x^{\prime} \rightarrow \pm \infty$.

[^481]:    ${ }^{6}$ Note that this packet is equivalent to Eq. (16) and hence is properly normalized to 1 - see Eq. (3). Hence the wave packet introduction offers a natural solution to the problem of infinite wave normalization, which was mentioned in Sec. 1.2.

[^482]:    ${ }^{7}$ See, e.g., brief discussions in CM Sec. 5.3 and EM Sec. 7.2.
    ${ }^{8}$ By the way, in the particular case of de Broglie wave described by dispersion relation (1.30), Eq. (28) is exact, because $\omega=E / \hbar$ is a quadratic function of $k=p / \hbar$, and all higher derivatives of $\omega$ over $k$ vanish for any $k_{0}$.

[^483]:    ${ }^{9}$ Its standard notation by letter $G$ stems from the fact that the propagator is essentially the spatial-temporal Green's function of Eq. (2.18), defined very similarly to Green's functions of other ordinary and partial differential equations describing various physics systems - see, e.g., CM Sec. 4.1 and/or EM Sec. 2.7 and 7.3.

[^484]:    ${ }^{10}$ Note that this initial condition is not equivalent to a $\delta$-functional initial probability density (2).

[^485]:    ${ }^{11}$ It was predicted theoretically by B. Josephson (then a graduate student!) in 1962 and observed experimentally in less than a year. More recently, analogs of this effect were also observed in superfluid helium and atomic BoseEinstein condensates.
    ${ }^{12}$ See, e.g., SM Sec. 3.4.
    ${ }^{13}$ For more on this notion see, e.g. SM Sec. 6.4.
    ${ }^{14}$ Later, Eq. (55) has been shown to be valid for other weak link types as well, though deviations from have also been found. These deviations, however, do not affect the fundamental $2 \pi$-periodicity of function $I(\varphi)$ - see, e.g., EM Sec. 6.4. As a result, no deviations from the fundamental relations (56)-(57) have been found (yet :-).

[^486]:    ${ }^{15}$ See, e.g., CM Sec. 4.4.
    ${ }^{16}$ If $\omega$ is not too high, this effect may be adequately described combining Eqs. (54)-(55). Let me leave this task for the reader.
    ${ }^{17}$ The most precise proof that the Josephson frequency-to-voltage ratio $f_{\mathrm{J}} / V$ does not depend on superconducting material (to at least 15 decimal places!) has been carried out by the group led by J. Lukens here at Stony Brook see J.-S. Tsai et al., Phys. Rev. Lett. 51, 316 (1983).

[^487]:    ${ }^{18}$ Note that this is not the eigenproblem like the one we have solved in Sec. 1.4 for a quantum well. Indeed, now energy $E$ is considered fixed - e.g., by the initial conditions that launch a long wave packet upon the potential step, from the left.

[^488]:    ${ }^{19}$ Our earlier discarding of the particular solution $\exp \{\kappa x\}$, now becoming $\exp \left\{-i k^{\prime} x\right\}$, is still valid, but now on a different grounds: this term would describe a wave packet incident on the potential step from the right, and this is not the problem under our consideration.
    ${ }^{20}$ These formulas are completely similar to those for the partial reflection of classical waves from a sharp interface between two uniform media, at normal incidence (see, e.g., CM Sec. 5.4 and EM Sec. 7.4), with the effective impedance $Z$ of de Broglie waves proportional to their wave number $k$.

[^489]:    ${ }^{21}$ See, e.g., G. Fursey, Field Emission in Vacuum Microelectronics, Kluwer, New York, 2005.
    ${ }^{22}$ See, e.g., G. Binning and H. Rohrer, Helv. Phys. Acta 55, 726 (1982).
    ${ }^{23}$ See, e.g., V. Sverdlov et al., IEEE Trans. on Electron Devices 50, 1926 (2003).

[^490]:    ${ }^{24}$ Philosophically, this space-domain method is very close to the time-domain rotating wave approximation (RWA) used, for example, in the classical and quantum theory of oscillations - see, e.g., CM Secs. 4.2-4.5, and Secs. 6.5, 7.6, 7.7, 9.2, and 9.4 of this course.
    ${ }^{25}$ Such perturbation theories will be discussed in Chapter 6.

[^491]:    ${ }^{26}$ For certainty, I will use the discretion given by Eq. (82) to define $k(x)$ as the positive root of its right-hand part.

[^492]:    ${ }^{27}$ An alternative way to solve the connection problem, without involving the Airy functions but using an analytical extension of WKB formulas to the plane of complex argument, may be found, e.g., in Sec. 47 of textbook by L. Landau and E. Lifshitz, Quantum Mechanics, Non-Relativistic Theory, 3rd ed. Pergamon, 1977.

[^493]:    ${ }^{28}$ The following (exact!) integral formulas,

    $$
    \operatorname{Ai}(\zeta)=\frac{1}{\pi} \int_{0}^{\infty} \cos \left(\frac{\xi^{3}}{3}+\zeta \xi\right) d \xi, \quad \operatorname{Bi}(\zeta)=\frac{1}{\pi} \int_{0}^{\infty}\left[\exp \left\{-\frac{\xi^{3}}{3}+\zeta \xi\right\}+\sin \left(\frac{\xi^{3}}{3}+\zeta \xi\right)\right] d \xi
    $$

[^494]:    ${ }^{29}$ Note that at motion in more than one dimension, a closed classical trajectory may have no turning points. In this case, the constant $1 / 2$ in the parentheses of Eq. (109), arising from the turns, should be dropped. The simplest example is the circular motion of the electron about the proton in Bohr's picture of the hydrogen atom, for which the modified quantization (109) condition takes form (1.10) postulated by N. Bohr. (A similar relation for the radial motion is sometimes called the Sommerfeld-Wilson quantization rule.)

[^495]:    ${ }^{30}$ Sorry, but the same letter, $d$, is used here for the barrier thickness (defined in this case as the classically forbidden region length, $x_{c}{ }^{\prime}-x_{c}$ ), and the constant in one of the wave amplitudes - see Eq. (116). Let me hope that the difference between these uses is absolutely evident from the context.

[^496]:    ${ }^{31}$ Note, however, that in the most important case $T_{\mathrm{wKB}} \ll 1$, Eq. (117) may be simply derived from Eqs. (105) an exercise left for the reader.
    ${ }^{32}$ It was carried out by E. Kemble in 1935. Notice that mathematically the Kemble formula is similar to the Fermi distribution in statistical physics, with effective temperature $T_{\text {ef }}=\hbar \omega_{0} / 2 \pi k_{\mathrm{B}}$. This similarity has some interesting implications for the statistics of Fermi gas tunneling.

[^497]:    ${ }^{34}$ In older literature, it is sometimes called the Ramsauer (or "Townsend", or "Ramsauer-Townsend") effect. However, it is currently more common to use that name(s) only for a similar 3D effect, especially at scattering of low-energy electrons on rare gas atoms - this is how it was first observed, independently, by C. Ramsauer and J. Townsend in the early 1920s.
    ${ }^{35}$ See also , e.g., EM Sec.7.9.
    ${ }^{36}$ The exact equality $T_{\max }=1$ is correct only if both component barriers are exactly equal.
    ${ }^{37}$ Probability $W(t)$ should not be confused with the delta-functional barrier's "area" $w$, defined by Eq. (122).

[^498]:    ${ }^{38}$ This almost evident assumption finds its formal justification in the perturbation theory to be discussed in Chapter 6.

[^499]:    ${ }^{39}$ Essentially the only requirement is to have the attempt time $\Delta t_{A}$ to be much longer than the effective time (instanton time, see Sec. 5.3 below) of tunneling through the barrier. In the delta-functional approximation for the barrier, the latter time vanishes, so that this requirement is always fulfilled.

[^500]:    ${ }^{40}$ Here I dare to refer the reader to my own old work K. Likharev, Int. J. Theor. Phys. 21, 311 (1982) that presented a constructive proof that at reversible computation (introduced in 1973 by C. Bennett) the energy dissipation may be lower than this apparent "quantum limit".
    ${ }^{41}$ See, e.g., a detailed discussion of this issue in the monograph by V. Braginsky and F. Khalili, Quantum Measurement, Cambridge U. Press, 1992.
    ${ }^{42}$ This argument is especially convincing if the particle detection time is much shorter than the time $t_{c}=2 v_{\mathrm{gr}} t / c$, where $c$ is the speed of light in vacuum, i.e. the maximum velocity of any information transfer ("signaling").

[^501]:    ${ }^{43}$ This formula will be easier to prove after we have discussed properties of Pauli matrices in Chapter 4.

[^502]:    ${ }^{44}$ Historically, the development of the fully quantum theory of $\mathrm{H}_{2}$ bonding by W. Heitler and F. London in 1927 was the breakthrough decisive for the acceptance of then-emerging quantum mechanics by chemists.
    ${ }^{45}$ Due to the opposite spins, the Pauli principle allows them to be in the same orbital ground state - see Chapter 8 .

[^503]:    ${ }^{46}$ Unit reminder: $1 \mathrm{~kJ} / \mathrm{mol} \approx 0.0434 \mathrm{eV}$.

[^504]:    WKB
    result for coupling energy

[^505]:    ${ }^{47}$ Since it is not true for potential (167), one should not be surprised that the resulting Eq. (189) is invalid for our initial problem, giving $\delta_{n}$ twice larger than the correct expression (178).

[^506]:    ${ }^{48}$ In solid state (especially semiconductor) physics and electronics, term bandgaps is more common.
    ${ }^{49}$ This expectation is implicitly confirmed by Fig. 20: at $\alpha \gg 1$, the highest resonance peak in each group tends to $k a=\pi n$, and the lowest peak also tend to a position independent of $N$ (though dependent on $\alpha$ ).

[^507]:    ${ }^{50}$ I am ashamed to confess that, due to the lack of time, this was virtually the only "lecture demonstration" in my QM courses.
    ${ }^{51}$ Named after F. Bloch who applied this concept to wave mechanics in 1929, i.e. very soon after its formulation. Admittedly, in mathematics, an equivalent statement, usually called the Floquet theorem, has been known since at least 1883.
    ${ }^{52}$ I will address this rigor in two steps. Later in this section, we will see that the function obeying Eq. (193) is indeed $a$ solution of the Schrödinger equation. However, to save time/space, it will be better for us to postpone the proof that any eigenfunction of the equation, with periodic boundary conditions, obeys the Bloch theorem, until Chapter 4. As a partial reward for the delay, that proof will be valid for an arbitrary spatial dimensionality.
    ${ }^{53}$ Product $\hbar q$, which has the dimensionality of momentum, is called either the quasi-momentum or (especially in the solid state physics) the "crystal momentum" of the particle.

[^508]:    ${ }^{54}$ Perhaps a more important reason for taking $q$ as the argument is that for motion in a general potential $U(x)$, particle's momentum $\hbar k$ is not a constant of motion, while (according to the Bloch theorem), the quasi-momentum $\hbar q$ is.

[^509]:    ${ }^{55}$ Below, we will see several other examples of this behavior. This alternation rule is also in accordance with the Bohr-Sommerfeld quantization condition

[^510]:    ${ }^{56}$ The benefits of my unusual choice of the summation index ( $l$ " instead of, say, $l$ ) will be clear in a few lines.

[^511]:    ${ }^{57}$ Note that we have essentially proved that the Bloch wavefunction (210) is indeed $a$ solution of Eq. (61), provided that the quasi-momentum $q$ is selected in a way to make the system of linear equation (215) compatible, i.e. is a solution of its characteristic equation - see, e.g., Eq. (223) below.
    ${ }^{58}$ Besides the constant potential $U_{0}$ that, as we know from Sec. 2, may be included into energy in a trivial way, so that we may take $U_{0}=0$.
    ${ }^{59}$ This method is so powerful that its multi-dimensional version is not much more complex than the 1D version described here - see, e.g., Sec. 3.2 in the classical textbook by J. M. Ziman, Principles of the Theory of Solids, $2^{\text {nd }}$ ed., Cambridge U. Press, 1979.

[^512]:    ${ }^{62}$ From that figure, it is also clear that in the weak potential limit, width $\Delta E_{n}$ of the $n$-th energy band is just $E^{(n)}-$ $E^{(n-1)}$ - see Eq. (221). Note that this is exactly the distance between adjacent energy levels of the simplest 1D quantum well of infinite depth - cf. Eq. (1.77).
    ${ }^{63}$ See, e.g., CM Sec. 5.1 and in particular Fig. 5.2.
    ${ }^{64}$ Actually, we could obtain this diagram earlier in this section, for the system of two weakly coupled quantum wells (Fig. 23), if we assumed the wells to be slightly dissimilar.

[^513]:    ${ }^{65}$ This equation, first studied in the 1860 s by É. Mathieu in the context of a rather practical problem of vibrating elliptical drumheads (!), has many other important applications in physics and engineering, notably including the parametric excitation of oscillations - see, e.g., CM Sec. 4.5.

[^514]:    ${ }^{66}$ Such plots, for several particular values of parameters, may be found, for example, in Figs. 8.11-8.13 of E. Merzbacher's textbook cited above.

[^515]:    67 A generalization of this expression to the case of essential interband transitions is not difficult using the Heisenberg picture of quantum mechanics (which will be discussed in Chapter 4 of this course) - see, e.g., Sec. 55 in E. M. Lifshitz and L. P. Pitaevskii, Statistical Physics, Part 2, Pergamon, 1980.

[^516]:    ${ }^{68}$ For a Gaussian packet, the spreading is described by Eq. (39), with the replacement $k \rightarrow q$; it is curious that at the inflection points with $d^{2} \omega / d q^{2}=0$ (which are present in each energy band) the packet does not spread.
    ${ }^{69}$ The proof of Eq. (237) is not difficult, but becomes more compact in the bra-ket formalism, to be discussed in Chapters 4 and 5. This is why I recommend the proof to the reader as an exercise after reading those two chapters.

[^517]:    ${ }^{70}$ The language is which the hole has a positive charge and mass has an additional convenience for states on the top of the valence band whose single-particle states are normally filled. Then the simplest, single-particle excitation of this multi-particle ground state may be created by giving one electron enough energy to lift it to a reference (e.g., Fermi-energy) level $E_{\mathrm{F}}$ that is, by definition of the valence band, is higher than all values $E(q)$. Then it is natural to prescribe to the excitation a positive mass $m_{\mathrm{ef}}$, because the energy $\Delta E=E_{\mathrm{F}}-E_{-}(q)$ necessary for the excitation grows with the deviation of $q$ from $q_{m}$.
    ${ }^{71}$ Intuition tells us (and statistical physics duly confirms :-) that this may be readily done, for example, by weakly coupling the system to a low-temperature environment, and letting it to relax to the lowest possible energy.

[^518]:    72 This phenomenon may be also discussed from the point of view of the reduced zone picture, but then it requires the introduction of instant jumps between the Brillouin zone boundary points (see the dashed red line in Fig. 32) that correspond to physically equivalent states of the particle. Evidently, this language is more artificial.

[^519]:    ${ }^{73}$ See, e.g., CM Sec. 1.5.
    ${ }^{74}$ In semiconductor device physics and engineering, such plots are called the band edge diagrams, and are the virtually unavoidable components of any discussion or publication.

[^520]:    ${ }^{75}$ In systems with many independent particles (such as semiconductors), the detection problem is exacerbated by phase incoherence of the Bloch oscillations performed by each particle. This drawback is absent in atomic BoseEinstein condensates whose Bloch oscillations (in a periodic potential created by standing optical waves) were eventually observed by M. Ben Dahan et al., Phys. Rev. Lett. 76, 4508 (1996).
    ${ }^{76}$ A simple analysis of phase locking of a classical oscillator may be found, e.g., in CM Sec. 4.4.
    ${ }^{77}$ A qualitative theory of such transitions will be discussed in Sec. 6.6 and then in Chapter 7.
    ${ }^{78}$ E. Mendez et al., Phys. Lev. Lett. 60, 2426 (1988).
    ${ }^{79}$ L. Kuzmin and D. Haviland, Phys. Rev. Lett. 67, 2890 (1991).

[^521]:    ${ }^{80}$ This unfortunate slip in the formula numbering can hardly lead to any misunderstanding.
    ${ }^{81}$ Of course, the dimensionality of $m_{\text {ef }}$ so defined is different from kg .
    ${ }^{82}$ This term has originated from the fact that the right-hand part of Eq. (253) equals to the single quantum unit $\left(\Phi_{0}\right)$ of the magnetic flux in superconductors - see Sec. 3.1 below.
    ${ }^{83}$ See, e.g., P. Bunyk et al., Int. J. on High Speed Electronics and Systems 11, 257 (2001).

[^522]:    ${ }^{84}$ Eq. (254) tells us that quasi-charge $Q$ has the simple physical sense of the external electric charge being inserted into the junction by the external current $I_{\text {ex }}$ - just like the physical sense of quasi-momentum $\hbar q$ of a mechanical particle, according to Eq. (237), is the contribution to particle's momentum by the external force $F$.
    ${ }^{85}$ D. Averin et al., Sov. Phys. - JETP 61, 407 (1985).
    ${ }^{86}$ Phase locking of the Bloch oscillations, with frequency (258), as well as that of very similar SET oscillations of frequency $f_{\mathrm{SET}}=I / e$, by a signal of well characterize frequency, enable fundamental standards of dc current. The experimentally achieved accuracy of such standards is close to $10^{-8}$, a few times worse than that of a less direct way - using the Josephson voltage standard and the resistance standard based on the quantum Hall effect.

[^523]:    ${ }^{87}$ It was predicted independently by L. D. Landau, Phys. Z. Sowjetunion 2, 46 (1932) and C. Zener, Proc. R. Soc. London A 137, 696 (1932).

[^524]:    ${ }^{88}$ Note that Eq. (264) is still limited to the hyperbolic dispersion relation, i.e. (in the band theory) to the weak potential limit. In the opposite, tight-binding limit, the interband tunneling may be treated as an excitation of the upper band states by sinusoidal Bloch oscillations, and is completely suppressed at $\hbar \omega_{\mathrm{B}}<\Delta_{1}$.

[^525]:    ${ }^{89}$ In Chapter 6, Eq. (266) will be derived using a different method based on the Golden Rule of quantum mechanics.
    ${ }^{90}$ See, e.g., SM Secs. 1.5 and 6.4.

[^526]:    ${ }^{91}$ See, e.g., CM Sec. 4.4.
    ${ }^{92}$ If not yet, I am inviting him or her to check this fact now by the direct substitution of solution (269) into the differential equation (268), simultaneously proving Eq. (270).
    ${ }^{93}$ Quantitatively, as was already mentioned in Sec. 2.1, $x_{0}=\sqrt{ } 2 \delta x=\left\langle 2 x^{2}\right\rangle^{1 / 2}$.

[^527]:    ${ }^{94}$ See, e.g., http://www.ligo.caltech.edu/, and a recent update by T. Feder, Phys. Today 68, No. 9, 20 (2015).
    ${ }^{95}$ According to the recent announcement by B. Abbott et al., Phys. Rev. Lett. 116, 061102 (2016), this sensitivity was sufficient for the first direct detection of gravitational waves emitted at a merger of two black holes.

[^528]:    ${ }^{96}$ These stationary states of the harmonic oscillator are sometimes called its Fock states, to distinguish them from other fundamental solutions (such as Glauber states) which will be discussed in Sec. 5.5 and beyond..
    ${ }^{97}$ In mathematics, a slightly more general statement, valid for a broader class of ordinary linear differential equations, is frequently called the Sturm oscillation theorem, and is a part of the Sturm-Liouville theory of such equations - see, e.g., Chapter 10 in the handbook by G. Arfken et al. recommended in MA Sec. 16.

[^529]:    ${ }^{98}$ The constant $P$ is called the force's impulse. (In higher dimensionalities, it is a vector - just as the force is.)
    ${ }^{99}$ Solving this problem is a good preparation to the use of the full variational method in the next two problems (and beyond).

[^530]:    100 With $F=m g$, this is just the well-known bouncing ball problem.
    ${ }^{101}$ See, e.g., Sec. 8.2 below.

[^531]:    ${ }^{102}$ In applications to electrons in solid-state crystals, the delta-functional quantum wells model the attractive potential of atomic nuclei, while $U_{0}$ represents the workfunction, i.e. the energy necessary for the extraction of an electron from the crystal to the free space - see, e.g., EM Sec. 2.6 and SM Sec. 6.4.

[^532]:    ${ }^{103}$ This system was used as the analytical mechanics "testbed problem" in the CM part of this series, and the reader is welcome to use any relations derived there - but remember that they pertain to the classical mechanics domain!

[^533]:    ${ }^{1}$ See, e.g., MA Eq. (10.9).

[^534]:    ${ }^{2}$ For a proof of Eq. (8), see, e.g., EM Sec. 8.5.
    ${ }^{3}$ A possible (and reasonable) concern about the application of Eq. (7) to the field in the slits is that it ignores the effect of opaque parts of the partition. However, as we know from Chapter 2, the main role of the classically forbidden region is providing the reflection of the incident wave towards its source (i.e. to the left in Fig. 1). As a result, the contribution of this reflection to the field inside the slits is insignificant is $A_{1,2} \gg \lambda^{2}$, and even in the opposite case provides just some rescaling of the amplitudes $a_{1,2}$, which is unimportant for our conceptual discussion.

[^535]:    ${ }^{4}$ See, e.g., a detailed discussion in EM Sec. 8.4.
    ${ }^{5}$ See, e.g., Sec. 5.1. Note that Eq. (14), as well as all other formulas of this course, are in the SI units; in Gaussian units, all terms which include either $\boldsymbol{B}$ or $\mathbf{A}$ should be divided by $c$, the speed of light in free space.

[^536]:    ${ }^{6}$ See, e.g., EM Sec. 9.7.
    ${ }^{7}$ See, e.g., EM Sec. 6.7, in particular Eqs. (6.106).
    ${ }^{8}$ Just for reader's reference, the classical Lagrangian corresponding to Hamiltonian (19) is

[^537]:    ${ }^{10}$ See, e.g., EM Sec. 5.3.
    ${ }^{11}$ I personally prefer the latter, less personable name, because the effect had been actually predicted by W. Ehrenberg and R. Siday in 1949, before it was rediscovered by Y Aharonov and D. Bohm in 1959. To be fair to Aharonov and Bohm, it was their work that triggered a wave of interest to the phenomenon, resulting in its first

[^538]:    ${ }^{13}$ One more bad, though common, term - a wire can (super)conduct, but a quantum hardly can!

[^539]:    ${ }^{14}$ For more detail, see EM Sec. 6.3.
    ${ }^{15}$ It was predicted in 1949 by F. London and experimentally discovered (independently and virtually simultaneously) in 1961 by two experimental groups: B. Deaver and W. Fairbank, and R. Doll and M. Näbauer.
    ${ }^{16}$ A brief review of these effects, and recommendations for further reading may be found in EM Sec. 6.4.

[^540]:    ${ }^{17}$ It was first observed in 1980 by K. von Klitzing and coworkers.
    18 Discovered in 1879 by E. Hall.

[^541]:    ${ }^{19}$ Recently, the quantum Hall effect was observed at room temperature in the graphene (a virtually perfect 2D sheet of carbon atoms, see Sec. 4 below) - see K. Novoselov et al., Science 315, 1379 (2007).

[^542]:    ${ }^{20}$ The explanation of this paradox may be obtained in terms of the so-called quantum edge channels - the quasi1D regions of width (51), along the lines were the Landau levels cross the Fermi surface. Particle motion along these channels, which is responsible for electron transfer, is effectively one-dimensional and thus cannot be affected by modest uniformities of the potential distribution $U(x, y)$.
    ${ }^{21}$ This fractional quantum Hall effect was discovered in 1982 by D. Tsui, H. Stormer, and A. Gossard. In contrast, the effect described by Eq. (55) with integer $i$ (Fig. 7) is now called the integer quantum Hall effect.
    ${ }^{22}$ For a comprehensive discussion of these effects I can recommend, e.g., either the monograph by D. Yoshioka, The Quantum Hall Effect, Springer, 1998, or the review by D. Yennie, Rev. Mod. Phys. 59, 781 (1987).

[^543]:    ${ }^{23}$ See, e.g., CM Sec. 3.7.
    ${ }^{24}$ In optics, this limit is called the Fraunhofer diffraction - see, e.g., EM Secs. (8.6) and (8.8).
    ${ }^{25}$ For example, in the simplest task of derivation of the so-called Rutherford formula for scattering of a charged non-relativistic particle by a point fixed charge, due to their Coulomb interaction - see, e.g., CM Sec. 3.7.

[^544]:    Born approximation

[^545]:    ${ }^{26}$ Named after M. Born, who was the first one to apply this approximation in quantum mechanics. However, the basic idea of this approach had been developed much earlier (in 1881) by Lord Rayleigh in the context of electromagnetic wave scattering - see, e.g., EM Sec. 8.3. Note that the contents of that section repeats much of our current discussion - regrettably but unavoidably so, because the Born approximation is a centerpiece of scattering theory for both electromagnetic and de Broglie waves.

[^546]:    ${ }^{27}$ Please notice both the similarity and difference between this Green's function and the propagator discussed in Sec. 2.1. In both cases, we use the linear superposition principle to solve wave equations, but while Eq. (68) gives the solution of the inhomogeneous equation (67), Eq. (2.44) does that for a homogeneous Schrödinger equation in which the wave sources are presented by initial conditions rather than by equation's right-hand part.
    ${ }^{28}$ See, e.g., EM Sec. 1.2.

[^547]:    ${ }^{29}$ See, e.g., EM Sec. 8.2.

[^548]:    ${ }^{30}$ It is easy to prove that this form is an asymptotic form of any solution $\psi_{s}$ of the scattering problem (even that beyond the Born approximation) at sufficiently large distances $r \gg a, k^{-1}$.
    ${ }^{31}$ Note that function $f$ has the dimension of length, and does not account for the incident wave. This is why sometimes a dimensionless function, $S=1+2 i k f$, is used instead. This function $S$ is called the scattering matrix, because it may be considered as a natural generalization of the 1D matrix S, defined by Eq. (2.133), to higher dimensionality.
    ${ }^{32}$ See, e.g., MA Eq. (10.8).

[^549]:    ${ }^{33}$ Note that according to Eq. (88), in the Born approximation the scattering intensity does not depend on the sign of potential $U$, and also that scattering in a certain direction is completely determined by a specific Fourier harmonic of function $U(\mathbf{r})$, namely by the harmonic with the wave vector equal to the scattering vector $\mathbf{q}$.

[^550]:    ${ }^{34}$ The construction of such series may be facilitated by the following observation. If we retain $\psi_{s}$ in the righthand part of Eq. (66), we may write a relation formally similar to Eq. (68) for the full wavefunction $\psi=\psi_{0}+\psi_{s}$ :

    $$
    \psi(\mathbf{r})=\psi_{0}(\mathbf{r})+\frac{2 m}{\hbar^{2}} \int U\left(\mathbf{r}^{\prime}\right) \psi\left(\mathbf{r}^{\prime}\right) G\left(\mathbf{r}, \mathbf{r}^{\prime}\right) d^{3} r^{\prime}
    $$

    This is one of forms of the Lipmann-Schwinger equation that is exactly equivalent to the differential Schrödinger equation (66) but is more convenient for some applications, in particular for the calculation of higher approximations $\psi_{n}$. Unfortunately, I will have not time to discuss this approach in detail and have to refer the reader, for example, to either Chapter 9 of the textbook by L. Schiff, Quantum Mechanics, $3^{\text {rd }}$ ed., McGraw-Hill, 1968, or (for even more details) to monograph by J. Taylor, Scattering Theory, Dover, 2006.

[^551]:    ${ }^{35}$ Named after A. Bravais, the crystallographer who introduced this notion in 1850.
    ${ }^{36}$ The strongest motivation for the band theory is provided by properties of solid crystals. Thus it is not surprising that perhaps the most clear, well illustrated introduction to the Bravais lattices may be found in Chapters 4 and 7 of the famous textbook by N. Ashcroft and N. Mermin, Solid State Physics, Saunders College, 1976.

[^552]:    ${ }^{37}$ It may be best understood as the sum of two fcc lattices of side $a$, mutually shifted by vector $\{1,1,1\} a / 4$, so that the distances between each point of the combined lattice and its 4 nearest neighbors (see the thick gray lines in Fig. 11c) are all equal.
    ${ }^{38}$ This structure is presently very popular due to the recent discovery of graphene - isolated monolayer sheets of carbon atoms arranged in a honeycomb lattice with the interatomic distance of 0.142 nm .
    ${ }^{39}$ A harder case is presented by quasicrystals (whose idea may be traced down to medieval Islamic tilings, but was discovered in natural crystals, by D. Shechtman et al., only in 1984), which obey high (say, 5 -fold) rotational symmetry, but cannot be described by a Bravais lattice with any finite primitive unit cell. For a popular review of quasicrystals see, for example, P. Stephens and A. Goldman, Sci. Amer. 264, \#4, 24 (1991).

[^553]:    ${ }^{40}$ For the 2D case ( $j=1,2$ ), one may use, for example, the first two formulas of Eq. (111) with $\mathbf{a}_{3}=\mathbf{a}_{1} \times \mathbf{a}_{2}$.
    ${ }^{41}$ See, e.g., MA Eq. (7.6).
    ${ }^{42}$ This notion is also the main starting point of X-ray diffraction studies of crystals, because it allows rewriting the well-known Bragg condition for diffraction peaks in an extremely simple form of the momentum conservation law: $\mathbf{k}=\mathbf{k}_{0}+\mathbf{Q}$, where $\mathbf{k}_{0}$ and $\mathbf{k}$ are the wave vectors of the, respectively, incident and diffracted photon.

[^554]:    ${ }^{43}$ See, e.g., MA Sec. 16 (iv).

[^555]:    ${ }^{44}$ Actually, using the same values of $\delta_{n}$ in both directions implies some sort of symmetry of the quasi-localized states. For example, $s$-states of axially-symmetric potentials (see the next section) always have such a symmetry.

[^556]:    ${ }^{45}$ This term is based on a (pretty loose) analogy with the Dirac theory of relativistic quantum mechanics, to be discussed in Chapter 9 below. Namely, in the vicinity of a Dirac point (122), Schrödinger equations (119), and hence the dispersion relation (122), may be obtained from the effective Hamiltonian $\hat{H}_{n}=\hbar v_{n} \hat{\boldsymbol{\sigma}} \cdot \hat{\widetilde{\mathbf{q}}}$. (Since vector $\widetilde{\mathbf{q}}$ is two-dimensional, this Hamiltonian employs only two of three Pauli matrices.) This expression reminds the first term of Dirac's Hamiltonian (9.97), which is defined, however, in a different Hilbert space.
    ${ }^{46}$ See, e.g., a recent review by A. Castro Neto et al., Rev. Mod. Phys. 81, 109 (2009). Note that transport properties of graphene are determined by coupling of $2 p_{z}$ electron states of carbon atoms, whose wavefunctions are proportional to $\exp \{ \pm i \varphi\}$ rather than are axially-symmetric as implied by Eqs. (120). However, due to the lattice symmetry this fact does not affect the dispersion relation $E(\mathbf{q})$.

[^557]:    ${ }^{47}$ This is a reasonable model for the confinement of light atoms, notably hydrogen, in some organic compounds.

[^558]:    ${ }^{48}$ See, e.g., MA Eq. (10.5).

[^559]:    ${ }^{49}$ This effect, whose qualitative features remain the same for all 2D or 3D localized states (see Chapter 6 below), is frequently referred to as the orbital diamagnetism. In magnetic materials consisting of particles with uncompensated spins, this effect competes with another effect, spin paramagnetism - see, e.g., EM Sec. 5.5.
    ${ }^{50}$ It is straightforward to check that Eqs. (133) and hence (135) remain valid even if the magnetic field lines do not touch the particle's trajectory, and the field is localized well inside rotator's ring.
    ${ }^{51}$ Such persistent, macroscopic diamagnetic currents in non-superconducting systems may be experimentally observed, for example, by measuring the weak magnetic field generated by electrons in a system of a large number $\left(\sim 10^{7}\right)$ of similar conducting rings - see, e.g., L. Lévy et al., Phys. Rev. Lett. 64, 2074 (1990). Due to the

[^560]:    ${ }^{55}$ Noting that for the planar rotator（Fig．16）$l / R=\varphi$ ，we can present Eq．（129）in a similar form．This is natural， because the rotator is just a particular case of our current problem－with a rigid confinement along axis $\rho$ ． ${ }^{56}$ See，e．g．，CM Sec．3．5．

[^561]:    ${ }^{57}$ A short summary of properties of these function, plus a few plots and a useful table of values, may be found in EM Sec. 2.4. For more on of Bessel functions, see the literature recommended in MA Sec. 16(ii).
    ${ }^{58}$ See, e.g., MA Eq. (10.9).

[^562]:    ${ }^{59}$ Here, rather regrettably, I had to replace the notation of the integer from $n$ to $m$, in order to comply with the generally accepted convention for this so-called magnetic quantum number. Let me hope that the difference between this integer and particle's mass is absolutely clear from the context.
    ${ }^{60}$ It was carried out by A.-M. Legendre (1752-1833). Just as a historic note: besides many original mathematical results, Dr. Legendre has authored the famous textbook Éléments de Géométrie, which dominated teaching geometry through the 19th century.

[^563]:    ${ }^{61}$ Derived independently by B. O. Rodrigues in 1816, J. Ivory in 1824, and C. Jacobi in 1827.
    ${ }^{62}$ In this behavior, we readily recognize the standing wave pattern typical for all 1D eigenproblems - cf. Fig. 1.7. The quantitative deviation from the sinusoidal waveform is due to the different metric of the sphere.

[^564]:    ${ }^{63}$ Such real functions $Y_{l m}$, which also form the full set of orthonormal eigenfunctions and are frequently called the real spherical harmonics, are more convenient than the complex functions $Y_{l}^{m}$ for several applications, especially when the variables of interest are real by definition.

[^565]:    ${ }^{64}$ The letter names for states with different values of $l$ stem from the history of optical spectroscopy - for example, letter " s ", used for $l=0$, originally denoted the "sharp" optical line series, etc. The sequence of the letters is as follows: $s, p, d, f, g, h$, and further in the alphabetical order.

[^566]:    ${ }^{65}$ Historically，the solution of this problem in 1928，that reproduced the main result（1．8）－（1．9）of the＂old＂ quantum theory developed by N．Bohr in 1912，without its restrictive assumptions，was the decisive step for the general acceptance of Schrödinger＇s wave mechanics．
    ${ }^{66}$ These two scales are obtained from relations $E_{0} \equiv \hbar^{2} / m r_{0}{ }^{2} \equiv C / r_{0}$ ，i．e．from the equality of the natural scales of the potential and kinetic energies，dropping all numerical coefficients．For the most important case of the hydrogen atom，$C=e^{2} / 4 \pi \varepsilon_{0}$ ，these scales are reduced，respectively，to the Bohr radius $r_{\mathrm{B}}(1.13)$ and the Hartree energy $E_{\mathrm{H}}$（1．9）．Note also that for a hydrogen－like atom（or rather ion），with $C=Z\left(e^{2} / 4 \pi \varepsilon_{0}\right)$ ，these two key parameters are rescaled as $r_{0}=r_{\mathrm{B}} / Z, E_{0}=\mathrm{Z}^{2} E_{\mathrm{H}}$ ．

[^567]:    ${ }^{67}$ In Eqs. (187)-(188), $p$ and $q$ are non-negative integers, with no relation whatsoever to particle's momentum or electric charge. Sorry for this notation, but it is absolutely common, and can hardly result in any confusion. ${ }^{68}$ Named after the same B. O. Rodrigues, and belonging to the same class as his another key result, Eq. (165).

[^568]:    ${ }^{69}$ See, e.g., MA Eq. (2.5a).
    ${ }^{70}$ Forgetting for a minute about such new "dark clouds" on the horizon of the modern physics as the hypothetical dark matter and dark energy.
    ${ }^{71}$ Note that even at the largest value of $l$, equal to $(n-1)$, term $l(l+1)$ in Eq. (200) cannot compensate term $3 n^{2}$.

[^569]:    ${ }^{72}$ The first of these relations may be also readily proved using the Heller-Feynman theorem (see Chapter 1); this proof is left for reader's exercise. Note also that the last of the expressions diverges at $l=0$, in particular in the ground state of the system (with $n=1, l=0$ ).
    ${ }^{73}$ Also called the Mendeleev table, after D. Mendeleev who put forward the concept of the periodicity of chemical element properties as functions of $Z$ phenomenologically in 1869. (The explanation of the periodicity had to wait for 60 more years until the quantum mechanics formulation in the late 1920s.)

[^570]:    ${ }^{74}$ Besides very small "fine-structure" corrections - to be discussed in Chapters 6 and 9.
    ${ }^{75}$ As will be discussed in detail in Chapter 8, electrons of the same atom are actually indistinguishable, and their quantum states are not independent, and frequently entangled. These factors are important for several properties of helium atoms (and heavier elements as well), especially for their response to external fields. However, for the atom classification purposes, they are not crucial.

[^571]:    ${ }^{76}$ Chemical valence is a relatively vague term describing the number of atom's electrons involved in chemical reactions. For the same atom, the number may depend on the chemical compound formed.

[^572]:    ${ }^{77}$ Another option is to return to the first column as soon an atom has one electron in $s$ state (like it is in $\mathrm{Cu}, \mathrm{Ag}$, and Au , in addition to the alkali metals).
    ${ }^{78}$ For a bit more detailed (but still very succinct) discussion of valence and other chemical aspects of atomic structure, I can recommend Chapter 5 of the classical text by L. Pauling, General Chemistry, Dover, 1988.

[^573]:    ${ }^{79}$ See, e.g., CM Sec. 8.5 or EM Sec. 2.8.

[^574]:    ${ }^{80}$ See, e.g., CM Sec. 3.7, in particular Eq. (3.72).

[^575]:    ${ }^{81}$ See, e.g., EM Sec. 3.1.

[^576]:    ${ }^{82}$ See, e.g., any of the handbooks recommended in MA Sec. 16(ii).

[^577]:    ${ }^{83}$ Such a fast change happens, for example, at the beta-decay, when one of nucleus' neurons suddenly becomes a proton, emitting a high-energy electron and a neutrino which leave the system very fast (instantly on the atomic time scale), and do not participate in the atom transition's dynamics.

[^578]:    ${ }^{1}$ To my knowledge, the concept of spin as an internal rotation of a particle was first suggested by R. Kronig, then a 20 -year-old student, in January 1925, a few months before two other students, G. Uhlenbeck and S. Goudsmit to whom the idea is usually attributed. The concept was then accepted and developed quantitatively by W. Pauli.
    ${ }^{2}$ See, e.g., EM Sec. 5.4, in particular Eq. (5.100).
    ${ }^{3} \mathrm{~A}$ convenient mnemonic rule is that it is close to $1 \mathrm{~K} / \mathrm{T}$. In the Gaussian units, $\mu_{\mathrm{B}} \equiv \hbar e / 2 m_{e} c \approx 0.9274 \times 10^{-20}$.

[^579]:    ${ }^{4}$ An attentive reader could notice my smuggling term "system" instead of "particle" which was used in the previous chapters. Indeed, the bra-ket formalism allows the description of quantum systems much more complex than a single spinless particle that is a typical (though not the only possible) subject of wave mechanics.
    ${ }^{5}$ As was expressed nicely by A. Peres, one of pioneers of the quantum information theory, "quantum phenomena do not occur in the Hilbert space, they occur in a laboratory".
    ${ }^{6}$ Terms bra and ket were suggested to reflect the fact that pair $\langle\beta|$ and $|\alpha\rangle$ may be considered as the set of parts of combination $\langle\beta \mid \alpha\rangle$ (see Eq. (11) below), which reminds an expression in the usual angle brackets.
    ${ }^{7}$ The Hilbert space of a given system is defined as the set of all its possible state vectors. As should be clear from this definition, it is not advisable to speak about a "Hilbert space of quantum states".

[^580]:    ${ }^{8}$ Mathematicians like to say that the ket- and bra-vectors of the same quantum system are defined in two isomorphic Hilbert spaces.
    ${ }^{9}$ This is one of the differences of bra- and ket-vectors from the usual (geometrical) vectors whose scalar product is always a real scalar.

[^581]:    ${ }^{10}$ If we consider $c$-numbers as a particular type of operators, then according to Eqs. (11) and (21), for them the Hermitian conjugation is equivalent to the simple complex conjugation, so that only a real $c$-number may be considered as a particular case of the Hermitian operator (22).
    ${ }^{11}$ Here "legitimate" means "having a clear sense in the bra-ket formalism". Some examples of "illegitimate" expressions: $|\alpha\rangle \hat{A}, \hat{A}\langle\alpha|,|\alpha\rangle|\beta\rangle,\langle\alpha|\langle\beta|$. Note, however, that the last two expressions may be legitimate if $\alpha$ and $\beta$ are states of different systems, i.e. if their state vectors belong to different Hilbert spaces. We will run into such tensor products of bra- and ket vectors (sometimes denoted, respectively, as $|\alpha\rangle \otimes|\beta\rangle$ and $\langle\alpha| \otimes\langle\beta|$ ) in Chapters 6-8.

[^582]:    ${ }^{12}$ Another popular notation for the anticommutator is $[\hat{A}, \hat{B}]_{+}$; it will not be used in these notes.

[^583]:    ${ }^{13}$ For the sake of formula compactness, below I will use the shorthand notation in which the operands of this equality are just $A_{j j}^{\dagger}$, and $A^{*}{ }_{j j}$. I believe that it leaves little chance for confusion, because the Hermitian conjugation sign $\dagger$ may pertain only to an operator (or its matrix), while the complex conjugation sign * to a scalar - say a matrix element.
    ${ }^{14}$ This equation should look familiar to the reader - see the stationary Schrödinger equation (1.60), which was the focus of our studies in the first three chapters. We will see soon that that equation is just a particular (coordinate) representation of Eq. (66) for the Hamiltonian as the operator of energy.
    ${ }^{15}$ The reciprocal statement is also true: if all eigenvalues of an operator are real, it is Hermitian (in any basis). This statement may be readily proved by applying Eq. (93) below to the case when $A_{k k^{\prime}}=A_{k} \delta_{\mathrm{kk}}$, with $A_{k}{ }^{*}=A_{k}$.

[^584]:    ${ }^{16}$ An alternative way to express Eq. (76) is to write $\hat{U}^{\dagger}=\hat{U}^{-1}$, but I will try to avoid this language.
    ${ }^{17}$ Quod erat demonstrandum (Lat.) - what needed to be proved.

[^585]:    19 A possible slight complication here are degenerate cases when characteristic equation gives certain equal eigenvalues corresponding to different eigenvectors. In this case the requirement of the mutual orthogonality of these states should be additionally enforced.

[^586]:    ${ }^{20}$ Note that though this particular unitary matrix is Hermitian, this is not true for an arbitrary choice of phases $\varphi$. ${ }^{21}$ This is the key point in the electron's spin description, developed by W. Pauli in 1925-1927.
    ${ }^{22}$ For an electron, with its negative charge $q=-e$, the gyromagnetic ratio is negative: $\gamma_{e}=-g_{e} e / 2 m_{\mathrm{e}}$, where $g_{e} \approx 2$ is the dimensionless $g$-factor. Due to quantum electrodynamics effects, the factor is slightly higher than $2: g_{e}=$ $2(1+\alpha / 2 \pi+\ldots) \approx 2.002319304 \ldots$, where $\alpha \equiv e^{2} / 4 \pi \varepsilon_{0} \hbar c \equiv\left(E_{\mathrm{H}} / m_{e} c^{2}\right)^{1 / 2} \approx 1 / 137$ is the fine structure constant. (The origin of its name will be clear from the discussion in Sec. 6.3.)

[^587]:    ${ }^{23}$ If you think about it, word "understand" typically means that we can explain a new, more complex notion in terms of those discussed earlier and considered "known". In our example, we cannot express the spin states by some wavefunction $\psi(\mathbf{r})$, or any other mathematical notion discussed earlier. The bra-ket formalism has been invented exactly to enable mathematical analysis of such "new" quantum states.
    ${ }^{24}$ Here again, just like in Sec. 1.2, the statement implies the abstract (mathematical) notion of "ideal experiments", postponing the discussion of real (physical) measurements until Sec. 7.7.
    ${ }^{25}$ As a reminder, in the end of Sec. 3 we have already proved that such eigenstates corresponding to different $A_{j}$ are orthogonal. If any of these values is degenerate, i.e. corresponds to several different eigenstates, they should be also selected orthogonal, in order for Eq. (118) to be valid.
    ${ }^{26}$ This key relation, in particular, explains the most common term for the (generally, complex) coefficients $\alpha_{j}$, the probability amplitudes.

[^588]:    ${ }^{27}$ This equality reveals the full beauty of Dirac's notation. Indeed, initially the quantum-mechanical brackets just reminded the angular brackets used for statistical averaging. Now we see that in this particular (but most important) case, the angular brackets of these two types may be indeed equal to each other!
    ${ }^{28}$ Note that Eq. (120) may be rewritten in the form similar to Eq. (125): $W_{j}=\langle\alpha| \hat{\Lambda}_{j}|\alpha\rangle$, where $\hat{\Lambda}_{j} \equiv\left|a_{j}\right\rangle\left\langle a_{j}\right|$ is the operator (42) of projection upon the $j^{\text {th }}$ eigenstate $a_{j}$.

[^589]:    ${ }^{29}$ Note that both sides of Eq. (140) are state-specific; the uncertainty relation statement is that this inequality should be valid for any possible quantum state of the system.
    ${ }^{30}$ This inequality is the quantum-mechanical analog of the usual vector algebra result $\alpha^{2} \beta^{2} \geq|\alpha \cdot \beta|^{2}$.

[^590]:    ${ }^{31}$ Moreover, we will be able to derive Eq. (1.25) from Eq. (154) - see Sec. 5.2.
    ${ }^{32}$ Here I intentionally use index $n$ rather than $j$, to emphasize the special role played by the stationary eigenstates $a_{n}$ in quantum dynamics.

[^591]:    ${ }^{33}$ See, e.g., EM Eq. (5.100). As a reminder, we have already used this expression for the derivation of Eq. (3). ${ }^{34}$ See, e.g., CM Sec. 6.5, in particular Eq. (6.72), and EM Sec. 5.5, in particular Eq. (5.114) and its discussion.

[^592]:    ${ }^{35}$ Note also that if the product $\gamma \mathcal{B}$ is positive, so is $\Omega$, so that $E_{\uparrow}$ is negative, while $E_{\downarrow}$ is positive. This is in the correspondence with the classical picture of a magnetic dipole $\mathbf{m}$ having negative potential energy when it is aligned with the external magnetic field $\mathcal{B}$ - see Eq. (162).

[^593]:    ${ }^{36}$ This is one more (hopefully, redundant :-) illustration of the difference between averaging over the statistical ensemble and over time: in Eqs. (170), (173)-(174), and quite a few relations below, only the former averaging has been performed, so the results are still functions of time.
    ${ }^{37}$ Such composite particles as nuclei (and, from the point of view of high-energy physics, even such hadrons as protons) may be characterized by a certain net spin (and hence by certain $\gamma$ ) only if during the considered process their internal degrees of freedom remain in a certain (usually, ground) quantum state.

[^594]:    ${ }^{38}$ We will run into such situations in Chapter 7, but will not need to apply Eq. (186).
    ${ }^{39}$ It may be found, for example, in Chapter 5 of J. Sakurai's textbook - see References.
    ${ }^{40}$ Note this relation is similar in structure to the symbolic Eqs. (94).

[^595]:    ${ }^{41}$ We could of course use this equation result, together with Eq. (157), to obtain all the above results for this system within the Schrödinger picture. In our simple case, the use of Eqs. (161) for this purpose was more straightforward, but in some cases (e.g., for time-dependent Hamiltonians) an explicit calculation of the timeevolution matrix may be the only practicable way to proceed.

[^596]:    ${ }^{42}$ Due to the same reason, $\hat{H}_{\mathrm{H}} \equiv \hat{u}^{\dagger} \hat{H}_{\mathrm{S}} \hat{u}=\hat{u}^{\dagger} \hat{u} \hat{H}_{\mathrm{S}}=\hat{H}_{\mathrm{S}}$; this is why the index of the Hamiltonian operator may be dropped in Eqs. (198)-(199).
    ${ }^{43}$ Reportedly, this equation was derived by P. A. M. Dirac, who was so generous that he himself gave the name of his colleague to this key result, because "Heisenberg was saying something like this".
    ${ }^{44}$ Using commutation relations (155), this equation may be readily generalized to the case of arbitrary magnetic field $\mathcal{B}(t)$ and arbitrary state basis - the exercise highly recommended to the reader.

[^597]:    ${ }^{45}$ See, e.g., CM Eq. (10.17). Also, please excuse my use, for the Poisson bracket, the same (traditional) symbol $\{\ldots, \ldots\}$ as for the anticommutator. We will not run into the Poisson brackets again in the course, leaving very little chance for confusion.
    ${ }^{46}$ Since we have run into the commutator of Heisenberg-picture operators, let me note emphasize again that the "values" of such an operator at different moments of time often do not commute. Perhaps the simplest example is the operator $\hat{x}$ of coordinate of a free 1D particle, with Hamiltonian $\hat{H}=\hat{p}^{2} / 2 m$. Indeed, in this case Eq. (199) yields equations $i \hbar \dot{\hat{x}}=[\hat{x}, \hat{H}]=i \hbar \hat{p} / m$ and $i \hbar \dot{\hat{p}}=[\hat{p}, \hat{H}]=0$, with simple solutions (similar to those for classical motion of the corresponding observables): $\hat{p}(t)=$ const $=\hat{p}(0), \quad \hat{x}(t)=\hat{x}(0)+\hat{p}(0) t / m$, so that $[\hat{x}(0), \hat{x}(t)]=[\hat{x}(0), \hat{p}(0)] t / m=\left[\hat{x}_{\mathrm{S}}, \hat{p}_{\mathrm{S}}\right] t / m=i \hbar t / m \neq 0$, if $t \neq 0$.

[^598]:    ${ }^{47}$ See, e.g., MA Eqs. (13.1) and (13.2).
    ${ }^{48}$ See, e.g. MA Eq. (2.9).

[^599]:    ${ }^{1}$ To recall why this condition is crucial, please revisit the beginning of Sec. 2.3. Note also that, in particular, the mutual phase shifts between different qubits are very important for quantum information processing (see Chapter 7 below), so that most discussions of these applications have to start from Eq. (3) rather than Eq. (4).

[^600]:    ${ }^{2}$ Named after the same F. Bloch who has pioneered the energy band theory that was discussed in Chapters 2-3.
    ${ }^{3}$ In the quantum information literature, ket-vectors $|\uparrow\rangle$ and $|\downarrow\rangle$ of these two states of a qubit are usually denoted as $|1\rangle$ ("quantum one") and $|0\rangle$ ("quantum zero").

[^601]:    ${ }^{4}$ Still, it is crucial to appreciate the difference between the expectation values (5), i.e. c-numbers, and the actual observables $S_{x}, S_{y}$, and $S_{z}$ which are described in quantum mechanics by operators. For example, according to Eq. (4.156), for any position on the Bloch sphere, it is impossible to have exact values of Cartesian components, as it is in the classical picture.
    ${ }^{5}$ The same is true for the angular momentum $\mathbf{L}$ at the classical torque-induced precession - see, e.g., CM Sec.6.5 and in particular Eq. (6.71).
    ${ }^{6}$ In this aspect as well, the information processing systems based on qubits are closer to classical analog computers rather then classical digital ones.

[^602]:    ${ }^{7}$ Notice that in the contrast to the discrete spectrum case, the dimensionality of the bra- and ket-vectors so normalized is different from 1 .

[^603]:    ${ }^{8}$ I do not quite like expressions like $\langle x \mid \Psi\rangle$ used in some papers and even textbooks. Of course, one is free to replace $\alpha$ with any other letter ( $\Psi$ including) to denote a quantum state, but then it is better not to use the same letter to denote the wavefunction, i.e. an inner product of two state vectors, to avoid confusion.

[^604]:    Space-
    local operators

[^605]:    ${ }^{9}$ Of all the operators we will encounter in this course, only the statistical operator $\hat{w}$ is substantially non-local see Sec. 7.2.
    ${ }^{10}$ In the second equality, I have use Eq. (9) for variable $x$.

[^606]:    ${ }^{11}$ The equivalence of the two forms of Eq. (28) may be readily proven, for example, by comparison of their effect on any differentiable function $f\left(x, x^{\prime}\right)$, using its Taylor expansion over argument $x$ at point $x^{\prime}=x$ - a simple but good exercise for the reader.

[^607]:    ${ }^{12}$ In some systems of quantum mechanics postulates, the Schrödinger equation (1.28) itself is considered as a sort of eigenstate/eigenvalue problem (34) for operator $i \hbar \partial / \partial t$. Notice that such construct is very close to that of the momentum operator $-i \hbar \partial / \partial x$, and similar arguments may be given for both expressions, starting from the invariance of the quantum state of a free particle with respect to translations in time and space, respectively.
    ${ }^{13}$ It is not important whether we speak about the Schrödinger or Heisenberg picture here. Indeed, if three operators in the former picture are related as $\left[\hat{A}_{\mathrm{S}}, \hat{B}_{\mathrm{S}}\right]=\hat{C}_{\mathrm{s}}$, then according to Eq. (4.190), in the latter picture

    $$
    \left.\left[\hat{A}_{\mathrm{H}}, \hat{B}_{\mathrm{H}}\right]=\mid \hat{U}^{\dagger} \hat{A}_{\mathrm{H}} \hat{U}, \hat{U}^{\dagger} \hat{B}_{\mathrm{H}} \hat{U}\right]=\hat{U}^{\dagger} \hat{A}_{\mathrm{H}} \hat{U} \hat{U}^{\dagger} \hat{B}_{\mathrm{H}} \hat{U}-\hat{U}^{\dagger} \hat{B}_{\mathrm{H}} \hat{U} \hat{U}^{\dagger} \hat{A}_{\mathrm{H}} \hat{U}=\hat{U}^{\dagger}\left[\hat{A}_{\mathrm{S}}, \hat{B}_{\mathrm{S}}\right] \hat{U}=\hat{U}^{\dagger} \hat{C}_{\mathrm{S}} \hat{U}=\hat{C}_{\mathrm{H}}
    $$

[^608]:    ${ }^{14}$ Since this Hamiltonian is time-independent, we may replace the partial derivative over time $t$ with the full one.

[^609]:    ${ }^{15}$ Indeed, acting exactly as at derivation of Eq. (36), for a space-local Heisenberg operator we get

    $$
    \langle A\rangle(t)=\int \Psi^{*}\left(x, t_{0}\right) \hat{A}_{\mathrm{H}}\left(t, t_{0}\right) \Psi\left(x, t_{0}\right) d x .
    $$

    ${ }^{16}$ The set of equations (49) constitute the Ehrenfest theorem.
    ${ }^{17}$ From this point on, for the sake of brevity I will drop index $x$ in the notation of the momentum - just as it was done in Chapter 2.

[^610]:    18 Repeating the calculation for each Cartesian component of a plane monochromatic wave of arbitrary dimensionality $d$, we get $\psi_{\mathbf{p}}=(2 \pi \hbar)^{-d / 2} \exp \{i(\mathbf{p} \cdot \mathbf{r} / \hbar+\varphi)\}$.

[^611]:    ${ }^{19}$ According to Feynman's memories, his work was motivated by a "mysterious" remark by P. A. M. Dirac in his pioneering 1930 textbook on quantum mechanics.
    ${ }^{20}$ For a more thorough discussion of the path-integral approach, see the famous text R. Feynman and A. Hibbs, Quantum Mechanics and Path Integrals first published in 1965. (For its latest edition by Dover in 2010, the book was emended by D. Styler.) For a more recent monograph that reviews more applications, see L. Schulman, Techniques and Applications of Path Integration, Wiley, 1981.

[^612]:    ${ }^{21}$ A strict proof of this intuitively evident statement would take more space and time than I can afford.

[^613]:    ${ }^{22}$ See, e.g., CM Sec. 2.1.
    ${ }^{23}$ See, e.g., CM Sec. 10.3.

[^614]:    ${ }^{24}$ This fact may be proved by expanding the difference ( $S-S_{\mathrm{cl}}$ ) in the Taylor series in path variations (leaving only the leading quadratic terms) and working out the resulting Gaussian integrals. It is interesting that the integration, together with the pre-exponential coefficient in Eq. (83a), gives exactly the pre-exponential factor that we have already found in Sec. 2.4 when refining the WKB approximation.
    ${ }^{25}$ The same trick is often used in analytical classical mechanics - say, for proving the Hamilton principle, and for the derivation of the Hamilton - Jacobi equations (see, e.g. CM Secs. 10.3-4).

[^615]:    ${ }^{26}$ One can argue that the pre-exponential coefficient in Eq. (91) should be close to 1, just like in Eq. (2.117), especially if the potential is smooth in the sense of Eq. (2.107), where $x$ is the coordinate along the trajectory.
    ${ }^{27}$ For a concise introduction to the field see, e.g., I. Gelfand and S. Fomin, Calculus of Variations, Dover, 2000, or L. Elsgolc, Calculus of Variations, Dover, 2007.
    ${ }^{28}$ In quantum field theory, the instanton concept may be formulated somewhat differently, and has more complex applications - see, e.g. R. Rajaraman, Solitons and Instantons, North Holland, 1987.

[^616]:    ${ }^{29}$ See, e.g., M. Buttiker and R. Landauer, Phys. Rev. Lett. 49, 1739 (1982), and references therein.
    ${ }^{30}$ This normalization is not really necessary, it just makes the following calculations less bulky - and thus more aesthetically appealing.

[^617]:    ${ }^{31}$ For the electromagnetic field oscillators, such excitations are called photons; for the mechanical wave field oscillators, phonons, etc.

[^618]:    ${ }^{32}$ Please note again the radical difference between the null-state in the right-hand part of Eq. (118) and the state described by ket-vector $|0\rangle$ in the left-hand side of that relation. The latter state does exist and, moreover, presents the most important, ground state of the system, with $n=0$ - see Eq. (2.269).

[^619]:    ${ }^{33}$ A useful mnemonic rule is that the $c$-number coefficient in any of these relations is equal to the square root of the largest number of the two states it relates.

[^620]:    ${ }^{34}$ The first line of Eq. (127), evidently valid for any time-independent system, is the simplest of the so-called sum rules, which will be repeatedly discussed below.
    ${ }^{35}$ Still note that operators of the partial (potential and kinetic) energies do not commute with either each other or with the full-energy (Hamiltonian) operator, so that the Fock states $n$ are not their eigenstates.

[^621]:    ${ }^{36}$ See, e.g., CM Chapter 4, especially Eqs. (4.4) and Fig. 4.9 and its discussion.

[^622]:    ${ }^{37}$ I have to confess that such geometric mapping of a quantum state on the phase plane $[x, p]$ is not exactly defined; you may think about colored areas in Fig. 6 as regions of pairs $\{x, p\}$ most probably obtained in measurements. A quantitative definition of such a mapping will be given in Sec. 7.3 using the Wigner function, though, as we will see, even such imaging definition has certain internal contradictions. Still such cartoons may have considerable cognitive/heuristic value, if their limitations are kept in mind.
    ${ }^{38}$ In the quantum theory of measurements, Eqs. (138) are frequently referred to as the standard quantum limit.
    ${ }^{39}$ Named after R. J. Glauber who studied these states in detail in 1965, though they had been discussed in brief by E. Schrödinger as early as in 1926. Another popular name, "coherent", for the Glauber states is very misleading, because all the quantum states we have studied so far (including the Fock states) may be presented as coherent (pure) superpositions of the basis states.

[^623]:    ${ }^{40}$ As will be discussed in Chapter 7, the ground state may be readily formed, for example, by providing a weak coupling of the oscillator to a low-temperature ( $k_{\mathrm{B}} T \ll \hbar \omega_{0}$ ) environment.

[^624]:    ${ }^{41}$ The proof of Eq. (148) may be readily achieved by expanding operator $\hat{f}(\lambda) \equiv \exp \{+\lambda \hat{A}\} \hat{B} \exp \{-\lambda \hat{A}\}$ in the Taylor series in the $c$-number parameter $\lambda$, and then evaluating the result at $\lambda=1$.

[^625]:    ${ }^{42}$ It is also rather counter-intuitive. Indeed, according to Eq. (122), the annihilation operator $\hat{a}$, acting on a Fock state $n$, "beats it down" to the lower-energy state ( $n-1$ ) - see Eq. (119). However, according to Eq. (155), its action on a Glauber state $\alpha$ does not lead to the state change and hence to an energy decrease! The resolution of this paradox may be achieved via representation of the Glauber state as a series of Fock states - see Eq. (165) below. Operator $\hat{a}$ indeed transfers each Fock component to a lower-energy state, but it also re-weighs each term of the expansion, so that the complete energy of the Glauber state remains constant.
    ${ }^{43}$ Note that the spectrum of eigenvalues $\alpha$ of eigenproblem (155) is continuous - it may be any complex number!

[^626]:    ${ }^{44}$ For a discussion and classical theory of this effect, see, e.g., CM Sec. 4.5.
    ${ }^{45}$ See, e.g., Chapter 7 in C. Gerry and P. Knight, Introductory Quantum Optics, Cambridge U. Press, 2005, and the spectacular measurements of the Glauber and squeezed states of electromagnetic (light) oscillators by G. Breitenbach et al., Nature 387, 471 (1997), very large (ten-fold) squeezing in such oscillators by H. Vahlbruch et al., Phys. Rev. Lett. 100, 033602 (2008); and recent first measurements of the (so far, slight) squeezing in mechanical resonators, with eigenfrequency $\omega_{0} / 2 \pi$ as low as 3.6 MHz , by E. Wollman et al., Science 349, 952 (2015).

[^627]:    ${ }^{46}$ See, e.g., MA Eq. (13.2).
    ${ }^{47}$ The importance of this issue stems from the following fact: it is easy (and is hence left to the reader :-) to use Eqs. (5.178) to prove that operators of all $L_{j}$ and of $L^{2}$ commute with the Hamiltonian of a particle in the spherically-symmetric potential $U(r)$, and hence all their eigenstates are the stationary states in such a field.
    ${ }^{48}$ This is just a particular example of Venn diagrams (introduced in the 1880 s by J. Venn) that show possible relations (such as intersections, unions, complements, etc.) between various sets of objects, and are a very useful tool in the general set theory.
    ${ }^{49}$ Note that this particular result is consistent with the classical picture of the angular momentum vector: even when is length is fixed, the vector may be oriented in various directions, corresponding to different values of its Cartesian components. However, in the classical picture, all these component may be fixed simultaneously, while in the quantum picture this is not true.

[^628]:    Spin operators: commutation relations

[^629]:    ${ }^{50}$ The reader is challenged to use the commutation relations discussed above to prove one more important property of the common eigenstates of operators $\hat{L}_{z}$ and $\hat{L}^{2}$ :

    $$
    \langle l, m| \hat{r}_{j}\left|l^{\prime}, m^{\prime}\right\rangle=0, \quad \text { if either } l^{\prime} \neq l \pm 1 \text {, or } m \neq m^{\prime} \text {, or both. }
    $$

    This property is the basis of the selection rules for dipole quantum transitions, to be discussed later in the course, especially in Sec. 9.3.

[^630]:    ${ }^{51}$ As a reminder, in the Standard Model of particle physics, such hadrons as mesons and baryons (notably including protons and neutrons) are essentially composite particles, with the spin equal to the sum of its component quark spins. However, at non-relativistic energies, protons and neutrons may be considered fundamental particles with $s=1 / 2$.

[^631]:    ${ }^{52}$ One may think that Eq. (207) is a trivial corollary of Eq. (199). However, now we should be a bit more careful, because in the Clebsch-Gordan coefficients, these quantum numbers characterize different groups of eigenstates.

[^632]:    ${ }^{53}$ For arbitrary spin $s$, the calculations and even the final expressions for the Clebsch-Gordan coefficients are rather bulky. They may be found, typically in a table form, mostly in special monographs - see, e.g., A. R. Edmonds, Angular Momentum in Quantum Mechanics, Princeton U. Press, 1957.

[^633]:    ${ }^{54}$ For the interested reader I can recommend, either Sec. 17.7 in E. Merzbacher, Quantum Mechanics, $3^{\text {rd }}$ ed., Wiley, 1998, or Sec. 3.10 in J. Sakurai, Modern Quantum Mechanics, Addison-Wesley, 1994.
    ${ }^{55}$ Cf. Problems 4.22, 4.23, 5.2.
    ${ }^{56}$ See, e.g., CM Problem 1.12.

[^634]:    ${ }^{57}$ Named after G. Gamow, who made this calculation as early as in 1928.

[^635]:    ${ }^{58}$ Note that the last task is just a particular case of Problem 4.17 (see also Problem 1).

[^636]:    ${ }^{1}$ Please note its similarity with Eq. (2.215) of the 1D band theory. Indeed, the latter equation is not much more than a particular form of Eq. (6) for 1D wave mechanics, and a specific (periodic) potential $U(x)$ considered as perturbation. Moreover, the approximate treatment of the weak potential limit in Sec. 2.7 was essentially a particular case of the more general perturbation theory we are discussing now.
    ${ }^{2}$ Note that, by definition, $\left\langle n^{,(0)} \mid n\right\rangle^{(0)}=\delta_{n^{\prime} n}$.

[^637]:    ${ }^{4}$ This is exactly the reason why such perturbation theories run into serious problems for systems with continuous spectrum, and other approximate techniques (such as the WKB approximation) are often necessary.
    ${ }^{5}$ Note that the choice of the basis is to some extent arbitrary, because due to the linearity of equations of quantum mechanics, any linear combination of states $n^{\prime(0)}$ is also an eigenstate of the unperturbed Hamiltonian. However, for using Eq. (24), these combinations have to be orthonormal, as was suggested at the derivation of Eq. (6).

[^638]:    ${ }^{6}$ For brevity, I am dropping the upper index (1) in the matrix elements.

[^639]:    ${ }^{7}$ Alternatively, if $a_{x}=0$, then $| \pm\rangle=(1 / \sqrt{ } 2)\left(\left|1^{(0)}\right\rangle \pm i\left|2^{(0)}\right\rangle\right)$. Note that besides a phase coefficient, these states are similar in that they present a coherent superposition of the unperturbed states, with a $50 / 50$ chance to find the perturbed system in any of those states. In that sense, the effects of perturbation coefficients $a_{x}$ and $a_{y}$ are similar. ${ }^{8}$ Since the hydrogen atoms are much lighter, it is more fair to speak about their correlated tunneling around the (nearly immobile) nitrogen atom.
    ${ }^{9}$ In particular, these molecules were used in the demonstration of the first maser by C. Townes' group in 1954.

[^640]:    ${ }^{10}$ If there is any doubt why, please revisit the discussion of Eq. (2.247), in which we should now take $F=q \varepsilon$.

[^641]:    ${ }^{11}$ See, e.g., MA Eq. (6.7d).

[^642]:    ${ }^{12}$ This value approximately corresponds to the threshold of electric breakdown in air, due to the impact ionization on the surface of typical metallic electrodes. (Reducing air pressure only enhances the ionization and lowers the breakdown threshold.) As a result, experiments with higher fields are rather difficult.
    ${ }^{13}$ See, e.g., EM Sec. 9.3, in particular Eq. (9.78) - or any undergraduate text on special relativity.

[^643]:    ${ }^{14}$ See, e.g., EM Sec. 5.1, in particular, Eq. (5.24).
    ${ }^{15}$ It was carried out first by L. Thomas in 1926; see, e.g., R. Harr and L. Curtis, Am. J. Phys. 55, 1044 (1987). ${ }^{16}$ See, e.g., CM Sec. 3.6.

[^644]:    ${ }^{17}$ The factor $l$ in the denominator does not give a divergence at $l=0$, because in this case $j=s=1 / 2$, and the numerator turns into 0 as well. A careful analysis of this case (which may be found, e.g., in G. K. Woolgate, Elementary Atomic Structure, $2^{\text {nd }}$ ed., Oxford, 1983), as well as the exact solution of the Bohr atom problem within the Dirac theory (Chapter 9) show that the final result (60), which is independent of $l$, is valid even in this case.
    ${ }^{18}$ This is natural, because the magnetic interaction of charged particles is an essentially relativistic effect, of the same order $\left(\sim v^{2} / c^{2}\right)$ as the kinetic correction (49a) - see, e.g., EM Sec. 5.1, in particular Eq. (5.3).

[^645]:    ${ }^{19}$ See the Selected Physical Constants appendix for the more exact value of this constant. Its expression in Gaussian units, $\alpha=e^{2} / \hbar c$, makes even more evident the fact that $\alpha$ is the just fundamental constant ratio which characterizes the strength (or rather the weakness :-) of electromagnetic effects in quantum mechanics - that in particular makes the perturbative quantum electrodynamics possible. The alternative expression $\alpha=E_{H} / m_{e} c^{2}$, where $E_{\mathrm{H}}$ is the Hartree energy (1.9), i.e. the scale of all energies $E_{n}$, is also very revealing.
    ${ }^{20}$ It was discovered experimentally in 1896 by P. Zeeman who, amazingly, was fired from the University of Leiden for an unauthorized use of lab equipment for this work - just to receive a Nobel Prize for it in a few years.

[^646]:    ${ }^{21}$ Despite its smallness, the quadratic term is necessary for description of the negative contribution of the orbital motion to the magnetic susceptibility $\chi_{m}$ (the so-called orbital diamagnetism, see EM Sec. 5.5), whose analysis, using Eq. (63), is left for reader's exercise.
    ${ }^{22}$ See, e.g., EM Sec. 5.4, in particular Eqs. (5.95) and (5.100).

[^647]:    ${ }^{23}$ In almost-hydrogen-like, but more complex atoms (such as those of alkali metals), the degeneracy in $l$ is lifted by electron-electron interaction even in the absence of the external magnetic field.

[^648]:    ${ }^{24}$ This formula is frequently used with capital letters $J, S$, and $L$, which denote the quantum numbers of the atom as a whole.

[^649]:    ${ }^{25}$ For a more complete discussion of the Stark, Zeeman, and fine-structure effects in atoms, I can recommend, for example, either the monograph by G. Woolgate cited above, or the one by I. Sobelman, Theory of Atomic Spectra, Alpha Science, 2006.
    ${ }^{26}$ See, e.g., CM Sec. 10.2.

[^650]:    ${ }^{27}$ Even if the problem under analysis may be described by the wave-mechanics Schrödinger equation (1.25), a direct numerical integration of that partial differential equation is typically less convenient than that of the ordinary differential equations (79).
    ${ }^{28}$ This is of course just a more general form of Eq. (1.61) of wave mechanics of time-independent systems.

[^651]:    ${ }^{29}$ The notation of the amplitude operators in Eq. (86) is justified by the fact that the perturbation Hamiltonian has to be self-adjoint (Hermitian), and hence each term in the right-hand part of that relation has to be a Hermitian conjugate of its counterpart, which is evidently true only if the amplitude operators are also the Hermitian conjugates of each other. Note, however, that each of the amplitude operators is generally not Hermitian.

[^652]:    ${ }^{30}$ Strictly speaking, another condition is that the number of "resonant" levels is also not too high - see Sec. 6.
    ${ }^{31}$ The notion of detuning is also very useful in the classical theory of oscillations - see, e.g., CM Chapter 4.
    ${ }^{32}$ Such omission of non-resonant terms is usually called the Rotating Wave Approximation (RWA); it is very instrumental not only in quantum mechanics, but also in the classical theory of oscillations - see, e.g., CM Secs. 4.3-4.5.

[^653]:    ${ }^{33}$ It was derived in 1952 by I. Rabi, in the context of his group's pioneering experiments with microwave excitation of quantum states, using molecular beams in vacuum.
    ${ }^{34}$ In the quantum information science language, this is just a logic operation NOT performed on a single qubit.
    ${ }^{35} \mathrm{We}$, of course, already know what happens to the ground state of an oscillator at its external sinusoidal (or any other) excitation: it turns into the Glauber state, i.e. a superposition of all Fock states - see Sec. 5.5.

[^654]:    ${ }^{36}$ See, e.g., EM Sec. 7.3, in particular, the correspondence between Eqs. (7.55) and (7.56).
    ${ }^{37}$ For introductions see, e.g., J. Wertz and J. Bolton, Electron Spin Resonance, $2^{\text {nd }}$ ed., Wiley, 2007; J. Keeler, Understanding NMR Spectroscopy, $2^{\text {nd }}$ ed., Wiley, 2010.

[^655]:    ${ }^{41}$ Here we have run again, in a more general context, into the "energy-time uncertainty relation" which was already discussed in the end of Sec. 2.5. Let me advise the reader to revisit that important discussion.

[^656]:    ${ }^{42}$ This situation is very much similar to the entropy increase in macroscopic systems, which is postulated in thermodynamics, and justified in statistical physics, even though it is based on time-reversible laws of mechanics - see, e.g., SM Sec. 1.2 and Sec. 2.2.

[^657]:    ${ }^{43}$ The normalization to infinite volume, using Eq. (5.55), is also possible, but less convenient in such problems.

[^658]:    ${ }^{44}$ The condition of its validity is again given by Eq. (117), but with $\omega \rightarrow 0$ in the upper limit.
    ${ }^{45}$ It is straightforward to show that in this form, the estimate is valid for a similar problem of any spatial dimensionality, not just the 1D case we have analyzed.
    ${ }^{46}$ This qualitative picture may be verified, for example, using the experimentally observable effects of dispersive electromagnetic environment on electron tunneling - see P. Delsing et al., Phys. Rev. Lett. 63, 1180 (1989).

[^659]:    ${ }^{47} \operatorname{Sign} \otimes$ is used to denote the formation of a joint ket-vector from kets of independent systems ("belonging to different Hilbert spaces"). Evidently, the order of operands in such a "product" may be changed at will.
    ${ }^{48}$ See, e.g., EM Sec. 3.1, in particular Eq. (3.16), in which letter $\mathbf{p}$ is used for the electric dipole moment.

[^660]:    ${ }^{49}$ The process is evidently spontaneous, i.e. does not require any external agent, and starts as soon as either the interaction (127) has been turned on, or (if it is always on) as soon as system $a$ is placed into the excited state $n^{\prime}{ }_{a}$. ${ }^{50}$ As a reminder, its proof for the particular case of wave mechanics was the subject of Problem 1.4.

[^661]:    ${ }^{51}$ See, e.g., CM Sec. 4.2.

[^662]:    ${ }^{52}$ See, e.g., EM Sec. 5.5, in particular Eqs. (5.127) and (5.112).

[^663]:    ${ }^{1}$ For a broader discussion of statistical mechanics and physical kinetics, including those of quantum systems, the reader is referred to the SM part of this lecture note series.
    ${ }^{2}$ Most of the mixed ensemble analysis in this chapter will pertain also to the cases when the systems of interest are not in a contact with the environment currently, and our knowledge about them is incomplete by some other reason - for example, if they had been in such a contact at some time between their perfect preparation (in a certain quantum state) and the observation, or if such a perfect preparation is impossible (or impracticable, or undesirable :-).
    ${ }^{3}$ See, e.g., SM Sec. 2.1.

[^664]:    ${ }^{4}$ In the opposite case, the very partition of the Universe into the system and the environment is impossible.
    5 Whether this assumption is true is an interesting issue, still being debated (more by philosophers than by physicists), but it is widely believed that its solution is not critical for the validity of the results of this approach. In Sec. 6, I will offer a strong argument for this opinion - albeit not its strict proof.
    ${ }^{6}$ Actually, such coexistence has been implied (but well hidden :-) in the derivation of the quantum-mechanical Golden Rule, which in all fairness, also belongs to the open systems class.

[^665]:    ${ }^{7}$ First suggested in 1927 by J. von Neumann.
    ${ }^{8}$ Of course the "bra-kets" in this expression are not $c$-numbers, because state $\alpha$ is defined in a larger Hilbert space (of the environment plus the system of interest) than the basis states $e_{k}$ (of the environment only).

[^666]:    9 This is essentially an alternative formulation of the basic postulate of statistical physics, called the microcanonical distribution - see, e.g., SM Sec. 2.2.
    ${ }^{10}$ See. e.g., SM Sec. 2.4. The Boltzmann constant $k_{\mathrm{B}}$ is only needed if temperature is measured in non-energy units, say in kelvins.

[^667]:    ${ }^{11}$ See, e.g., SM Sec. 2.8.
    ${ }^{12}$ See, e.g., SM Sec. 2.5 - but mind a different energy reference level, $E_{0}=\hbar \omega$, used in Eqs. (2.68)-(2.69), affecting the expression for $Z$. Actually, the calculation is so straightforward (just the summation of a geometric progression for the enumeration of $Z$ ) that it is highly recommended to the reader as a simple exercise.
    ${ }^{13}$ See, e.g., SM Sec. 2.8.
    ${ }^{14}$ Because of the fundamental importance of Eq. (26) for many fields of physics, let me remind the reader of its main properties. At low temperatures, $k_{\mathrm{B}} T \ll \hbar \omega_{0}$, there are virtually no thermal excitations, $\langle n\rangle \rightarrow 0$, and the average energy of the oscillator is dominated by that of its ground state. In the opposite limit of high temperatures, $\langle n\rangle \rightarrow k_{\mathrm{B}} T / \hbar \omega_{0} \gg 1$, and $\langle E\rangle$ approaches the classical value $k_{\mathrm{B}} T$ (following, for example, from the equipartition theorem, which assigns energy $k_{\mathrm{B}} T / 2$ to each quadratic contribution to system's energy - in the 1 D oscillator case, to one potential and one kinetic energy term).

[^668]:    ${ }^{15}$ For now, I will focus on a fixed time instant (say, $t=0$ ), and hence write $\psi(x)$ instead of $\Psi(x, t)$.
    ${ }^{16}$ This fact is the historic origin of density matrix' name.

[^669]:    ${ }^{17}$ Due to the delta-normalization of the eigenfunction, the density matrix for the free particle (and any system with continuous eigenvalue spectrum) is normalized as

    $$
    \int_{-\infty}^{+\infty} w\left(x, x^{\prime}\right) Z d x^{\prime}=\int_{-\infty}^{+\infty} w\left(x, x^{\prime}\right) Z d x=1
    $$

[^670]:    ${ }^{18}$ I will have no time to discuss this technique, and have to refer the interested reader to special literature. Probably, the most famous text of that field is A. Abrikosov, L. Gor'kov, and I. Dzyaloshinski, Methods of Quantum Field Theory in Statistical Physics, Prentice-Hall, 1963. (Later reprintings are available from Dover.)

[^671]:    ${ }^{19}$ I have to confess that this notation is imperfect, because from the point of view of rigorous mathematics, $w(x$, $x^{\prime}$ ) and $w(x)$ are different functions, and so are $w\left(p, p^{\prime}\right)$ and $w(p)$ used below. In the perfect world, I would use different letters for them all, but I desperately want to stay with " $w$ " for all the probability densities, and there are not so many good different fonts for this letter. Let me hope that the difference between these functions is clear from their arguments, and from the context.
    ${ }^{20}$ It was introduced in 1932 by E. Wigner on the basis of a general (Weyl-Wigner) transform suggested by H. Weyl in 1927, and re-derived in 1948 by J. Ville on a different mathematical basis.

[^672]:    ${ }^{21}$ Note that the last line of Eq. (5.67) is invalid for the density operator $\hat{w}$, because it is not local!
    ${ }^{22}$ Such density, which would express the probability $d W$ to find the system in a small area of the phase plane as $d W=\rho(X, P) d X d P$, is the basic notion of (1D) classical statistics - see, e.g., SM Sec. 2.1.

[^673]:    ${ }^{23}$ Please note that in notations of that section, arguments $\{X, P\}$ of the Wigner function should be replaced with $\{x, p\}$, and capital letters saved for the Cartesian coordinates of the central point (5.133), i.e. the classical complex amplitude of the oscillations.
    ${ }^{24}$ Spectacular experimental measurements of this function (for $n=0$ and $n=1$ ) were carried out recently by E. Bimbard et al., Phys. Rev. Lett. 112, 033601 (2014).

[^674]:    ${ }^{25}$ In many texts, it is called the "Liouville equation", due to the philosophical proximity to the classical Liouville theorem for the distribution function $\rho(X, P)$ or its multi-dimensional analog - see, e.g., SM Sec. 6.1, in particular Eq. (6.5).

[^675]:    ${ }^{26}$ Another example when $W_{j}$ are constant in time, and hence Eq. (66) is valid, is the thermodynamic equilibrium. However, in this case the statistical operator is diagonal in the stationary state basis and hence commutes with the Hamiltonian. Hence the right-hand part of Eq. (66) vanishes, and it shows that the density matrix does not evolve in time at all - as it should.
    27 Though this model works very well in many cases (see the examples given below), it is not adequate for a particle interacting with the environment of similar particles. In this case the methods discussed in the next chapter are more relevant.

[^676]:    ${ }^{28}$ This can be done because we may consider the whole system, including the environment, as a Hamiltonian one - see Eq. (68).

[^677]:    ${ }^{29}$ This assumption is not in any contradiction with the quantum treatment of the two-level system, because a typical environment has very dense energy spectrum, so that the distances between them may be readily bridged by thermal excitations of energies $\sim k_{\mathrm{B}} T \ll 2 a_{z}$, often making its essentially classical.

[^678]:    ${ }^{30}$ The theory of this phenomenon, first observed experimentally by biologist R. Brown in the early 1800 s , was pioneered by A. Einstein in 1905 (see in particular Eq. (206) below) and developed in detail by M. Smoluchowski in 1906-1907, and A. Fokker in 1913.

[^679]:    ${ }^{31}$ This result is valid only if approximation (82) may be applied at time interval $d t$ which, in turn, should be much smaller than $T_{2}$, i.e. if the dephasing time is much longer that the environment's correlation time $\tau_{c}$. This requirement is usually well satisfied, because in most environments, $\tau_{c}$ very short. For example, in the original Brownian motion experiments with few- $\mu \mathrm{m}$ ink particles in water, it is of the order of the average interval between sequential molecular impacts, of the order of $10^{-21} \mathrm{~s}$.
    ${ }^{32}$ See, e.g., MA Eq. (1.2a).

[^680]:    ${ }^{33}$ The most frequent example of violation of these conditions is environment's overheating by the energy flow from the subsystem. I leave it to the reader to estimate the overheating of a standard physical laboratory room by a typical dissipative quantum process - the emission of an optical photon by an atom. (Hint: extremely small.)
    ${ }^{34}$ The FDT was first derived by H. Callen and T. Welton in 1951, on the background of an earlier derivation of its classical limit by H. Nyquist in 1928, and the pioneering 1905 work by A. Einstein - see below.
    ${ }^{35}$ The FDT may be proved in several ways which are different from, and shorter than the one given in this section - see, e.g., either SM Secs. 5.5 and 5.6 (based on H. Nyquist's arguments), or the original paper by H. Callen and T. Welton, Phys. Rev. 83, 34 (1951) - wonderful in its clarity. The longer approach I describe here, besides giving the important Kubo formula (109) as a byproduct, is a very useful exercise in the operator manipulation and the perturbation theory in its integral form, different from the differential form used in Chapter 6. If the reader is not interested in this exercise, he or she may skip the derivation and jump directly to the result expressed by Eq. (134), which uses the notions defined by Eqs. (114) and (123).
    ${ }^{36}$ We can always do that if the local environment is large enough, so that the processes in our subsystem would not depend on the type of boundary between it and the external environment; in particular we may assume the total system closed, i.e. Hamiltonian.
    ${ }^{37}$ For usual ("ergodic") environments, without intrinsic long-term memories, this statistical averaging over an ensemble of environments is equivalent to averaging over relatively short times - much longer than the correlation time $\tau_{c}$ of the environment, but still much shorter than the characteristic time of evolution of the system under analysis, such as the dephasing time $T_{2}$ and the energy relaxation time $T_{1}$ - both still to be calculated. As was already mentioned, in most practical environments, $\tau_{c}$ is very short. Thus, for relatively "massive" (inertial) systems of interest the separation of the averaging into two steps is well justified.

[^681]:    ${ }^{38}$ Here we assume that for the equilibrium, Eq. (92) has zero average, because if this is not so, this average part of force may be always included into the Hamiltonian of subsystem $s$.

[^682]:    ${ }^{39}$ A good sanity check here is that at $\tau=0$, the difference (99) between $K_{F}(\tau)$ and $K_{F}(-\tau)$ vanishes.

[^683]:    ${ }^{40}$ For a more detailed discussion of this function and the causality principle, see, e.g., CM Sec. 4.1.
    ${ }^{41}$ This relation, called the Kubo (or "Green-Kubo") formula, after the works by M. Green (1954) and R. Kubo (1957), does not come up in the easier derivations of the FDT, discussed in the beginning of this section.
    ${ }^{42}$ Due to their practical importance, and certain mathematical issues with their justification for random functions, Eqs. (112)-(113) have their own grand name, the Wiener-Khinchin theorem, though the math rigor aside, they are just a straightforward corollary of the Fourier integral transform (115) - see, e.g., SM Sec. 5.4.

[^684]:    ${ }^{44}$ Using, e.g., MA Eq. (6.5a). (The imaginary parts of the integrals vanish, because integration in infinite limits may be always re-centered to finite points $\pm \hbar \omega$.) A mathematically enlightened reader may have noticed that the integrals might be taken without the introduction of small $\varepsilon$, using the Cauchy theorem - see MA Eq. (15.1).

[^685]:    ${ }^{45}$ Integration in Eq. may be extended to the whole time axis, $-\infty<\tau<+\infty$, if we complement definition (107) of $G(\tau)$ for $\tau>0$ with its definition as $G(\tau)=0$ for $\tau<0$, in correspondence with the causality principle.
    ${ }^{46}$ In order to prove this relation, it is sufficient to plug expression $\hat{x}_{s}=\hat{x}_{\omega} e^{-i \omega t}$, or any sum of such exponents, into Eqs. (107) and then use definition (123). This simple exercise is highly recommended to the reader.
    ${ }^{47}$ The expression $P=F \dot{x}=F v$ used for the instant power flow is evident if $x$ is the usual Cartesian coordinate of a mechanical system. According to analytical mechanics (see, e.g., CM Chapters 2 and 10), it is valid for any generalized coordinate - generalized force pair which forms the interaction Hamiltonian (90).

[^686]:    ${ }^{48}$ A curious feature of the FDT is that Eq. (134) includes the exactly same function of temperature as the average energy (26) of a quantum oscillator of frequency $\omega$, though, as the reader could witness, the notion of the

[^687]:    ${ }^{54}$ See, e.g., CM Sec. 4.1.
    ${ }^{55}$ See, e.g., MA Eq. (6.5a).

[^688]:    ${ }^{56}$ By the way, the simplest way to calculate $S_{F}(\omega)$, i.e. to derive the FDT, is to require that Eqs. (48) and (150) give the same result for an oscillator with any eigenfrequency $\omega$. This is exactly the approach used by H. Nyquist (for the classical case) - see also SM Sec. 5.5.
    ${ }^{57}$ See, for example, R. Koch et al., Phys. Lev. B 26, 74 (1982)..

[^689]:    ${ }^{58}$ Its natural generalizations enable analyses of fluctuations in arbitrary linear systems, i.e. the systems described by linear differential (or integro-differential) equations of motion, including those with many degrees of freedom, and distributed systems (continua).
    ${ }^{59}$ For some calculations, this problem may be avoided by linearization: if we are only interested in small fluctuations, the Heisenberg equations of motion may be linearized about their expectation values (see, e.g., CM Sec. 4.2), and the linear equations for variations solved either as has been shown above, or (if the expectation values evolve in time) by their Fourier expansions.

[^690]:    ${ }^{60}$ As in Sec. 4, the reader not interested in the derivation of the basic equation (181) for the density matrix evolution may immediately jump to the discussion of this equation and its applications.

[^691]:    ${ }^{62}$ A similar analysis of a more general case, when the interaction with environment may be represented as a sum of products of the type (90), may be found in a monograph by K. Blum, Density Matrix Theory and Applications, $3^{\text {rd }}$ ed., Springer, 2012.

[^692]:    ${ }^{63}$ Named after A. Markov (1856-1922; in older literature, "Markoff"), because the result of this approximation is a particular case of the Markov process whose future development is completely determined by its present state.
    ${ }^{64}$ Rather reluctantly, I will use this standard notation, $E_{n}$, for the eigenenergies of our system of interest $(s)$, in hope that the reader would not confuse these discrete energy levels with the quasi-continuous energy levels of its environment, participating in particular in Eqs. (108) and (111). As a reminder, by this stage of our calculations the environment levels have disappeared, leaving behind their "trace functions" $K_{F}(\tau)$ and $G(\tau)$.

[^693]:    ${ }^{65}$ This is essentially the same rotating-wave approximation (RWA) that is so instrumental in other fields of not only quantum mechanics, but classical physics as well - see, e.g., CM Secs. 4.2-4.5.
    ${ }^{66}$ As was already discussed in Sec. 4, the lower-limit substitution $\left(t^{\prime}=-\infty\right)$ in integrals (174) gives zero, due to the finite-time "memory" of the system, expressed by the decay of the correlation and response functions at large values of the time delay $\tau=t-t$ '.

[^694]:    ${ }^{67}$ The master equations, first introduced to quantum mechanics in 1928 by W. Pauli, are sometimes called the "Pauli master equations", or "kinetic equations", or "rate equations".
    ${ }^{68}$ As Eq. (193) shows, the term with $m=n$ would vanish, and thus may be legitimately excluded from the sum.

[^695]:    ${ }^{69}$ As Eq. (193) shows, the result for $\Gamma_{n \rightarrow n^{\prime}}$ is described by Eq. (195) as well, provided that indices $n$ and $n$ ' are swapped in all components of its right-hand part, including the swap $\omega_{n n^{\prime}} \rightarrow \omega_{n^{\prime} n}=-\omega_{n n^{\prime}}$.
    ${ }^{70}$ It is straightforward to show that at relatively low temperatures $\left(k_{\mathrm{B}} T \ll\left|E_{n},-E_{n}\right|\right)$, Eq. (196) gives the same result as the Golden Rate formula (6.134) - see Exercise 2. (The low temperature limit is necessary to ensure that the initial occupancy of the excited level is negligible, as was assumed at the derivation of Eq. (6.134).)

[^696]:    ${ }^{71}$ Because of the reason explained above, this (relatively :-) simple result is not valid for systems with equidistant energy spectra, most importantly, for the harmonic oscillator (while Eq. (7.194) is). For the oscillator, with its simple matrix elements $x_{n n^{\prime}}$, it is straightforward to repeat the above calculations, starting from (7.183), to obtain an equation similar to Eq. (7.200), but with two other terms, proportional to $w_{n \pm 1, n^{\prime} \pm 1}$, in its right-hand part. Since for the harmonic oscillator the Heisenberg-Langevin approach allows obtaining most results in a much simpler way, I will skip the derivation of this equation and the discussion of its solutions. The interested reader may find such a discussion, for example, in a paper by B. Zeldovich et al., Sov. Phys. JETP 28, 308 (1969).
    ${ }^{72}$ Sometimes Eq. (200) (in any of its numerous alternative forms) is called the Redfield equation, after the 1965 work by A. Redfield. Note, however, that several other authors, notably including (in the alphabetical order) H. Haken, W. Lamb, M. Lax, W. Louisell, and M. Scully, also made key contributions into the very fast development of the density-matrix approach to open quantum systems in the mid-1960s.
    ${ }^{73}$ This correction is frequently called the Lamb shift, because it was first observed experimentally in 1947 by W. Lamb and R. Retherford, as a minor, $\sim 1 \mathrm{GHz}$ shift between energy levels of $2 s$ and $2 p$ states of hydrogen, due to the electric-dipole coupling of hydrogen atoms to the free-space electromagnetic environment. (These levels are equal not only in the non-relativistic theory (Sec. 3.6), but also in the relativistic, Dirac theory (Sec. 9.7), if the

[^697]:    ${ }^{75}$ The tunneling may be described without altering Eq. (70), just by adding, to the unperturbed Hamiltonian (69), terms proportional to other Pauli matrices. The reader is encouraged to spell out the equations for the time evolution of the density matrix elements of this system, and analyze their main properties - at least in the lowtemperature limit.

[^698]:    ${ }^{76}$ It was the main result of A. Einstein's pioneering analysis of such Brownian motion in 1905. (The development of this analysis in 1906-1908 by M. Smoluchowski has led in 1912 to the Fokker-Planck theory.)

[^699]:    ${ }^{81}$ Besides the trivial case $\alpha_{j}=\delta_{j j^{\prime}}$ (so that $W_{j}=\delta_{j j^{\prime}}$ ), when the system is in a certain eigenstate $\left(a_{j^{\prime}}\right.$ ) of operator $\hat{A}$. ${ }^{82}$ The reader in doubt is invited to compare entropy $S=-\Sigma_{j} W_{j} \ln W_{j}$, the measure of system's disorder (see, e.g., SM Sec. 2.2) of the pure state $(S=0)$ with that in any state with several nonvanishing values of $W_{j}(S>0)$.

[^700]:    ${ }^{83}$ This scheme may be implemented, for example, using a simple Josephson-junction circuit called the balanced comparator - see, e.g., T. Walls et al., IEEE Trans. on Appl. Supercond. 17, 136 (2007), and references therein. Experiments by V. Semenov et al., IEEE Trans. Appl. Supercond. 7, 3617 (1997) have demonstrated that this system may have measurement accuracy dominated by quantum-mechanical uncertainty at relatively modest cooling (to $\sim 1 \mathrm{~K}$ ). One of advantages of such implementation of this measurement scheme is that it is based on externally-shunted Josephson junctions - devices whose quantum-mechanical model is in a quantitative agreement with experiment - see, e.g., D. Schwartz et al., Phys. Rev. Lett. 55, 1547 (1985). Colloquially, the balanced comparator is an instrument with a "well-documented Hamiltonian" including its part describing coupling to environment.
    ${ }^{84}$ As a reminder, dynamics of this system was discussed in Sec. 2.6 and then again in Sec. 6.1.

[^701]:    ${ }^{85}$ Somewhat counter-intuitively, the latter growth plays a positive role for measurement fidelity. Indeed, it does not affect the intrinsic "signal-to-noise ratio" $\delta x_{s} /\left\langle x_{s}\right\rangle$, while making the intrinsic (say, quantum-mechanical) uncertainty much larger that possible noise contribution by the latter measurement stage(s).

[^702]:    ${ }^{86}$ This name, coined by E. Sudarshan and B. Mishra in 1997 (though the paradox had been discussed in detail by A. Turing in 1954); is due to the apparent similarity of this paradox to classical paradoxes by ancient Greek philosopher Zeno of Elea. By the way, just to have a minute of fun, let us have a look what happens when Mother Nature is discussed by people to do not understand math and physics. The most famous of the classical Zeno paradoxes is the Achilles and Tortoise case: a fast runner Achilles can apparently never overtake a slower Tortoise, because (in the words by Aristotle) "the pursuer must first reach the point whence the pursued started, so that the slower must always hold a lead". For a physicist, the paradox has a trivial resolution, but let us listen what a philosopher (D. Burton) writes about it - not in some year BC, but in 2010 AD: "Given the history of 'final resolutions', from Aristotle onwards, it's probably foolhardy to think we've reached the end." For me, this is a sad symbol of modern philosophy.

[^703]:    ${ }^{87}$ For a detailed survey of this field see, e.g., either V. Braginsky and F. Khalili, Quantum Measurements, Cambridge U. Press, 1992, or H. Wiseman and G. Milburn, Quantum Measurement and Control, Cambridge u. Press, 2010.
    ${ }^{88}$ S. Peil and G. Gabrielse, Phys. Rev. Lett. 83, 1287 (1999).
    ${ }^{89}$ Similar to the one discussed in EM Sec. 2.4 (see in particular Eq. (2.77) and Fig. 2.7), but with additional rotation about one of the axes - either $x$ or $y$.

[^704]:    ${ }^{90}$ I am simplifying the real situation a bit. Actually, in the experiment there was an electron spin's contribution to the interaction Hamiltonian as well, but since the large magnetic field polarized the spins quite reliably, their only role was a constant shift of frequency $\omega_{z}$.

[^705]:    ${ }^{91}$ This simple equation is limited to 1D systems with Hamiltonians of the type (2.50), but the reader should agree that this is a pretty general form.
    ${ }^{92}$ See, e.g., CM Sec. 4.1. Note in particular that function $\sin \omega_{0} \tau\left(\right.$ with $\left.\tau \equiv t-t^{\prime}\right)$ under the integral, divided by $\omega_{0}$, is nothing more than the temporal Green's function $G(\tau)$, of a loss-free harmonic oscillator.

[^706]:    ${ }^{93}$ The physical sense of these relations should be clear from Fig. 5.6: they define a system of coordinates rotating clockwise with angular velocity $\omega$, so that the point representing unperturbed classical oscillations with that frequency is at rest in that rotating frame. (The "probability cloud" presenting a Glauber state is also stationary in coordinates $\left[x_{1}, x_{2}\right]$.) The reader familiar with the classical theory oscillations may notice that $x_{1}$ and $x_{2}$ are essentially the RWA variables $u$ and $v$, i.e. the Poincaré plane coordinates - see, e.g., CM Sec. 4.3-4.6, and especially Fig. 4.9.
    ${ }^{94}$ See, e.g., P. Grangier et al., Nature 396, 537 (1998), and references therein. This was, however, not the first QND implementation in optics - for a review see J. Roch et al., Appl. Phys. B 55, 291 (1992).
    ${ }^{95}$ As it is, for example, for gravitational wave detectors - see the discussion and references in Sec. 2.10.
    ${ }^{96}$ See, e.g., CM Sec. 4.5.
    ${ }^{97}$ For the exact definition of the latter parameter, suitable for the quantum sensitivity range $\left(\Theta_{N} \sim \hbar \omega\right)$ as well, see, e.g., I. Devyatov et al., J. Appl. Phys. 60, 1808 (1986). In the classical noise limit ( $\Theta_{N} \gg \hbar \omega$ ), it coincides with $k_{\mathrm{B}} T_{N}$, where $T_{N}$ is a more popular measure of electronics noise, called the noise temperature.

[^707]:    ${ }^{98}$ This fact was recognized very early - see, e.g., H. Haus and J. Mullen, Phys. Rev. 128, 2407 (1962).
    ${ }^{99}$ See, e.g., the spectacular experiments by B. Yurke et al., Phys. Rev. Lett. 60, 764 (1988).
    ${ }^{100}$ See, e.g., D. Averin, Phys. Rev. Lett. 88, 207901 (2002).

[^708]:    ${ }^{1}$ An important conceptual question is why not treat one particle of such a collection as an open quantum system, and apply to it the powerful methods discussed in the last chapter, based on the separation of the whole Universe into the "system of our interest" and the "environment" - see Fig. 7.1. Such separation is very natural and works very well in cases when one, relative "massive" (inertial) particle, or a specific collective degree of freedom (also relatively inertial), is surrounded by a sea of "lighter particles", which serve the role of an environment frequently in or close to thermal equilibrium. On the other hand, in most systems of identical particles, such separation is more artificial and may lead to errors, because the quantum state of the "particle of interest" may be substantially correlated (in particular, entangled) with that of similar particles of its "environment" - see the discussion later in this section.

[^709]:    ${ }^{2}$ Here by "elementary particles" I mean any of the following two options:
    (i) particles like electrons, which (at least at this stage of development of physics) are considered as structure-less entities;
    (ii) any object (e.g., a hadron or meson) which may be considered as a system of "more elementary" particles (e.g., quarks), but still may be reliably placed in a definite (say, ground) quantum state.

    From that point of view, even complex atoms or molecules of a certain chemical element, each in its ground state, may be considered on the same footing as elementary particles.
    ${ }^{3}$ A very legitimate question is why, in this situation, we need to introduce particle's number to start with. A partial answer is that in this approach it is much simpler to derive (or guess) problem Hamiltonians from the correspondence principle. For example for a system of two spinless particles, each in an external potential $U(\mathbf{r})$, and with the interaction energy $U_{\text {int }}\left(\left|\mathbf{r}_{1}-\mathbf{r}_{2}\right|\right)$, the correct Hamiltonian is

    $$
    \hat{H}=\frac{\hat{p}_{1}^{2}}{2 m}+\frac{\hat{p}_{2}^{2}}{2 m}+U\left(\hat{\mathbf{r}}_{1}\right)+U\left(\hat{\mathbf{r}}_{2}\right)+U_{\mathrm{int}}\left(\left|\hat{\mathbf{r}}_{1}-\hat{\mathbf{r}}_{2}\right|\right)
    $$

    Later in this chapter, we will discuss an alternative approach (the so-called "second quantization") in which tracing a certain particle is avoided. While for indistinguishable particles this is more logical, in that approach writing adequate Hamiltonians (which, in particular, would avoid spurious self-interaction of the particles) is much more challenging - see Sec. 3 below.

[^710]:    ${ }^{4}$ As in many situations we met before, kets (10) and (11) may be multiplied by $\exp \{i \varphi\}$ with an arbitrary real phase $\varphi$. However, until we discuss coherent superpositions of various states $\alpha$, there is no good motivation for taking the phase different from 0 ; that would only clutter the notation.

[^711]:    ${ }^{5}$ Traditionally, people speak about two different "statistics": the Bose-Einstein statistics of bosons, and FermiDirac statistics of fermions, because their statistical distributions in thermal equilibrium are indeed different - see, e.g., SM Sec. 2.8. However, as evident from the above discussion, their difference is deeper, and actually we are dealing with two different quantum mechanics.
    ${ }^{6}$ For a quantitative discussion of the Bose-Einstein condensation see, e.g., SM Sec. 3.4.
    ${ }^{7}$ Such possibility follows from the fact that for the Bose-Einstein condensate of $N \gg 1$ particles, the Heisenberg uncertainty relation may be reduced to $\delta N \delta \varphi>1$, where $\varphi$ is the condensate wavefunction's phase, so that it may have $\delta N /\langle N\rangle \ll 1$ and $\delta \varphi \ll 1$ simultaneously.
    ${ }^{8}$ It was formulated by W. Pauli in 1925, on the basis of less general rules suggested by G. Lewis (1916), I. Langmuir (1919), N. Bohr (1922), and E. Stoner (1924) for the explanation of experimental spectroscopic data.

[^712]:    ${ }^{9}$ Note that in the sense of Eq. (5.197), all three triplet states of a two-electron system behave as a single integer spin with $s=1$; for example, $S^{2}$ equals $2 \hbar^{2}$, rather than 0 as one could expect for the last component of Eq. (21) see Problem 1.
    ${ }^{10}$ In this chapter, I try to use lower-case letters for observables of single particles (in particular, $\varepsilon$ for their energies), in order to distinguish them as clearly as possible from system's variables, including the total energy $E$ of the system, typeset in capital letters.

[^713]:    ${ }^{11}$ It is also very important, since helium makes up more than $20 \%$ of all "ordinary" matter of our Universe.
    ${ }^{12}$ Evidently, the positive ion $\mathrm{He}^{+1}$ of such atom, with just one electron, is very well described by the hydrogenlike atom theory with $Z=2$, whose ground-state energy, according to Eq. (3.191), is $-Z^{2} E_{\mathrm{H}} / 2=-2 E_{H} \approx-55.4 \mathrm{eV}$.

[^714]:    ${ }^{13}$ See also Problems 2.6-2.8, 2.34, and 3.3.

[^715]:    ${ }^{14}$ This example explains why the variational method is broadly used for approximate treatment of complex quantum systems, although it is based more or less intuitive guesses of trial functions, i.e. in contrast with the perturbation theories discussed in Chapters 6 and 7, does not guarantee asymptotically correct results in any particular limit, unless such correctness is manually incorporated into the trial state choice.

[^716]:    ${ }^{15}$ See, e.g., EM Sec. 1.3, in particular Eq. (1.54).
    ${ }^{16}$ Note that the result for $E_{\text {dir }}$ correctly reflects the basic fact that a charged particle does not interacts with itself, even if its wavefunction is quantum-mechanically spread over a finite space volume. Unfortunately, this is not true for some other approximate theories of multi-particle systems - see Sec. 4 below.

[^717]:    ${ }^{17}$ It was invented (first for photons and then for arbitrary bosons) by P. Dirac in 1927, and then modified in 1928 for fermions by E. Wigner and P. Jordan. The term "second quantization" is rather misleading for the nonrelativistic applications we are discussing, but finds certain justification in the quantum field theory.

[^718]:    ${ }^{18}$ The resulting Dirac state is not an eigenstate of every multiparticle Hamiltonian. However, we will see below that for a set of non-interacting particles it is an eigenstate, and thus may be used in the basis for perturbation theories of systems of weakly interacting particles.

[^719]:    ${ }^{19}$ See, e.g., MA Eq. (2.3).

[^720]:    ${ }^{20}$ A by-product of this calculation is a proof that operator (64) counts the number of particles $N_{j}$ (now equal to either 1 or 0 ), just at it does for bosons.

[^721]:    ${ }^{21}$ Equations of motion for creation operators $\hat{a}_{1,2}^{\dagger}$ are just the Hermitian-conjugates of Eqs. (98), and do not add any new information about system's dynamics.

[^722]:    ${ }^{22}$ For the second well's occupancy, the result is complementary, $N_{2}(t)=N_{1}(0) \sin ^{2} \Omega t+N_{2}(0) \cos ^{2} \Omega t$, giving in particular a good sanity check: $N_{1}(t)+N_{2}(t)=N_{1}(0)+N_{2}(0)=$ const.

[^723]:    ${ }^{23}$ For a review of the 1D version of this problem, see, e.g., J. Pendry, Adv. Phys. 43, 461 (1994).
    ${ }^{24}$ To complete this section, I have to note, at least in passing, a different form of the second-quantization formalism, based on the so-called field operators. It will be more natural for me to discuss it in the next chapter.
    ${ }^{25}$ Another important example is the so-called Hubbard model in which there may be only two particles on each of localized sites, with the negligible interaction of particles on different sites - which are only connected by the next-neighbor tunneling - see Eq. (104).
    ${ }^{26}$ The only new feature is a specific order of the indices of the creation operators. Note the mnemonic rule of writing this expression, similar to that for Eq. (79): each term corresponds to moving a pair of particles from states $l$ and $l$ ' to states $j^{\prime}$ and $j$, factored with the corresponding two-particle matrix element (107).

[^724]:    Energy
    correction due to
    fermion interaction

[^725]:    ${ }^{27}$ Constructs (117) are also close to spinors (14), besides that the spin $s$ of a single particle is fixed, so that the spin-orbital should be indexed by spin's orientation $m \equiv m_{s}$ rather than the full spin $s$. Also, the orbital index should be clearly distinguished from $j$ (which, again, is the set of that orbital index and $m$ ). This is why I believe that the frequently met notation of spinors as $\psi_{j, s}(\mathbf{r})$ may lead to confusion.

[^726]:    ${ }^{32}$ See, e.g., A. Szabo and N. Ostlund, Modern Quantum Chemistry, McGraw-Hill, 1989.
    ${ }^{33}$ That method, in particular, allows the calculation of proper linear superpositions of the Dirac states (such as the excited singlet state for $N=2$, discussed above) which are missing in the generic Hartree-Fock approach.
    ${ }^{34}$ It was developed by W. Kohn and coauthors in the mid-1960s, and eventually (in 1998) awarded with a Nobel prize in chemistry.
    ${ }^{35}$ For a uniform, degenerate Fermi-gas of electrons (with the Fermi energy $\varepsilon_{\mathrm{F}} \gg k_{\mathrm{B}} T$ ), the exchange potential may be calculated analytically, giving $u_{\mathrm{ex}}=(3 / 4 \pi) e^{2} k_{\mathrm{F}} / 4 \pi \varepsilon_{0}$, where $k_{\mathrm{F}}$ is the Fermi-surface wave number that defines both the Fermi energy $\varepsilon_{\mathrm{F}}=\left(\hbar k_{\mathrm{F}}\right)^{2} / 2 m$ and the electron density (per unit volume) $n=2(4 \pi / 3) k_{\mathrm{F}}^{3} /(2 \pi)^{3} \equiv$ $k_{\mathrm{F}}^{3} / 3 \pi^{2}$.
    ${ }^{36}$ See, e.g., G. te Velde et al., J. Comp. Chem. 22, 931 (2001), and/or M. D. Segall et al., J. Phys. - Cond. Matt. 14, 2717 (2002), and references therein.

[^727]:    ${ }^{37}$ This popularity is enhanced by the availability of several advanced DFT software packages, some of them (such as SIESTA, http://icmab.cat/leem/siesta/) in public domain.
    ${ }^{38}$ See, e.g., N. Simonian et al., J. Appl. Phys. 113, 044504 (2013).
    ${ }^{39}$ Since these fields are much related, they are often referred to together, under the (somewhat misleading) title of "quantum information".
    ${ }^{40}$ Despite many recent book titles in the field, one of its first surveys, by M. Nielsen and I. Chuang, Quantum Computation and Quantum Information, Cambridge U. Press, 2000, is perhaps still the best one.
    ${ }^{41}$ In some texts, the term qubit (or "Qbit", or "Q-bit") is used instead for the information contents of a two-level system - very much like the classical bit of information (in this context, frequently called "Cbit" or "C-bit") describes the information contents of a classical bistable system - see, e.g., SM Sec. 2.2.
    ${ }^{42}$ The slightly odd aspect of this notation is that at the Bloch sphere representation (Fig. 5.1), the North Pole state (that is traditionally denoted as $\uparrow$ in other fields of quantum mechanics) is taken for 0 , while the South Pole state $\downarrow$ for 1 , so that Eqs. (5.4) take the form $a_{0}=\cos (\theta / 2), a_{1}=\sin (\theta / 2) \exp \{i \varphi\}$.

[^728]:    ${ }^{43}$ Here and in most instances below I use the same shorthand notation as was used in the beginning of this chapter - cf. Eq. (8.1). In this short form, qubit's number is coded by the order of its state index inside the single ketvector, while in the long form, such as in Eq. (129), it is coded by the order of the ket-vector.
    ${ }^{44}$ It follows from the requirement that the sum of two probabilities $W_{j}=\langle\alpha| \hat{P}_{j}|\alpha\rangle$ (where $\hat{P}_{j}=|j\rangle\langle j|$ is the corresponding projection operator, see Sec. 4.5) to find one of qubits in one of its two possible states $j$, equals 1. It is remarkable that the application of this condition to any of the qubits results in the same Eq. (127).

[^729]:    ${ }^{45}$ Numerous modifications of this baseline scheme have been suggested, for example with the number of output qubits different from that of input qubits, etc. Some other options are discussed in the end of this section.
    ${ }^{46}$ The notion of "wires" stems from the similarity between these diagrams and the drawings used to describe classical computation circuits (see, e.g., Fig. 3a below); in the latter case the lines may be indeed understood as physical wires connecting physical devices: logic gates and/or memory cells. In this context note that classical computer components also have nonvanishing time delays, so that even in this case the left-to-right device ordering is useful to indicate the timing of (and frequently the causal relation between) the signals.
    ${ }^{47}$ As we know from Chapter 7, the preparation of pure state (125) is (conceptually :-) straightforward. Placing a qubit into a weak contact with an environment of temperature $T \ll \Delta / k_{\mathrm{B}}$, where $\Delta$ is the difference between energies of eigenstates $|0\rangle$ and $|1\rangle$, we may achieve its relaxation into the lowest-energy state. (Otherwise, the relaxation may be to one of states with equal, or nearly-equal energies, combined with its measurement - see Fig. 7.8 and its discussion.) Then, if the qubit must be set into the opposite state, it may be driven there by the application of a pulse of a proper external classical "force". For example, if actual spin- $1 / 2$ particles are used as qubits, a constant magnetic field may be applied in the $[x, y]$ plane for a half-period of the torque-induced spin precession - see Fig. 5.1c. However, for most qubit implementations, the basis state reversal using a half-period of rf-induced Rabi oscillations (Sec. 6.5) is more convenient.

[^730]:    ${ }^{48}$ Named after D. Deutsch, whose 1985 paper (motivated by an inspirational but not very specific publication by R. Feynman in 1982) launched the whole field of quantum computation.

[^731]:    ${ }^{49}$ Alternatively, we may perform two sequential experiments on the same black box $f$, first recording and then recalling their results.

[^732]:    50 In order to exclude any chance of confusion between the Hadamard transform's operator $\hat{\notin t}$ and the Hamiltonian operator $\hat{H}$, I have typeset them using different fonts.
    ${ }^{51}$ Note that according to Eq. (138), the operator $\hat{H}$ does not belong to the limited class $\hat{U}$ described by Eq. (132). ${ }^{52}$ Since states 0 and 1 form a full basis of the single qubit, Eqs. (139) may be summarized as an operator equality: ${\hat{\mathcal{H}^{2}}}^{2}=\hat{I}$.

[^733]:    ${ }^{53}$ This means that the last Hadamard transform of the target qubit (i.e. the Hadamard gate shown in the lower right corner of Fig. 3b) is not necessary for the Deutsch problem solution - though it should be included if we want the whole circuit to satisfy the general condition (132).

[^734]:    ${ }^{54}$ To comply with our current notation, coefficients $a_{n}$ ' and $a_{n}$ of Sec. 6.5 should be replaced with $a_{0}$ and $a_{1}$. Also note that their definition (6.82) implies that the trivial time evolution (6.81) of unperturbed qubits has been already excluded from these expansion coefficients.

[^735]:    ${ }^{55}$ The assumption of simultaneous time independence of the basis state vectors and the interaction operator (within the time interval $0<t<T$ ) is possible only if the basis state energy difference $\Delta$ of both qubits is exactly the same. For this case, the simple physical explanation of the time evolution (149) follows from Fig. 8.5, which shows the spectrum of the total energy $E=E_{1}+E_{2}$ of the two-bit system. In the absence of interaction, the energies of two basis states, $|01\rangle$ and $|10\rangle$, are equal, enabling even a weak qubit interaction to cause their substantial evolution in time - see Sec. 6.7. If the qubit energies are different (Fig. 5c), the interaction may still be reduced, in the rotating-wave approximation, to Eq. (149), by compensating the energy difference $\left(\Delta_{1}-\Delta_{2}\right)$ with an external rf signal of frequency $\omega=\left(\Delta_{1}-\Delta_{2}\right) / \hbar$ - see Sec. 6.5.

[^736]:    ${ }^{56}$ It Eq. (4.175) shows, each of component unitary transforms $\hat{I} \exp \left\{i \theta^{\prime} \hat{\sigma}_{z}\right\}$ may be created by applying to each qubit, for a time period $T^{\prime}=\hbar \theta^{\prime} / \kappa^{\prime}$, a constant external field described by Hamiltonian $\hat{H}=-\kappa^{\prime} \hat{\sigma}_{z}$. We already know that for a charged, spin- $1 / 2$ particle, such Hamiltonian may be created by applying $z$-oriented external constant magnetic field - see Eq. (4.163). For most other physical implementations of qubits, the organization of such Hamiltonian is also straightforward - see, e.g., Fig. 7.4 and its discussion.
    ${ }^{57}$ As was discussed above, this gate is identical to quantum gate $f$ for $f=f_{3}$, i.e. $f(j)=j$. The implementation of $f$ for 3 other functions $f$ requires straightforward modifications whose analysis is left for reader's exercise.
    ${ }^{58}$ This fundamental importance of the CNOT gate was perhaps a major reason why D. Wineland, the leader of the NIST group that had demonstrated the first experimental implementation in 1995 (following the theoretical suggestion by J. Cirac and P. Zoller), was awarded the 2012 Nobel Prize (shared with S. Haroche, the leader of another leading group working towards quantum computation).
    ${ }^{59}$ For that, the reader may be referred to either the monograph by Nielsen and Chuang, cited above, or to a shorter (but more formal) textbook by N. Mermin, Quantum Computer Science, Cambridge U. Press, 2007.

[^737]:    ${ }^{60}$ His original paper was published only in proceedings of a meeting, but a clear description of the algorithm may be found in several accessible sources including Wikipedia (http://en.wikipedia.org/wiki/Shor's algorithm).
    ${ }^{61}$ Named after R. Rivest, A. Shamir, and L. Adleman, the authors of the first open publication of the code in 1977, but actually invented earlier (in 1973) by C. Cocks.
    ${ }^{62}$ For more details, and a discussion of other possible implementations (such as quantum dots and dopants in crystals) see, e.g., T. Ladd et al., Nature 464, 45 (2010), and references therein.
    ${ }^{63} \mathrm{~A}$ brief discussion of such interactions (so-called Cavity QED) will be given in Sec. 9.4 below.
    ${ }^{64}$ In this field, the condition $\omega=\omega_{10}$, discussed above, is called the nuclear magnetic resonance, or NMR - the term well known due to the broad application of this effect in chemistry and medicine.
    ${ }^{65}$ See Eq. (4.5) and its discussion.
    ${ }^{66}$ This challenge may be partly mitigated using ingenious spin manipulation techniques such as refocusing - see, e.g., either Sec. 7.7 in Nielsen and Chuang, or J. Keeler's monograph cited in the end of Sec. 6.5.
    ${ }^{67}$ B. Lanyon et al., Phys. Rev. Lett. 99, 250505 (2001).

[^738]:    ${ }^{68}$ For the purposes of $E_{J}$ control reasons, it is more convenient to use two-junction configurations called Bloch transistors. Unfortunately, I do not have time to go into these details.
    ${ }^{69}$ See, e.g., EM Sec. 6.4 and references therein.
    ${ }^{70}$ This expression directly follows from combining EM Eqs. (6.57), (6.59), and (6.70).

[^739]:    ${ }^{71}$ This is even more true for the so-called "transmons" (or "Xmons") - the phase qubits versions in which a Josephson junction is just a part of an external resonator, providing it with small nonlineartity (anharmonism) see, e.g., R. Barrens et al., Nature 508, 500 (2014) and references therein.
    ${ }^{72}$ E. Lucero et al., Nature Physics 8, 719 (2012).
    ${ }^{73}$ E. Knill et al., Nature 409, 46 (2001).
    ${ }^{74}$ E. Martin-López et al., Nature Photonics 6, 773 (2012).

[^740]:    ${ }^{75}$ Amazingly, this no-cloning theorem was discovered as late as in 1982 (independently by W. Wooters and W. Zurek, and by D. Dieks) - in the context of work toward quantum cryptography.

[^741]:    ${ }^{76}$ This does not mean that several qubits cannot be put into the same, arbitrary quantum state - theoretically, with arbitrary precision. Indeed, they may be first set into their lowest-energy stationary states as was discussed above, and then driven into an arbitrary state (125) by exerting on them similar classical external "forces". So, the nocloning theorem pertains to only an unknown state $\alpha$ of a qubit.
    ${ }^{77}$ Such state is also the 3-qubit example of the so-called Greeenberger-Horne-Zeilinger (GHZ) states, which are frequently called the "most entangled" states of a system of $N>2$ qubits.

[^742]:    ${ }^{78}$ For example, in the Hilbert space of the qubit, the model Hamiltonian (7.70), which was explored in Sec. 7.3, is diagonal in the $z$-basis of states 0 and 1 , so that the unitary transform it provides during interval $T$ is also diagonal, giving the phase shifts described by Eq. (163), with $\varphi=\frac{1}{\hbar} \int_{0}^{T} f\{\lambda\} d t$. Let me emphasize again that Eq. (162) is valid only if the interaction with environment is a pure dephasing, i.e. does not include the energy relaxation of the qubit or its thermal activation to the higher eigenstate - see Chapter 7 .

[^743]:    ${ }^{79}$ Note that qualifier "quantum" is important here, to distinguish this research direction from the option of classical adiabatic (or "reversible") computation - see, e.g., SM Sec. 3.3 and references therein.

[^744]:    ${ }^{80}$ See, e.g., the experiments on factoring of number $143=13 \times 11$, using nuclear spin relaxation, by $\mathrm{N} . \mathrm{Xu}$ et al., Phys. Rev. Lett. 108, 130501 (2012), though by the moment of this writing, their results remained controversial.
    ${ }^{81}$ Due to the same reason, the implementation is so far limited to most scalable, Josephson-junction (flux) qubits - see, e.g., M. Johnson et al., Nature 473, 194 (2011).
    ${ }^{82}$ For its classical version, see, e.g., SM Eq. (4.23) and its discussion.
    ${ }^{83}$ See S. Boxio et al., Nature Physics 10, 218 (2014) and T. Ronnow et al., arXiv:1401.2910 [quant-ph].
    ${ }^{84}$ This field was pioneered in the 1970s by S. Wisener.
    ${ }^{85}$ This procedure had been first suggested in 1993 by the same C. Bennett, and then repeatedly demonstrated experimentally - see, e.g., the recent paper by L. Steffen et al., Nature 500, 319 (2013), and literature therein.

[^745]:    ${ }^{86}$ All four states (172) are eigenstates of both these operators, so that the measurements do not affect each other and may be done in any order.

[^746]:    ${ }^{87}$ BB84 suggested in 1984 by C. Bennett and G. Brassard, and EPRBE suggested in 1991 by A. Ekert. For details, see, e.g., either Sec. 12.6 in Nielsen and Chuang, or the review by N. Gizin et al., Rev. Mod. Phys. 74, 145 (2002).
    ${ }^{88}$ For their discussion see, e.g., EM Sec. 7.8.
    ${ }^{89}$ See P. Hiskett et al., New J. Phys. 8, 193 (2006), and R. Ursin et al., Nature Physics 3, 481 (2007).

[^747]:    ${ }^{90}$ For more discussion of this and other models of ferromagnetism and antiferromagnetism see SM Chapter 4.
    ${ }^{91}$ For similar particles (in particular, with $\gamma_{1}=\gamma_{2}$ ) the problem is reduced to the previous one.

[^748]:    92 The anomalously large value of its $g$-factor may be qualitatively understood as a result of the three-quark structure of this particle. (The exact quantitative calculation of $g_{p}$ still remains a challenge for quantum chromodynamics.)
    ${ }^{93}$ Correct in the sense of the $1^{\text {st }}$ order of the perturbation theory.

[^749]:    ${ }^{1}$ Note that some material of this chapter is frequently taught as a part of the QFT. I will focus on a few most important results that may be obtained without starting heavy QFT engines.
    ${ }^{2}$ See, e.g., EM Chapter 9.
    ${ }^{3}$ By now this fact has been verified experimentally with an accuracy of at least $\sim 10^{-22} m_{e}-$ see S . Eidelman et al., Phys. Lett. B 592, 1 (2004).
    ${ }^{4}$ In the case of finite energy absorption in the walls, or in the wave propagation media (say, described by complex constants $\varepsilon$ and $\mu$ ), the system would not be energy-conserving (Hamiltonian), i.e. would interact with the dissipative environment. Specific cases of such interaction will be considered in Sections 2 and 3 below.
    ${ }^{5}$ See, e.g., EM Eq. (7.3), for the particular case $\varepsilon=\varepsilon_{0}, \mu=\mu_{0}, v^{2} \equiv 1 / \varepsilon \mu=1 / \varepsilon_{0} \mu_{0} \equiv c^{2}$.

[^750]:    ${ }^{6}$ See, e.g., various problems discussed in EM Chapter 7, especially in Sec. 7.9.
    ${ }^{7}$ See, e.g., EM Sec. 9.8, in particular, Eq. (9.225). I am using use SI units, with $\varepsilon_{0} \mu_{0} \equiv c^{-2}$; in the Gaussian units, coefficients $\varepsilon_{0}$ and $\mu_{0}$ disappear, but there is an additional common factor $1 / 4 \pi$ in the equation for energy. If we modify the normalization conditions accordingly, all the subsequent results look similar in any system of units.

[^751]:    ${ }^{8}$ See, e.g., EM Eq. (7.6).
    ${ }^{9}$ With different normalizations of functions $\mathbf{e}_{j}(\mathbf{r})$ and $\mathbf{b}_{j}(\mathbf{r})$, we could readily arrange any value of $m_{j}$, and the choice corresponding to $m_{j}=1$ is the best one just for the notation simplicity. Note also that I am using notation $q_{j}$ instead of $x_{j}$ for the generalized coordinate of the field oscillator, in order to emphasize the difference between the former variable, defined by Eq. (8), and one of the Cartesian coordinates, i.e. one of arguments of $c$-number functions $\mathbf{e}$ and $\mathbf{b}$.

[^752]:    ${ }^{10}$ It was predicted in 1948 by H. Casimir and D. Polder, and confirmed semi-quantitatively in experiments by M. Sparnaay, Nature 180, 334 (1957) and others. A decisive error bar reduction (to about $\sim 5 \%$ ), providing a quantitative confirmation of the Casimir formula (23), was achieved by S. Lamoreaux, Phys. Rev. Lett. 78, 5 (1997) and U. Mohideen and A. Roy, Phys. Rev. Lett. 81, 004549 (1998).

[^753]:    Casimir
    effect

[^754]:    ${ }^{11}$ For realistic metals, the reduction of $d$ below $\sim 1 \mu \mathrm{~m}$ causes significant deviations from this simple model, and hence from Eq. (23). The reason is that at the important frequencies $\omega \sim c / d$, the depth of field penetration into the metal (see, e.g., EM Secs. 2.1 and 6.2) becomes comparable with $d$, and a theory of the Casimir effect has to involve a certain model of field penetration. (It is curious that in-depth analyses of this problem, pioneered in 1956 by E. Lifshitz, have revealed a deep relation between the Casimir effect and the long-range London dispersion forces which were the subject of Problems 3.7, 5.10 and 6.8 - for a review see, e.g., either I. Dzhyaloshinskii et al., Sov. Phys. Uspekhi 4, 153 (1961), or K. Milton, The Casimir Effect, World Scientific, 2001.) Recent experiments in the $100 \mathrm{~nm}-2 \mu \mathrm{~m}$ range of distances $d$, with accuracy better than $1 \%$, allowed even to distinguish the difference between alternative approximate models of field penetration - see D. Garcia-Sanchez et al., Phys. Rev. Lett. 109, 027202 (2012).

[^755]:    ${ }^{12}$ As a reminder: this relation, with the single-particle expression $\mathbf{d}=q \mathbf{r}$, has already been used several times see, e.g., Eqs. (6.32) and (6.149). In contrast to the former of those cases, now we have to account for the quantum nature of the electromagnetic field $\boldsymbol{\varepsilon}$, so in Eq. (24) it is represented by the (vector) operator (16a).
    ${ }^{13}$ Please note that (as was promised) we have gradually slipped to the analysis of open, irreversible systems, with the detector(s) playing the role of a continuous-spectrum environment for the quantized electromagnetic field.
    ${ }^{14}$ In a multimode field, the modes are typically incoherent, so that the total transition rate may be calculated as the sum of the partial rates of each mode - as we will do for a certain case below.
    ${ }^{15}$ By the way, this expression shows that for the single-particle transitions from the ground state to $n^{\text {th }}$ Fock state, the absorption rate is indeed proportional to the oscillator strength $\left.f_{n} \equiv\left(2 m / \hbar^{2}\right)\left(E_{n}-E_{0}\right)|\langle n| x| 0\right\rangle\left.\right|^{2}$ of the transition, where $x$ is particle's coordinate in the direction of the external field. As was discussed in Chapter 5, the strengths obey the Thomas-Reiche-Kuhn sum rule $\Sigma_{n} f_{n}=1$.

[^756]:    ${ }^{16}$ This is essentially the same rotating wave approximation (RWA) which was already used in Sec. 6.3 - see the transition from Eq. (6.90) to the first of Eqs. (6.94).

[^757]:    ${ }^{17}$ It was pioneered as early as in the mid-1950s (i.e. before the advent of lasers!), by R. Hanbury Brown and R. Twiss. Their first experiment was also remarkable for the rather unusual light source they used - star Sirius! (It was a part of an attempt to improve astrophysics interferometry techniques.)
    ${ }^{18}$ The reader may be interested what is the first-order correlation function. It is usually defined as

    $$
    g^{(1)}(\tau) \equiv\left\langle\hat{\varepsilon}\left(\mathbf{r}_{1}, t\right) \hat{\varepsilon}^{\dagger}\left(\mathbf{r}_{2}, t-\tau\right)\right\rangle /\left[\left\langle\hat{\varepsilon}\left(\mathbf{r}_{1}, t\right) \hat{\varepsilon}^{\dagger}\left(\mathbf{r}_{1}, t\right)\right\rangle\left\langle\hat{\varepsilon}\left(\mathbf{r}_{2}, t\right) \hat{\varepsilon}^{\dagger}\left(\mathbf{r}_{2}, t\right)\right\rangle\right]^{1 / 2}
    $$

    In the single-mode case, and the rotating-wave approximation, the function is proportional to the $c$-number product $\mathbf{e}\left(\mathbf{r}_{1}\right) \mathbf{e}^{*}\left(\mathbf{r}_{2}\right)$, with all creation-annihilation operators cancelled, i.e. is suitable for characterizing interference patterns (30), but not the quantum state of the electromagnetic field.

[^758]:    ${ }^{19}$ H. J. Kimble et al., Phys. Rev. Lett. 39, 691 (1977). For a detailed review of phonon antibunching, see, e.g., H. Paul, Rev. Mod. Phys. 54, 1061 (1982).

[^759]:    ${ }^{20}$ For some field states, including the squeezed ground states $\xi$ discussed in the end of Sec. 5.5 , values $g^{(2)}(0)$ may be even higher than 2 - the so-called super-bunching. Analysis of one particular case of super-bunching is offered to the reader - see the exercise problem list.

[^760]:    ${ }^{21}$ Here I have smuggled back the sum over all electromagnetic field modes $j$ - see Eq. (16). Since in the quasistationary approximation, $k_{j} a \ll 1$, which is necessary for the interaction presentation by Eq. (24), matrix elements (49) are independent on $k_{j}$, the summation is reduced to the calculation of the total $\rho_{\text {fin }}$ for all modes.
    ${ }^{22}$ Note the essential dependence of Eq. (50), and hence of Eq. (53) on the field geometry; all following formulas of this section are valid for free 3D space only. If the same atom is place into a high- $Q$ resonant cavity (see, e.g., EM 7.9), the rate of its photon emission is strongly suppressed at frequencies between the cavity resonances (where $\rho_{\text {fin }} \rightarrow 0$ ) - see, e.g., the review of first experiments by S. Haroche and D. Klepner, Phys. Today 42, 24 (Jan. 1989). On the other hand, the emission is strongly (by a factor $\sim\left(\lambda^{3} / V\right) Q$, where $V$ is cavity's volume) enhanced at resonance frequencies - the so-called Purcell effect, discovered by E. Purcell already in the 1940s. For a brief discussion of these and other quantum effects in cavities, see the next section.
    ${ }^{23}$ An equivalent expression was first obtained in 1930 by V. Weisskopf and E. Wigner, so that the whole calculation is sometimes referred to as the Weisskopf-Wigner theory.
    ${ }^{24}$ See, e.g., EM Sec. 8.2, in particular Eq. (8.28).

[^761]:    ${ }^{25}$ The scale $c \tau$ of the spatial extension of the corresponding wave packet is surprisingly macroscopic - in the range of a few millimeters. Such "human" size of the emitted photons makes the optical table the key component of many optical experiments.
    ${ }^{26}$ As was already mentioned in Sec. 5.6, for a single particle moving in a spherically-symmetric potential (e.g., a hydrogen-like atom), the selection rules are simple: the only allowed electric-dipole transitions are those with $\Delta l \equiv$ $l_{\text {fin }} l_{\text {ini }}= \pm 1$ and $\Delta m \equiv m_{\text {fin }}-m_{\text {ini }}=0$. The simplest example of the transition that does not satisfy this rule is that between states with $n=2$ and $n=1$, both with $l=0$; because of that, the lifetime of the lowest excited $s$-state in hydrogen is as long as $\sim 0.15 \mathrm{~s}$.
    ${ }^{27}$ See, e.g., EM Sec. 8.9.

[^762]:    ${ }^{28}$ Relations (56) and (58) were conjectured, from very general arguments, by A. Einstein as early as in 1916.

[^763]:    ${ }^{29}$ It is straightforward to show that this fact is also true if the field is initially in the Glauber state - which is more typical for lasers.
    ${ }^{30}$ This idea has been traced back at least to an obscure 1939 publication by V. Fabrikant.
    ${ }^{31}$ I can recommend, for example, P. W. Milloni and J. H. Eberly, Laser Physics, ${ }^{\text {nd }}$ ed., Wiley, 2010, and a less technical text by A. Yariv, Quantum Electronics, 3rd ed., Wiley, 1989.
    ${ }^{32}$ This path has been developed (also in the mid-1960s), by several researchers, notably including M. Sully and W. Lamb - see, e.g., M. Sargent III, M. Scully, and W. Lamb, Jr., Laser Physics, Westview, 1977. Note that

[^764]:    ${ }^{38}$ The exact choice of this component is not important, while the formulas simplify if it is proportional to either pure $\sigma_{x}$ or pure $\sigma_{y}$.
    ${ }^{39}$ D. Braak, Phys. Rev. Lett. 107, 100401 (2011).

[^765]:    ${ }^{40}$ It was first proposed and analyzed in 1963 by two electronic engineers, E. Janes and F. Cummings, and it took the physics community a while to recognize and acknowledge the fundamental importance of that work.
    ${ }^{41}$ In most applications, Hamiltonian (78) is augmented by additional term(s) describing, for example, incoming radiation and/or coupling to environment, say due to the electromagnetic energy loss in the cavity walls - see Eq. (7.68).

[^766]:    ${ }^{42}$ Besides the non-degenerate ground state level $E_{g}=-\hbar \Omega / 2$.

[^767]:    ${ }^{43}$ Another important corollary of the level structure shown in Fig. 5 is the Purcell effect already mentioned in Sec. 3. As we already know from Chapter 7, if the system is coupled to environment, the coupling suppresses its quantum coherence, in our case the coherence between components of each pair (82). As a result, if the atom is initially in state $\uparrow$ with higher energy (79), it may perform incoherent (dissipative) transition to the lower-energy state $\downarrow$, giving energy $\hbar \omega$ to the cavity $(n-1 \rightarrow n)$, which rapidly drains it into the environment. Since the total energies of these initial and final states are close (Fig. 5), the rate of such transitions may be much higher than in free space. The quantitative analysis of such enhancement is left for reader's exercise.
    ${ }^{44}$ I can recommend, for example, either C. Gerry and P. Knight, Introductory Quantum Optics, Cambridge U. Press, 2005' or G. Agarwal, Quantum Optics, Cambridge U. Press, 2012.
    ${ }^{45}$ This approach was suggested almost simultaneously in 1926-1927 by (at least) V. Fock, E. Schrödinger, O. Klein and W. Gordon, J. Kudar, T. de Donder and F.-H. van der Dungen, and L. de Broglie.
    ${ }^{46}$ Note that in the sense of Eq. (1), in the non-relativistic column of this table, the energy is referred to the rest energy $m c^{2}$, while in the relativistic column, to zero.

[^768]:    ${ }^{47}$ Due to the same P. A. M. Dirac!

[^769]:    ${ }^{48}$ After such generalization, Eq. (84) is usually called the relativistic Schrödinger equation.
    ${ }^{49}$ The task left for the reader.

[^770]:    ${ }^{50}$ After the "naturally-relativistic" form of the Klein-Gordon equation (84), this apparent return to the nonrelativistic Schrödinger equation may look very counter-intuitive. However, it becomes a bit less surprising taking into account the fact (whose proof is left for the reader) that Eq. (84) may be also recast into form (95) for a twocomponent column-vector (spinor) $\Psi$, with a Hamiltonian which may be represented by a $2 \times 2$ matrix - and hence expressed via the Pauli matrices (4.

[^771]:    ${ }^{52}$ It is straightforward to show that this result remains valid for a particle in the field of central potential $U(\mathbf{r})$.
    ${ }^{53}$ See, e.g., A. Calogeracos and N. Dombey, Contemp. Phys. 40, 313 (1999).
    ${ }^{54}$ For a review see, e.g., T. Robinson, Am. J. Phys. 80, 141 (2012).

[^772]:    ${ }^{55}$ This difference may be traced even by classical means - see, e.g., EM Sec. 5.1.
    ${ }^{56}$ With the $g$-factor still equal to exactly 2 - see Eq. (4.116) and its discussion. In order to describe the small deviation of $g_{e}$ from 2, the electromagnetic field should be quantized (just as this was done in Secs. 1-4), and its potentials $\mathbf{A}$ and $\phi$, participating in Eq. (112) should be treated as operators - rather than as $c$-number functions as was assumed above. The calculation of this deviation is one of the basic problems of quantum field theory. Other small but important effects of electromagnetic interactions, described by the theory, include the so-called Lamb shift of atomic levels - see the end of this chapter for references.

[^773]:    ${ }^{57}$ The only facts immediately evident from Eq. (121) are that the term we are discussing is proportional to the electric field, as required by Eq. (122), and that it is of the proper order of magnitude. Indeed, Eqs. (101)-(102) imply that in the Dirac theory, $c \hat{\boldsymbol{\alpha}}$ plays the role of the velocity operator, so that the expectation values of the term are of the order of $\hbar q v \varepsilon / 2 m c^{2}$. Since the expectation values of the operators participating in Hamiltonian (122) scale as $S \sim \hbar / 2$ and $L \sim m v r$, the spin-orbit interaction energy has the same order of magnitude.
    ${ }^{58}$ As a reminder, in this course the notion of spinor was introduced earlier for two-particle states - see Eq. (8.14). For a single particle, that definition is reduced to $\psi(\mathbf{r})|s\rangle$, whose representation in a particular spin- $1 / 2$ basis is a column similar to Eq. (123). Also note that spinors (123) may be expanded into a series over the spin-orbitals (8.117) discussed in Sec. 8.3, with index $j$ used for numbering both the two directions of spin (i.e. two components of spinor's column) and orbital eigenfunctions.

[^774]:    ${ }^{59}$ Strictly speaking, this requirement is imposed on the expectation values of $U(\mathbf{r})$ in the eigenstates to be found.

[^775]:    ${ }^{60}$ The first term gives a small, spin-independent shift of the energy spectrum, which is very difficult to verify experimentally.
    ${ }^{61}$ Good descriptions of the solution are available in many textbooks (the older the better :-), for example see Sec. 53 in L. Schiff, Quantum Mechanics, $3^{\text {rd }}$ ed., McGraw-Hill (1968).

[^776]:    ${ }^{62}$ For a gradual introduction see, e.g., either L. Brown, Quantum Field Theory, Cambridge U. Press (1994) or R. Klauber, Student Friendly Quantum Field Theory, Sandtrove (2013); on the other hand, M. Srednicki, Quantum Field Theory, Cambridge U. Press (2007) and A. Zee, Quantum Field Theory in a Nutshell, $2^{\text {nd }}$ ed., Princeton (2010), among many others, offer a steeper learning curve.
    ${ }^{63}$ See, e.g., MA Eq. (2.12).

[^777]:    ${ }^{64}$ Here $\psi$ is a function of both $\mathbf{r}$ and $t$, and the lower-case letter is used only to distinguish this two-component spinor from the scalar function $\Psi(\mathbf{r}, t)$ obeying the Klein-Gordon equation.

[^778]:    ${ }^{65}$ Actually, the key relation (3.192), $n \geq l+1$, mathematically stems from the fact that the "genuine" quantum number of the radial problem, $n_{r}$, can only take non-negative integer values.

[^779]:    ${ }^{1}$ I believe that another popular name for this group of issues, "foundations of quantum mechanics", is hardly appropriate. The only reliable foundation of physics (or any other genuine scientific discipline) is a set of experimental facts.
    ${ }^{2}$ As was discussed in Sec. 7.7, Stern-Gerlach-type experiments may be readily made almost "perfect", i.e. virtually unaffected by instrument imperfections, provided that we do not care about the state of the particle after a single-shot measurement.

[^780]:    ${ }^{3}$ This is possible, because the corresponding operators commute: $\left[\hat{p}_{1}-\hat{p}_{2}, \hat{x}_{1}+\hat{x}_{2}\right]=\left[\hat{p}_{1}, \hat{x}_{1}\right]-\left[\hat{p}_{2}, \hat{x}_{2}\right]=0$.
    ${ }^{4}$ Another convenient experimental technique of entangled state generation, frequently used in this field, is the four-wave mixing (FWM) of optical photons. Its brief discussion may be found, for example, in CM Sec. 5.5. ${ }^{5}$ As a reminder, it differs from Eq. (1) only by the sign in the parentheses - see, e.g., Eqs. (4.123).

[^781]:    ${ }^{6}$ In his pioneering book J. von Neumann, Mathematische Grundlagen der Quantenmechanik [Mathematical Foundations of Quantum Mechanics], Springer, 1932. (The first English translation was published only in 1955.)
    ${ }^{7}$ Evidently, it would not satisfy A. Einstein, but reportedly he did not know about von Neumann's result before signing the EPR paper.
    ${ }^{8}$ See, e. g., J. S. Bell, Rev. Mod. Phys. 38, 447 (1966), or J. S. Bell, Foundations of Physics 12, 158 (1982).

[^782]:    ${ }^{9}$ Important milestones on that way were experiments by A. Aspect et al., Phys. Rev. Lett. 49, 91 (1982) and M. Rowe et al., Nature 409, 791 (2001). A detailed review of the experimental situation was given, for example, by M. Genovese, Phys. Repts. 413, 319 (2005); see also more recent experiments by D. Matsukevich et al., Phys. Rev. Lett. 100, 150404 (2008) and D. Salart et al., Nature 454, 861 (2008). Presently, a low-noise demonstration of the Bell inequality violation has become a standard test in each experiment with entangled qubits used for quantum encryption research - see Sec. 8.5.

[^783]:    ${ }^{10}$ A detailed discussion of statistical ensemble's role may be found, e.g., in L. Balentine, Quantum Mechanics, World Scientific, 1998.
    ${ }^{11}$ D. Bohm, Phys. Rev. 85, 165; 180 (1952).
    ${ }^{12}$ If the reader is not satisfied with this "positivistic" approach, and wants to improve the situation, my earnest advice would be to start not from square one, but from reading what other (including some very clever!) people thought about it. A good starting point is the review collection by J. Wheeler and W. Zurek (eds.), Quantum Theory and Measurement, Princeton U. Press, 1983.

[^784]:    ${ }^{1}$ For remedial reading, I can recommend, for example (in the alphabetical order): C. Kittel and H. Kroemer, Thermal Physics, $2^{\text {nd }}$ ed., W. H. Freeman (1980); F. Reif, Fundamentals of Statistical and Thermal Physics, Waveland (2008); D. V. Schroeder, Introduction to Thermal Physics, Addison Wesley (1999).
    ${ }^{2}$ See, e.g., Sec. 4 below. (Note that in these notes, the chapter number is dropped in references to figures, formulas, and sections within the same chapter.)
    ${ }^{3}$ See, e.g., CM Chapters 8 and 9. (Acronyms CM, EM, and QM refer to other of my lecture note series.)
    ${ }^{4}$ See, e.g., QM Chapter 1.

[^785]:    ${ }^{5}$ See, e.g., CM Chapters 2 and 10.

[^786]:    ${ }^{6}$ The notion of entropy was introduced into thermodynamics in the 1850s by R. Clausius, on the background of an earlier pioneering work by S. Carnot (see Sec. 7 below), as a variable related to "useful thermal energy" rather than a measure of disorder. In the absence of any clue of entropy's microscopic origins (which had to wait for decades until the works by L. Boltzmann and J. Maxwell), this was an amazing intellectual achievement.
    ${ }^{7}$ Indeed, as recently as in the late XIX century, the very possibility of irreversible macroscopic behavior of microscopically reversible systems was questioned by some serious scientists, notably by J. Loschmidt in 1876.
    ${ }^{8}$ While quantum-mechanical effects, with their intrinsic uncertainty, are quantitatively important in this example, our qualitative discussion does not depend on them. A good example is the chaotic, but classical motion of a billiard ball on a 2D Sinai table - see CM Fig. 9.8.

[^787]:    ${ }^{9}$ Several other quantities, for example the heat capacity $C$, may be obtained as partial derivatives of the basic variables discussed above. Also, at certain conditions, the number of particles $N$ in the system is not fixed and may be also considered as an (extensive) variable.
    ${ }^{10}$ Admittedly, some of these proofs are based on other (but deeper) postulates, for example the central statistical hypothesis - see Sec. 2.2.
    ${ }^{11}$ Defined as a system completely isolated from the environment, i.e. the system with its internal energy fixed.
    ${ }^{12}$ Implicitly, this statement also postulates the existence, in a closed system, of thermodynamic equilibrium, an asymptotically reached state in which all thermodynamic variables, including entropy, remain constant.

[^788]:    ${ }^{13}$ Here we strongly depend on a very important (and possibly the least intuitive) aspect of the $2^{\text {nd }}$ law, namely that the entropy is the unique measure of disorder, i.e. its only measure which may affect the system's energy, or any other thermodynamic variable.

[^789]:    ${ }^{14}$ Here I have to mention a traditional unit of energy, still used in some fields related to thermodynamics: the calorie; in the most common definition (the so-called thermochemical calorie) it equals exactly 4.148 J .
    ${ }^{15}$ For more exact value of this and other constants, see appendix CA: Selected Physical Constants. Note that both $T$ and $T_{\mathrm{K}}$ define the absolute (also called "thermodynamic") scale of temperature, in contrast to such artificial temperature scales as degrees Celsius ("centigrades"), defined as $T_{\mathrm{C}} \equiv T_{\mathrm{K}}+273.15$, or degrees Fahrenheit: $T_{\mathrm{F}} \equiv$ $(9 / 5) T_{\mathrm{C}}+32$.

[^790]:    ${ }^{16}$ A general (not necessarily adiabatic) process conserving entropy is sometimes called isentropic.

[^791]:    Energy:
    differential

[^792]:    $1^{\text {st }}$ law of thermodynamics

[^793]:    ${ }^{17}$ Let me emphasize that an adiabatic process is reversible, but not vice versa.
    ${ }^{18}$ Such conservation, expressed by Eqs. (18)-(19), is sometimes called the $1^{\text {st }}$ law of thermodynamics. While it (in contrast with the $2^{\text {nd }}$ law) does not present any new law of nature on the top of mechanics, and in particular was already used de-facto to write the first of Eqs. (5) and Eq. (14), such grand name was quite justified in the mid$19^{\text {th }}$ century when the mechanical nature of the internal energy (thermal motion) was not at all clear. In this context, the names of two great scientists, J. von Mayer (who was first to conjecture the conservation of the sum of the thermal and macroscopic mechanical energies in 1841), and J. Joule (who proved the conservation experimentally two years later), have to be reverently mentioned.
    ${ }^{19}$ Actually, the $3^{\text {rd }}$ law (also called the Nernst theorem) as postulated by W. Nernst in 1912 was different - and really meaningful: "It is impossible for any procedure to lead to the isotherm $T=0$ in a finite number of steps." I will discuss this postulate in the end of Sec. 6.
    ${ }^{20}$ By this definition, the full heat capacity of a system is an extensive variable. The capacity per either unit mass or per particle (i.e., an intensive variable), is called the specific heat capacity or just the specific heat. Note, however, that in some texts, the last term is used for the heat capacity of the system as the whole as well, so that some caution is in order.

[^794]:    ${ }^{21}$ A similar duality is possible for other pairs $\left\{q_{j}, Z_{j}\right\}$ of generalized coordinates and forces as well. For example, if a long sample of a dielectric placed is into a parallel, uniform external electric field, value of field $\varepsilon$ is fixed, i.e. does not depend on sample's polarization. However, if a thin sheet of such material is perpendicular to the field, then value of field $D$ is fixed - see, e.g., EM Sec. 3.4.
    ${ }^{22}$ The same is true for work $\mathcal{W}$, and in some textbooks this fact is emphasized by using a special sign for differentials of these variables. I do not do this in my notes, because both $d w$ and $d Q$ are still very much usual differentials: for example, $d w$ is the difference between the mechanical work which has been done over our system by the end of the infinitesimal interval we are considering, and that done by the beginning of that interval.

[^795]:    ${ }^{23}$ From the point of view of mathematics, Eq. (27) is a particular case of the so-called Legendre transformations. Note also that the term $P V$ has a purely mechanical meaning, and that the transfer from $H$ to $E$ just reflects the transfer from the "usual" potential energy of the system to its Gibbs potential energy - see, e.g., CM Sec. 1.4. ${ }^{24}$ This function (as well as the Gibbs free energy G, see below), had been introduced in 1875 by J. Gibbs, though the term "enthalpy" was coined (much later) by H. Onnes.

[^796]:    ${ }^{25}$ Named after H. von Helmholtz (1821-1894). The last term was recommended by the most recent (1988) IUPAC's decision, but I will use the first term, which prevails is physics literature. The origin of the adjective "free" stems from Eq. (32): $F$ is may be interpreted as the internal energy's part that is "free" to be transferred to mechanical work - at a reversible, isothermal process only!

[^797]:    ${ }^{26}$ Note the similarity of this situation with that is analytical (classical) mechanics (see, e.g., CM Chapters 2 and 10): the Lagrangian function may be used to get simple equations of motion if it is expressed as a function of generalized coordinates and velocities, while is order to use the Hamiltonian function in a similar way, it has to be expressed as a function of the generalized coordinates and momenta.

[^798]:    ${ }^{27}$ There is also a wealth of other relations between thermodynamic variables that may be presented as second derivatives of the thermodynamic potentials, including four Maxwell relations such as $(\partial S / \partial V)_{T}=(\partial P / \partial T)_{V}$, etc. (They may be readily recovered from the well-known property of a function of two independent arguments, say, $f(x, y): \partial(\partial f / \partial x) / \partial y=\partial(\partial f / \partial y) / \partial x$.) In this chapter, I will list only the thermodynamic relations that will be used later in the course; a more complete list may found, e.g., in Sec. 16 of the textbook by L. Landau and E. Lifshitz, Statistical Physics, Part 1, $3^{\text {rd }}$ ed., Pergamon, 1980 (and later its re-printings).

[^799]:    ${ }^{28}$ See, e.g., CM Sec. 1.5.
    ${ }^{29}$ There are a few practical systems, notably including the so-called magnetic refrigerators (to be discussed in Chapter 4), when the natural growth of $S$ is so slow that the condition $S=$ const may be closely approached.
    ${ }^{30}$ This equation was first derived from experimental data by E. Clapeyron (in 1834) in the form $P V=n R T_{\mathrm{K}}$, where $n$ is the number of moles in the gas sample, and $R \approx 8.31 \mathrm{~J} / \mathrm{mole} \cdot \mathrm{K}$ is the so-called gas constant. This form is equivalent to Eq. (44), taking into account that $R=k_{\mathrm{B}} N_{\mathrm{A}}$, where $N_{\mathrm{A}} \approx 6.02 \times 10^{23} \mathrm{~mole}^{-1}$ is the so-called Avogadro number, i.e. the number of molecules per mole. (By definition of the mole, $N_{\mathrm{A}}$ is just the reciprocal mass, in grams, of a baryon - more exactly, by convention, of a $1 / 12^{\text {th }}$ part of the carbon- 12 atom.)

[^800]:    ${ }^{31}$ Note, however, that the difference $C_{P}-C_{V}=N$ (if temperature is measured in kelvins, $C_{P}-C_{V}=n R$ ) is independent of $f(T)$. (It is possible to show that the difference $C_{P}-C_{V}$ is fully determined by the equation of state for any medium.)

[^801]:    ${ }^{32}$ This name, of a historic origin, is a bit misleading: as evident from Eq. (52), $\mu$ has a clear physical sense of the average energy cost of adding one more particle to the system of $N \gg 1$ particles.
    ${ }^{33}$ Note that strictly speaking, Eqs. (9), (15), (31), (35) and (39) should be now generalized by adding one more lower index, $N$, to the corresponding derivatives.

[^802]:    ${ }^{34}$ Note that positive sign of the circular integral corresponds to the clockwise rotation of the point, so that work ($w$ done by the working gas is positive at the clockwise rotation (pertinent to heat engines) and negative in the opposite case (implemented in refrigerators and heat pumps).
    ${ }^{35}$ A cycle with an $[S, T]$ shape very close to the Carnot (rectangular) one may be implemented at the already mentioned magnetic (or "adiabatic-demagnetization") refrigeration, using the alignment of either atomic or

[^803]:    ${ }^{36}$ Such a hypothetical (and impossible!) heat engine, which would violate the $2^{\text {nd }}$ law of thermodynamics, is called the "perpetual motion machine of the $2^{\text {nd }}$ kind" - in contrast to the "perpetual motion machine of the $1^{\text {st }}$ kind" with would violate the $1^{\text {st }}$ law, i.e., the energy conservation.

[^804]:    ${ }^{37}$ For a detailed discussion of this issue see, e.g., J. Wilks, The Third Law of Thermodynamics, Oxford U. Press, 1961.

[^805]:    ${ }^{38}$ This name stems from the fact that the cycle is an approximate model of operation of the four-stroke internalcombustion engine, which was improved and made practicable (though not invented!) by N. Otto in 1876.

[^806]:    ${ }^{1}$ For the reader interested in reviewing a more rigorous approach, I can recommend, for example, Chapter 18 of the handbook by G. Korn and T. Korn - see MA Sec. 16(ii).

[^807]:    ${ }^{2}$ The most popular counter-example of a non-ergodic system is an energy-conserving system of particles placed in a potential which is a quadratic form of particle coordinates. Theory of oscillations tells us (see, e.g., CM Sec. 5.2) that this system is equivalent to a set of non-interacting harmonic oscillators. Each of these oscillators conserves its own initial energy $E_{j}$ forever, so that the statistics of $N$ measurements of one such system may differ from that of $N$ different systems with random distribution of $E_{j}$, even if the total energy of the system, $E=\Sigma_{j} E_{j}$, is the same. Such non-ergodicity, however, is a rather feeble phenomenon, and is readily destroyed by any of "mixing" mechanisms, such as weak interaction with environment (leading, in particular, to oscillation damping), nonlinear interaction of the components (see, e.g., CM Ch. 4), and chaos (CM Ch. 9), all of them strongly enhanced by increasing the number of particles in the system, i.e. the number of its degrees of freedom. This is why most real-life systems are ergodic; for those interested in non-ergodic exotics, I can recommend the monograph by V. Arnold and A. Avez, Ergodic Problems of Classical Mechanics, Addison-Wesley, 1989.
    ${ }^{3}$ Here, and everywhere in these notes, angle brackets $\langle\ldots\rangle$ mean averaging over a statistical ensemble, which is generally different from averaging over time - as it will be the case in quite a few examples considered below.

[^808]:    ${ }^{4}$ See, e.g., QM Sec. 7.1.

[^809]:    ${ }^{5}$ Here I use the Schrödinger picture of quantum mechanics in which the matrix elements $f_{n n}$, do not evolve in time.

[^810]:    ${ }^{6}$ The terms "microcanonical", as well as "canonical" (see Sec. 4 below) are apparently due to J. Gibbs, and I could not find out his motivation for these names. ("Canonical" in the sense of "standard" or "common" is quite appropriate, but why "micro"?)
    ${ }^{7}$ Formally, the main result of this section, Eq. (20), is valid for any $M$ (including $M=1$ ), it is just less informative for small $M$ - and trivial for $M=1$.
    ${ }^{8}$ Though I have to move on, let me note that the microcanonical distribution (20) is a very nontrivial postulate, and my advice to the reader to give some thought to this foundation of the whole building of statistical mechanics.

[^811]:    ${ }^{9}$ I will rely on reader's common sense and intuitive understanding what information is, because in the formal information theory this notion is also essentially postulated - - see, e.g., the wonderfully clear text by J. Pierce, An Introduction to Information Theory, Dover, 1980.
    ${ }^{10}$ This is of course just the change of a constant factor: $S(M)=\ln M=\ln 2 \times \log _{2} M=\ln 2 \times I(M) \approx 0.693 I(M)$. A review of Chapter 1 shows that nothing in thermodynamics prevents us from choosing such coefficient arbitrarily, with the corresponding change of the temperature scale - see Eq. (1.9). In particular, in the SI units, Eq. (24b) becomes $S=-k_{\mathrm{B}} \ln W_{m}$, so that one bit of information corresponds to the entropy change $\Delta S=k_{\mathrm{B}} \ln 2 \approx 0.693 k_{\mathrm{B}} \approx$ $0.965 \times 10^{-23} \mathrm{~J} / \mathrm{K}$. By the way, formula " $S=k \log W$ " is engraved on the tombstone of L. Boltzmann (1844-1906) who was the first one to recognize this intimate connection between the entropy and probability.

[^812]:    ${ }^{11}$ See, e.g., MA Eq. (2.3). Despite the intimidating name, Eq. (26) may be very simply derived. Indeed, $N$ ! is just the number of all possible permutations of $N$ balls, i.e. the ways to place them in certain positions - say, inside $M$ boxes. Now in order to take into account that the particular order of the balls in each box is not important, that number should be divided by all numbers $N_{n}$ ! of possible permutations of balls within each box - that's it.
    ${ }^{12}$ See, e.g., MA Eq. (2.10).

[^813]:    ${ }^{13}$ Strictly speaking, I should use notation $\langle S\rangle$ here. However, following the style accepted in thermodynamics, I will drop the averaging sign until we will really need them to avoid confusion. Again, this shorthand is not too bad because the relative fluctuations of entropy (as those of any macroscopic variable) are very small at $N \gg 1$.
    ${ }^{14}$ With the replacement of $\ln W_{m}$ for $\log _{2} W_{m}$ (i.e. division by $\ln 2$ ), Eq. (29) is the famous Shannon (or "Boltzmann-Shannon") formula for average information $I$ per symbol in a long communication string using $M$ different symbols, with probability $W_{m}$ each.
    ${ }^{15}$ In some textbooks, this simple argument is even accepted as the derivation of Eq. (29); however, it is evidently less strict than the one outlined above.

[^814]:    ${ }^{16}$ This is not to say that these definitions are fully equivalent. Despite all the wealth of quantitative relations given by thermodynamics, it still leaves a substantial uncertainty in the definition of entropy (and hence temperature), while Eq. (24) narrows this uncertainty to an unsubstantial constant.
    ${ }^{17}$ See, e.g., QM Secs. 2.10 and 5.4.

[^815]:    ${ }^{18}$ Let me hope that the reader knows that the zero-point energy is experimentally measurable - for example using the famous Casimir effect - see, e.g., QM Sec. 9.1. In Sec. 5.6 below we will discuss another method of experimental observation of that energy.

[^816]:    ${ }^{19}$ Let me offer a very vivid example how slowly does the logarithm function grow at large values of its argument: $\ln$ of the number of atoms in the visible Universe is less than 200.
    ${ }^{20}$ By the same reason, the notion of pressure $P$ in such a system is not clearly defined, and neither are any thermodynamic potentials but $E$ and $F$.
    ${ }^{21}$ Let me hope that using the same letter for the mass and the state number would not lead to reader's confusion. I believe that the difference between these uses is very clear from the context.

[^817]:    ${ }^{22}$ Note again that though we have committed the energy $E_{N}$ of $N$ oscillators to be fixed (in order to apply Eq. (36), valid only for a microcanonical ensemble at thermodynamic equilibrium), single oscillator's energy $E$ in our analysis may be arbitrary - within limits $\hbar \omega \ll E<E_{N} \sim N T$.
    ${ }^{23}$ As a reminder, the Hamiltonian of any system whose classical Lagrangian function is an arbitrary quadratic form its generalized coordinates and the corresponding generalized velocities, may be brought to form (49) by an appropriate choice of "normal coordinates" $q_{j}$ which are certain linear combinations of the original coordinates see, e.g., CM Sec. 5.2.
    ${ }^{24}$ This also means that in the classical limit, the heat capacity of a system is equal to one half the number of its half-degrees of freedom (in SI units, multiplied by $k_{\mathrm{B}}$ ).
    ${ }^{25}$ The reader is strongly urged to solve Exercise 2, whose task is to do a similar calculation for another key ("twolevel") physical system, and to compare the results.

[^818]:    ${ }^{26}$ See, e.g., CM Chapter 9 and literature therein.
    ${ }^{27}$ For the definition of $\lambda$, see, e.g., CM Eq. (9.9).
    ${ }^{28}$ For more discussion, see, e.g., either Sec. 6.2 of the monograph H. G. Schuster and W. Just, Deterministic Chaos, $4^{\text {th }}$ ed., Wiley-VHS, 2005, or the monograph by Arnold and Avez, cited in Sec. 1.
    ${ }^{29}$ While some of these concerns should be treated with due respect (because the ideas of entropy and disorder are indeed highly nontrivial), I have repeatedly run into rather shallow arguments which stemmed from arrogant contempt to the information theory as an "engineering discipline", and unwillingness to accept the notion of information on the equal footing with those of space, time, and energy. Fortunately, most leading physicists are much more flexible, and there are even opposite extremes such as J. A. Wheeler's "it from bit" (i.e. matter from information) philosophy - to which I cannot fully subscribe either.

[^819]:    ${ }^{30}$ This procedure of redefining the statistical ensemble is the central point of the connection between the information theory and physics, and is crucial in particular for any (meaningful :-) discussion of measurements in quantum mechanics - see, e.g., QM Secs. 2.5 and 7.7.

[^820]:    ${ }^{31}$ In the dominating CMOS technology, $\Delta E$ is close to twice the energy $C V^{2} / 2$ of recharging the total capacitance $C$ of the transistor gate electrodes and the wires interconnecting the gates, by the voltage $V$ representing the binary unity. As the technology progresses, $C$ decreases in approximate proportion with the minimum feature size, resulting in the almost proportional decrease of $\Delta E$. (The used voltage $V$ has almost saturated at $\sim 1 \mathrm{~V}-$ the value that stems from the bandgap of $\sim 1 \mathrm{eV}$ of the used semiconductor - silicon.)
    ${ }^{32}$ Unfortunately, this delusion has resulted in a substantial and unjustified shift of electron device research resources toward using "non-charge degrees of freedom" (such as spin) - as if they do not obey the general laws of statistical physics!

[^821]:    ${ }^{33}$ C. Bennett, IBM J. Res. Devel. 17, 525 (1973); see also a later review C. Bennett, Int. J. Theor. Phys. 21, 905 (1982). To the best of my knowledge, the sub- $7 \ln 2$ energy loss per logic step is still to be demonstrated experimentally, but at least one research team is closing at this goal.
    ${ }^{34}$ Reversible computation may also overcome the perceived "fundamental quantum limit", $\Delta E \Delta t>\hbar$, where $\Delta t$ is the time scale of the binary logic operation - see K. Likharev, Int. J. Theor. Phys. 21, 311 (1982).
    ${ }^{35}$ The situation is rather different for quantum computation which may be considered as a specific type of reversible but analog computation - see, e.g., QM Sec. 8.5 and references therein.

[^822]:    ${ }^{36}$ See also exercise problems listed in the end of this chapter.

[^823]:    ${ }^{37}$ Another way to arrive at the same conclusion is to note that the entropy of the canonical ensemble with fixed $E_{m}$ has to be a sum of entropies of its microcanonical sub-ensembles (with different $E_{\Sigma}$ ), which participate in Eq. (55). As a result, the logarithm of the probability $W_{m}$ for our system of interest to have energy $E_{m}$ in the whole (canonical) ensemble is just a sum of Eqs. (57) for sub-ensembles with different $E_{\Sigma}$.
    ${ }^{38}$ The temperature dependence of the type $\exp \{-E / T\}$, especially when showing up in rates of certain events, e.g., chemical reactions, is also frequently called the Arrhenius law - after chemist S. Arrhenius who has noticed this

[^824]:    law in experimental data. In all cases I am aware of, the Gibbs distribution is the underlying reason of the Arrhenius law.
    ${ }^{39}$ This opinion is shared by several authoritative colleagues, including R. Feynman who climbs on this summit already by page 4 (!) of his brilliant book Statistical Mechanics, $2^{\text {nd }}$ ed., Westview, 1998. (Despite its title, this monograph a collection of lectures on a few diverse, mostly advanced topics of statistical physics, rather than its systematic course, so that unfortunately I cannot recommend it as a textbook.)

[^825]:    ${ }^{40}$ In many multiparticle systems, the effect of an external field may be presented as a sum of its effects on each particle - frequently described by interaction energy with structure $-\mathcal{F}_{j} q_{j}^{(k)}$, where $q_{j}^{(k)}$ is a generalized coordinate of $k$-th particle. Generally, this energy has to be included directly into energies of particle states $E_{m}$, used in $Z$, and hence in the free energy $F$ (63). In this case, the thermodynamic equilibrium corresponds to the minimum of $F-$ see Eq. (1.42). On the other hand, for "linear" systems (whose energy is a quadratic-homogeneous form of its generalized coordinates and velocities), equivalent results may be obtained by accounting for the interaction at the thermodynamic level, i.e. by subtracting term $\mathcal{F}_{j}\left\langle q_{j}\right\rangle=\mathcal{F}_{j} N\left\langle q_{j}{ }^{(k)}\right\rangle$ from the free energy $F$ calculated in the absence of the field, and then finding the equilibrium as a minimum of the resulting Gibbs energy $G$ - see Eq. (1.43). In this case, any of the approaches is fine, provided only that the same interaction is not counted twice.
    ${ }^{41}$ A simpler task of making a similar calculation for another key quantum-mechanical object, the two-level system, is left for reader's exercise.

[^826]:    ${ }^{42}$ See, e.g., MA Eq. (2.8b).

[^827]:    ${ }^{43}$ It was first obtained in 1924 by S. Bose, and is frequently called the Bose distribution - a particular case of the Bose-Einstein distribution - to be discussed in Sec. 8 below.

[^828]:    ${ }^{44}$ See, e.g., QM Sec. 2.10.
    ${ }^{45}$ The calculation may be found, e.g., in QM Sec. 7.2.
    ${ }^{46}$ As a quantum mechanics reminder, the ground state energy of the oscillator is not only measurable, but is also responsible for several important phenomena, e.g., the Casimir effect - see, e.g., QM Sec. 9.1.

[^829]:    ${ }^{47}$ See, e.g., EM Sec. 7.9.
    ${ }^{48}$ See, e.g., QM Sec. 9.1.
    ${ }^{49}$ In our current context, the volume should be much larger than $(c \hbar / T)^{3}$, where $c \approx 3 \times 10^{8} \mathrm{~m} / \mathrm{s}$ is the speed of light. For room temperature ( $T \approx k_{\mathrm{B}} \times 300 \mathrm{~K} \approx 4 \times 10^{-21} \mathrm{~J}$ ), that lower bound is of the order of $10^{-16} \mathrm{~m}^{3}$.
    ${ }^{50}$ See, e.g., EM Sec. 7.9, or QM Sec. 1.6.
    ${ }^{51}$ Let me hope the reader knows that the law was first suggested in 1900 by M. Planck as an empirical fit for the experimental data on blackbody radiation, and this was the historic point at which the Planck constant $\hbar$ (or rather $h \equiv 2 \pi \hbar)$ was introduced - see, e.g., QM Sec. 1.1.

[^830]:    ${ }^{52}$ For a recent popular book of this topic, see, e.g., S. Singh, Big Bang: The Origins of the Universe, HarperCollins, 2005.

[^831]:    ${ }^{53}$ Note that the heat capacity $C_{V} \equiv(\partial E / \partial T)_{V}$, following from Eq. (88), is proportional to $T^{3}$ at any temperature, and hence does not obey the trend $C_{V} \rightarrow$ const at $T \rightarrow \infty$. This is the result of the unlimited growth, with temperature, of the number of thermally-exited field oscillators with $\hbar \omega<T$.
    ${ }^{54}$ See, e.g., MA Eqs. (6.8b), (6.6b), and (2.7b).

[^832]:    ${ }^{55}$ See, e.g., EM Sec. 9.8.
    ${ }^{56}$ Please note that according to Eqs. (1.44), (88), and (92), the difference between the equations of state of the photon gas and an ideal gas of non-relativistic particles, expressed in the more usual form - as $P=P(V, T)$, is much more dramatic: $P \propto T^{4} V^{0}$ instead of $P \propto T^{1} V^{1}$.

[^833]:    ${ }^{57}$ Due to low temperature expansion of solids, the difference between their $C_{V}$ and $C_{P}$ is small.
    ${ }^{58}$ In good conductors (e.g., metals), specific heat is contributed (and at low temperatures, dominated) by free electrons - see Sec. 3.3 below.
    ${ }^{59}$ See, e.g., CM Sec. 7.7.
    ${ }^{60}$ See, e.g., CM Sec. 5.3, in particular Fig. 5.5 and its discussion.

[^834]:    ${ }^{61}$ In SI units, Debye temperatures $T_{D}$ are of the order of a few hundred K for most simple solids (e.g., close to 430 K for aluminum and 340 K for copper), with somewhat lower values for crystals with heavy atoms ( $\sim 105 \mathrm{~K}$ for lead), and reach the highest value $\sim 2200 \mathrm{~K}$ for diamond with its relatively light atoms and very stiff lattice.

[^835]:    ${ }^{62}$ This is why there is a general "rule of thumb" in science: if you plot your data on a linear rather than log scale, you better have a good excuse ready. (A valid excuse example: the variable you are plotting changes sign within the important range.)
    ${ }^{63}$ This is the exact solution of a particular 1D model of such a crystal - see CM Chapter 5.
    ${ }^{64}$ This term stems from the fact that at $k \rightarrow 0$, the mechanical waves corresponding to these branches have phase velocities $v_{\mathrm{ph}} \equiv \omega(k) / k$ that are much higher than that of the acoustic waves, and may approach the speed of light. As a result, these waves can strongly interact with electromagnetic (practically, optical) waves of the same frequency, while the acoustic waves cannot.

[^836]:    ${ }^{65}$ The additional index in the new notation $E_{m, N}$ for the energy of the system of interest reflects the fact that its eigenvalue spectrum is generally dependent on the number $N$ of particles in it.

[^837]:    ${ }^{66}$ The average number of particles $\langle N\rangle$ is of course exactly what was called $N$ in thermodynamics (see Ch. 1), but I need to keep this explicit notation here to make a clear distinction between this average value of the variable, and its particular values participating in Eqs. (102)-(110).

[^838]:    ${ }^{67}$ The distribution was first suggested in 1877 by the founding father of statistical physic, L. Boltzmann. For the particular case when $\varepsilon$ is the kinetic energy of a free classical particle (and hence has a continuous spectrum), it is reduced to the Maxwell distribution - see Sec. 3.1 below.

[^839]:    ${ }^{68}$ See, e.g., QM Sec. 8.1.
    ${ }^{69}$ This invites a natural question: what particles are "elementary enough" for the identity? For example, protons and neutrons have an internal structure, in some sense consisting of quarks and gluons; they be considered elementary? Next, if protons and neutrons are elementary, are atoms? molecules? What about really large molecules (such as proteins)? viruses? The general answer to these questions, given by quantum mechanics (or rather experiment :-), is that any particles/systems, no matter how large and complex they are, are identical if they have exactly the same internal structure, and also are exactly in the same internal quantum state - for example, in the ground state of all their internal degrees of freedom.

[^840]:    ${ }^{70}$ As the reader certainly knows, for the electromagnetic field oscillators, such excitations are called photons; for mechanical oscillation modes, phonons. It is important, however, not to confuse these mode excitations with the oscillators as such, and be very careful in prescribing to them certain spatial locations - see, e.g., QM Sec. 9.1.

[^841]:    ${ }^{71}$ See, e.g., MA Eq. (2.2).
    ${ }^{72}$ See also MA Eq. (2.4).

[^842]:    ${ }^{73}$ This is essentially a simpler (and funnier :-) version of the particle scattering model used by L. Boltzmann to prove his famed H-theorem (1872). Besides all the historic significance of that theorem, the model used by Boltzmann (see Sec. 6.2 below) is almost as cartoonish.

[^843]:    74 See, e.g., QM Sec. 4.4. Note that both models assume that the particle's orbital motion (if any) does not contribute to its magnetic moment.
    ${ }^{75}$ See, e.g., EM Sec. 5.5, in particular Eq. (5.111).
    ${ }^{76}$ See, e.g., QM Sec. 5.7, in particular Eq. (5.197).

[^844]:    ${ }^{77}$ For its definition and main properties, see, e.g., MA Eqs. (6.6)-(6.9).
    ${ }^{78}$ It may be reduced to the so-called elliptic theta-function $\theta_{3}(z, \tau)$ for a particular case $z=0$ - see, e.g., Sec. 16.27 in the Abramowitz-Stegun handbook cited in MA Sec. 16(ii). However, you do not need that (or any other :-) handbook to solve this problem.
    ${ }^{79}$ This is a reasonable model of the constraints imposed on small atomic groups (e.g., ligands) by their environment inside some large molecules.

[^845]:    ${ }^{80}$ Note that by the same dispersion law is typical for elastic bending waves in thin rods - see, e.g., CM Sec. 7.8.
    ${ }^{81}$ See, e.g., CM Problem 1.12.
    ${ }^{82}$ In this context, weak junction means a tunnel junction with transparency so low that the tunneling electron's wavefunction looses its quantum-mechanical coherence before the electron has time to tunnel back. In a typical junction of a macroscopic area this condition is fulfilled if the effective tunnel resistance of the junction is much higher than the quantum unit of resistance (see, e.g., QM Sec. 3.2), $R_{Q} \equiv \pi \hbar / 2 e^{2} \approx 6.5 \mathrm{k} \Omega$.

[^846]:    ${ }^{1}$ In more realistic cases when particles do have internal degrees of freedom, but they are in certain (say, ground) quantum states, Eq. (3) is valid as well, with $\varepsilon_{k}$ referred to the internal ground-state energy.
    ${ }^{2}$ See, e.g., QM Sec. 1.2.

[^847]:    ${ }^{3}$ This formula was suggested by J. C. Maxwell as early as in 1860, i.e. well before the Boltzmann and Gibbs distributions. Note also that the term "Maxwell distribution" is often associated with the distribution of particle's momentum (or velocity) magnitude,

    $$
    d W=4 \pi C p^{2} \exp \left\{-\frac{p^{2}}{2 m T}\right\} d p=4 \pi C m^{3} v^{2} \exp \left\{-\frac{m v^{2}}{2 T}\right\} d v, \quad \text { with } 0 \leq p, v<\infty,
    $$

    which immediately follows from Eq. (5) combined with the expression $d^{3} p=4 \pi p^{2} d p$ due to the spherical symmetry of the distribution in the momentum/velocity space.
    ${ }^{4}$ See, e.g., MA Eq. (6.9b).
    ${ }^{5}$ See, e.g., MA Eq. (6.9c).

[^848]:    ${ }^{6}$ Since each particle belongs to the same portion of gas, i.e. cannot be distinguished from others by its spatial position, this requires some internal "pencil mark", for example a specific structure or a specific quantum state of its internal degrees of freedom.
    ${ }^{7}$ As a reminder, we have already used this rule (twice) in Sec. 2.6, with particular values of $g$.

[^849]:    ${ }^{8}$ For the opposite limit when $N=g=1$, Eq. (15) yields the results obtained, by two alternative methods, in Problems 2.5 and 2.6. For $N=1$, the "correct Boltzmann counting" factor $N$ ! equals 1 , so that the particle distinguishability effects vanish - naturally.

[^850]:    ${ }^{9}$ The result presented by Eq. (20), with function $f$ given by Eq. (16b), was obtained independently by O. Sackur and H. Tetrode in 1911, i.e. well before the final formulation of quantum mechanics in the late 1920s.
    ${ }^{10}$ By the way, if an ideal classical gas consists of particles of several different sorts, its full pressure is a sum of independent partial pressures exerted by each component - the so-called Dalton law. While this fact was an important experimental discovery in the early 1800s, from the point of view of statistical physics this is just a straightforward corollary of Eq. (18), because in an ideal gas, the component particles do not interact.

[^851]:    ${ }^{11}$ It is interesting that statistical mechanics of weak solutions is very similar to that of ideal gases, with Eq. (18) recast into the following formula (derived in 1885 by J. van't Hoff), $P V=c N T$, for the partial pressure of the solute. One of its corollaries is that the net force (called the osmotic pressure) exerted on a semipermeable membrane is proportional to the difference of solute concentrations it is supporting.
    ${ }^{12}$ Unfortunately, I do not have time for even a brief introduction into this important field, and have to refer the interested reader to specialized textbooks - for example, P. A. Rock, Chemical Thermodynamics, University Science Books, 1983; or P. Atkins, Physical Chemistry, $5^{\text {th }}$ ed., Freeman, 1994; or G. M. Barrow, Physical Chemistry, $6^{\text {th }}$ ed., McGraw-Hill, 1996.
    ${ }^{13}$ See, e.g., either Chapter 6 in A. Bard and L. Falkner, Electrochemical Methods, $2^{\text {nd }}$ ed., Wiley, 2000 (which is a good introduction to electrochemistry as the whole); or Sec. II.8.3.1 in F. Scholz (ed.), Electroanalytical Methods, $2^{\text {nd }}$ ed., Springer, 2010.
    ${ }^{14}$ In some textbooks, Eq. (26) is also called the Boltzmann distribution, though it certainly should be distinguished from the more general Eq. (2.111).

[^852]:    ${ }^{15}$ The mean free path may be defined by the geometric relation $n \sigma l=1$, where $\sigma$ is the full cross-section of the particle-particle scattering - see, e.g., CM 3.7.
    ${ }^{16}$ The reason of the drop is that the atmosphere, including molecules such as $\mathrm{H}_{2} \mathrm{O}, \mathrm{CO}_{2}$, etc., absorbs Sun's radiation at wavelengths $\sim 500 \mathrm{~nm}$ much smaller than those of the back-radiation of the Earth surface, with the spectrum centered at wavelength $\sim 10 \mu \mathrm{~m}$ - see Eq. (2.87) and its discussion.

[^853]:    ${ }^{17}$ In quantum mechanics, parameter $r_{\mathrm{c}}$ so defined is frequently called the correlation length - see, e.g., QM Sec. 7.2 and in particular Eq. (7.37).

[^854]:    ${ }^{18}$ See, e.g., MA Eq. (6.7a).
    ${ }^{19}$ For reader's reference only: for the upper sign, the integral in Eq. (40) is a particular form (for $s=1 / 2$ ) of a special function called the complete Fermi-Dirac integral $F_{s}$, while for the lower sign, it is a particular case (for $s$ $=3 / 2$ ) of another special function called the polylogarithm $\mathrm{Li}_{s .}$. (In what follows, I will not use these notations.)

[^855]:    ${ }^{20}$ Note that in the electronic engineering literature, $\mu$ is usually called the Fermi level, at any temperature.

[^856]:    ${ }^{21}$ See, e.g., CM Eq. (7.39).
    ${ }^{22}$ Recently, degenerate gases (with $\varepsilon_{F} \sim 5 T$ ) have been formed of weakly interacting Fermi atoms as well - see, e.g., K. Aikawa et al., Phys. Rev. Lett. 112, 010404 (2014) and references therein.
    ${ }^{23}$ See, e.g., QM Sec. 8.4.
    ${ }^{24}$ Note also a huge difference between the very high bulk modulus of metals ( $K \sim 10^{11} \mathrm{~Pa}$ ) and its very low values in usual gases (for them, at ambient conditions, $K \sim 10^{5} \mathrm{~Pa}$ ). About 4 orders of magnitude of this difference in due to that in particles, density $N / V$, but the balance is due to the electron gas' degeneracy. Indeed, in an ideal classical gas, $K=P=N T / V$, so that factor (2/3) $\varepsilon_{F}$ in Eq. (58), of the order of a few eV in metals, should be compared with factor $T \sim 25 \mathrm{meV}$ in the atomic gases at room temperature.

[^857]:    ${ }^{25}$ Data from N. Ashcroft and N. Mermin, Solid State Physics, W. B. Sounders, 1976.
    ${ }^{26}$ Named after A. Sommerfeld, who was the first (in 1927) to apply the then-emerging quantum mechanics to degenerate Fermi gases, in particular to electron in metals, and may be credited for most of the results discussed in this section.

[^858]:    ${ }^{27}$ See, e.g., MA Eqs. (6.8c) and (2.12b), with $n=1$.

[^859]:    ${ }^{28}$ Solids, with their low thermal expansion coefficients, present a virtually fixed-volume confinement for the electron gas, so that the specific heat measured at ambient conditions may be legitimately compared with calculated $c_{V}$.
    ${ }^{29}$ See, e.g., MA Eqs. (6.8b), (2.7b), and (6.6c) with $s=3 / 2$.

[^860]:    ${ }^{30}$ This is, of course, just another form of Eq. (71).

[^861]:    ${ }^{31}$ For the involved dimensionless integral see, e.g., MA Eqs. (6.8b), (2.7b) and (6.7e) with $s=5 / 2$.

[^862]:    ${ }^{32}$ Its detailed discussion may be found, e.g., in: C. Pethick and H. Smith, Bose-Einstein Condensation in Dilute Gases, 2nd ed., Cambridge U. Press, 2008.
    ${ }^{33}$ See, e.g., QM Sec. 8.3.

[^863]:    ${ }^{34}$ See, e.g., QM Eq. (3.28).
    ${ }^{35}$ This is the Meissner-Ochsenfeld (or just "Meissner") effect which may be also readily explained using Eq. (84), combined with the Maxwell equations - see, e.g., EM Sec. 6.3.

[^864]:    ${ }^{36}$ See QM Sec. 2.3, and EM Secs. 6.3 and 6.4. Recently, some of these effects were observed in the BoseEinstein condensates of diluted gases as well.
    ${ }^{37}$ A concise discussion of weak interactions in quantum gases may be found, for example, in Chapter 10 of K. Huang, Statistical Mechanics, $2^{\text {nd }}$ ed., Wiley, 2003.

[^865]:    ${ }^{38}$ Term "virial", from Latin viris (meaning "force"), was introduced to molecular physics by R. Clausius. The motivation for adjective "second" for $B(T)$ is evident from the last form of Eq. (94), with the "first virial coefficient", standing before the $N / V$ ratio and sometimes denoted $A(T)$, equal to 1 - see also Eq. (100) below.

[^866]:    ${ }^{39}$ Indeed, the independent fluctuation-induced components $\mathbf{p}(t)$ and $\mathbf{p}^{\prime}(t)$ of dipole moments of two particles have random mutual orientation, so that the time average of their interaction energy, proportional to $r^{-3}$, vanishes. However, the electric field $\varepsilon$ of each dipole $\mathbf{p}$, proportional as $r^{-3}$, induces a correlated component of $\mathbf{p}$, also proportional to $r^{-3}$, giving a potential energy of their interaction, proportional to $\mathbf{p}^{\prime} \cdot \varepsilon \propto r^{-6}$, with a non-vanishing time average. A detailed theory of this effect, closely related to the Casimir effect in quantum mechanics (see, e.g., QM Sec. 9.1) may be found, e.g., in Secs. 80-82 of E. Lifshitz and L. Pitaevskii, Statistical Mechanics, pt. 2, Pergamon, 1980.
    ${ }^{40}$ Note that the particular form of the first term in the approximation $U(r)=a / r^{12}-b / r^{6}$ (called the Lennard-Jones potential or the "12-6 potential"), suggested in 1924, lacks physical justification and was soon replaced, in professional physics, by better approximations, including the so-called exp-6 model (better fitting most experimental data) and the Morse potential (more convenient for quantum-mechanical calculations - see QM Chapter 2). However, the Lennard-Jones potential still travels from one undergraduate textbook to another, as a trick for simpler calculation of the equilibrium distance between the particles by differentiation.

[^867]:    ${ }^{41}$ The strong inequality between $U$ and $T$ in this model is necessary not only to make calculations simpler. A deeper reason is that if $\left(-U_{\min }\right)$ becomes comparable with, or larger than $T$, particles may become trapped in the potential well formed by this potential, forming a different phase - a liquid or a solid. In such phases, the probability to find more than two particles interacting simultaneously is high, so that approximation (92), on which all our further results are based, becomes invalid.
    ${ }^{42} \mathrm{~L}$. Boltzmann has used that way to calculate the $3^{\text {rd }}$ and $4^{\text {th }}$ virial coefficients for the hardball model - as much as can be done analytically.

[^868]:    ${ }^{43}$ This method was developed in 1937-38 by J. Mayer and collaborators for a classical gas, and generalized to quantum systems in 1938 by B. Kahn and G. Uhlenbeck.

[^869]:    ${ }^{44}$ Actually, the fact that in that case $Z=\langle N\rangle$, could have been noted earlier by comparing Eq. (104) with Eq. (39). ${ }^{45}$ Looking at Eq. (109), one may think that since $\xi=Z+Z^{2} I_{2} / 2+\ldots$ is of the order of at least $Z \sim\langle N\rangle \gg 1$, the expansion (113), which converges only if $|\xi|<1$, is illegitimate. However, the expansion is justified by its result (114), in which the $n$-th term is of the order of $\langle N\rangle^{n}\left(V_{0} / V\right)^{n-1} / n$ !, so that the series does converge if the gas density is sufficiently low: $\langle N\rangle / V \ll 1 / V_{0}$, i.e. $r_{\mathrm{A}} \gg r_{0}$. This is the very beauty of the cluster expansion, whose few first terms present a good approximation even for a gas with $\langle N\rangle \gg 1$ particles.

[^870]:    ${ }^{46}$ A discussion of the energy band theory may be found, e.g., in QM Sec. 2.7 and 3.4. Though the reader is highly encouraged to review the discussions of this (very important) topic, such a review is not required for solving this particular problem.

[^871]:    ${ }^{47}$ It was suggested in 1927, independently, by L. Thomas and E. Fermi.
    ${ }^{48}$ This is, for example, an approximate model for electrons in white dwarf stars, whose Coulomb interaction is mostly compensated by the charge of nuclei of fully ionized helium atoms.

[^872]:    ${ }^{1}$ The plasma phase, in which atoms are partly or completely ionized, in frequently mentioned in the same breath as the three phase listed above, but one has to remember that in contrast to them, a typical electroneutral plasma consists of particles of two different sorts - ions and electrons.
    ${ }^{2}$ Such classification schemes, started by P. Ehrenfest, have been repeatedly modified, and only the "first-order phase transition" is still a generally accepted term.
    ${ }^{3}$ For example, for water the latent heat of vaporization at ambient pressure is as high as $\sim 2.2 \times 10^{6} \mathrm{~J} / \mathrm{kg}$, i.e. $\sim 0.4$ eV per molecule, making this liquid indispensable for many practical purposes - including fire fighting. (The latent heat of water's ice melting is an order of magnitude lower.)

[^873]:    ${ }^{4}$ Due to the phenomenological character of the van der Waals model, one cannot say whether the condensed phase it predicts corresponds to a liquid or a solid. However, in most real substances at ambient conditions, gas coexists with liquid, hence the name I will use.
    ${ }^{5}$ The special choice of numerical coefficients in Eq. (3) is motivated by making the border between two regions to take place exactly at $t=1$, i.e. at temperature $T_{c}$, with the critical point coordinates equal to $P_{c}$ and $V_{c}$.

[^874]:    ${ }^{6}$ Actually, this assumption is not crucial for our analysis of mechanical stability, because if a fluctuation takes place in a small part of the total volume $V$, its other parts play the role of pressure-fixing environment.
    ${ }^{7}$ Frequently, especially for water gas diluted in air (vapor), $P_{0}(T)$ is called the saturated vapor pressure.

[^875]:    Maxwell's
    rule

[^876]:    ${ }^{8}$ An important question is: why does the phase-equilibrium line $P=P_{0}(T)$ stretch all the way from point 1 to point 2 (Fig. 2)? Indeed, branches 1-1' and 2-2' of the single-phase isotherm have negative derivative ( $\partial P / \partial V)_{T}$ and hence are mechanically stable to small perturbations. The answer is that these branches are actually metastable, i.e. have larger Gibbs energy per particle (i.e. $\mu$ ) than the counterpart phase and are hence unstable to larger perturbations - such as foreign microparticles (say, dust), confining wall protrusions, etc. In very controlled conditions, these single-phase "superheated" or "supercooled" states can survive virtually all the way to zeroderivative points 1 ' and 2 ', leading to sudden jumps of the system into the counterpart phase. (For fixed-pressure conditions, such jumps are shown by dashed lines in Fig. 2.) However, at more realistic conditions, perturbations result in the two-phase coexistence extending all the way between (or very close to) points 1 and 2 .

[^877]:    ${ }^{9}$ It is fascinating how well is this Arrhenius exponent hidden in the polynomial van der Waals equation (2)!

[^878]:    ${ }^{10}\left(\mathrm{CH}_{3}-\mathrm{CH}_{2}\right)-\mathrm{O}-\left(\mathrm{CH}_{2}-\mathrm{CH}_{3}\right)$, historically the first popular general anesthetic.
    ${ }^{11}$ It is interesting that very close to the critical point the substance suddenly becomes opaque - in the case of ether, whitish. The qualitative explanation of this effect, called the critical opalescence, is simple: at this point the difference of Gibbs energies per particle (i.e. chemical potentials) of the two phases becomes so small that the unavoidable thermal fluctuations lead to spontaneous appearance and disappearance of relatively large (a-few$\mu \mathrm{m}$-scale) single-phase regions in all the volume. Since the optical refraction coefficients of the phases are slightly different, large concentration of the region boundaries leads to strong light scattering.

[^879]:    ${ }^{12}$ Please note that $P_{t}$ for water is several orders of magnitude lower than $P_{c}$ of the water-vapor transition, so that Fig. 3 b is indeed very much not to scale!
    ${ }^{13}$ Perhaps the most practically important example is the air/water system. For its detailed discussion, based on Eq. (19), the reader may be referred, e.g., to Sec. 3.9 in F. Schwabl, Statistical Mechanics, Springer (2000). Other important applications include metallic alloys - solid solutions of metal elements.

[^880]:    ${ }^{14}$ For ferromagnets, this point is usually referred to at the Curie temperature, and for antiferromagnets, as the Néel temperature.

[^881]:    ${ }^{15}$ As follows from the discussion of Eqs. (1.1)-(1.3), for ferroelectric transitions between phases with different electric polarization, the role of pressure is played by the external electric field $\varepsilon$, while for the ferromagnetic transitions between phases with different magnetization, by the external magnetic field $\mathcal{H}$. As we will see very soon, such fields give such a phase transition a nonvanishing latent heat, making it the first order transition.
    ${ }^{16}$ Unfortunately, I will have no time for these interesting (and practically important) generalizations, and have to refer the interested reader to the famous monograph by R. Stratonovich, Topics in the Theory of Random Noise, in 2 vols., Gordon and Breach, 1963 and 1967, and/or the influential review by H. Haken, Ferstkörperprobleme 10, 351 (1970).

[^882]:    ${ }^{17}$ See, e.g., QM Sec. 4.4.
    ${ }^{18}$ At $J<0$, the first term of Eq. (21) gives a reasonable model of an antiferromagnet, but in this case the external magnetic field effects are more subtle, so I will not have time to discuss it.
    ${ }^{19}$ Named after E. Ising who explored the 1D version of the model in detail in 1925, though a similar model was discussed earlier (in 1920) by W. Lenz.
    ${ }^{20}$ For a more detailed discussion of phase transition theory (including other popular models of the ferromagnetic phase transition, e.g., the Potts model), see, e.g., either H. Stanley, Introduction to Phase Transitions and Critical Phenomena, Oxford U. Press, 1971; or A. Patashinskii and V. Pokrovskii, Fluctuation Theory of Phase Transitions, Pergamon, 1979; or B. McCoy, Advanced Statistical Mechanics, Oxford U. Press, 2010. For a much more concise text, I can recommend J. Yeomans, Statistical Mechanics of Phase Transitions, Clarendon, 1992.

[^883]:    ${ }^{21}$ See, e.g., EM Secs. 5.4-5.5.
    ${ }^{22}$ The form of all temperature functions is selected so that all critical exponents are non-negative.
    ${ }^{23}$ This variable models the real physical magnetic susceptibility $\chi_{m}$ of magnetic materials - see, e.g., EM Eq. (5.111).

[^884]:    ${ }^{24}$ There is some duality of terminology (and notation) in literature on this topic. Indeed, in the Ising model (as in the Heisenberg model), the magnetic field effects are usually accounted at the microscopic level, by the inclusion of the corresponding term into each particular value of energy $E_{m}$. Then, as was discussed in Sec. 1.4, system's equilibrium (at fixed external field $h$, and also $T$ and $N$ ) corresponds to the minimum of the Helmholtz free energy $F$. From this point of view, these problems do not feature either pressure or volume, hence we may take $P V=$ const, so that both thermodynamic potentials effectively coincide: $G \equiv F+P V=F+$ const. On the other hand, it is fair to say that the role of the magnetic field in these problems is very similar to that of pressure (or rather of $P$ ) in the "usual" thermodynamics. Due to this analogy, and taking into account that the equilibrium of a system at fixed $P$ corresponds to the minimum of the Gibbs free energy $G$, in some publications this name is used for the minimized potential. Still, on the microscopic level, there is a difference in the descriptions of field and pressure see the footnote in the end of Sec. 2.4. Due to this reason, I will follow the traditional, first point of view in most of my narrative, but will use the replacements $F \rightarrow G$ and $h \rightarrow-P$ to use thermodynamic formulas (1.39) and (37) when convenient.
    ${ }^{25}$ Admittedly, it belongs to Chapter 1, but I was reluctant to derive it there to avoid a narrative interruption.

[^885]:    ${ }^{26}$ Historically, the last term belongs to the later (1950) extension of the theory by V. Ginzburg and L. Landau see below.

[^886]:    ${ }^{27}$ According to Eq. (30), the correlation radius may be interpreted as the length distance at which the order parameter $\eta$ relaxes to its equilibrium value, if it is deflected from it at some point. Since the law of such spatial change may be obtained by a variational differentiation of $F$, for the actual relaxation law, all major terms of (46) have to be comparable.

[^887]:    ${ }^{28}$ In the phenomenological Ginzburg-Landau theory, charge $q$ remains unspecified, though the wording in their original paper clearly shows that the authors correctly anticipated that this charge might turn out to be different from the single electron charge.

[^888]:    ${ }^{29}$ See, e.g., EM Eq. (5.129).
    ${ }^{30}$ As a useful elementary sanity check, the minimization of $\Delta f$ in the absence of a superconductor, i.e. without the first 3 terms in the right-hand part of Eq. (56), immediately gives the correct result $\mathbf{B}=\mu_{0} \mathbf{H}$.
    ${ }^{31}$ See, e.g., QM Sec. 3.1.
    ${ }^{32}$ From the mathematics standpoint, such term, nonlinear in $|\psi|$, makes Eq. (58) a member of the family of "nonlinear Schrödinger equations". Another important member of this family is the Gross-Pitaevskii equation,

    $$
    a \tau \psi=b|\psi|^{2} \psi-\frac{\hbar^{2}}{2 m} \nabla^{2} \psi+U(\mathbf{r}) \psi
    $$

    which gives a very reasonable (albeit phenomenological and hence approximate) description of Bose-Einstein condensates of neutral atoms at $T \approx T_{\mathrm{c}}$. The differences between the Ginzburg-Landau and Gross-Pitaevskii equations reflect, first, the zero charge $q$ of the neutral atoms and, second, the fact that the atoms forming the

[^889]:    condensates may be readily placed in external potentials $U(\mathbf{r}) \neq$ const (e.g., those trapping the atoms), while in superconductors such potential profiles are much harder to create due to the screening of electric field by metals see, e.g., EM Sec. 2.1.
    ${ }^{33}$ Such penetration had been discovered experimentally by L. Shubnikov in the mid-1930s, but its quantitative explanation had to wait until A. Abrikosov's work (based on the Ginzburg-Landau equations) published in 1957.
    ${ }^{34}$ See, e.g., M. Tinkham, Introduction to Superconductivity, ${ }^{\text {nd }}$ ed., McGraw-Hill, 1996. A short discussion of the Josephson effects may be found in QM Sec. 2.3 and EM Sec. 6.4.
    ${ }^{35}$ See, e.g., Sec. 45 in E. Lifshitz and L. Pitaevskii, Statistical Physics, Part 2, Pergamon, 1980.
    ${ }^{36}$ Since in this naïve approach we neglect the thermal fluctuations of spin, i.e. their disorder, this assumption implies $S=0$, so that $F \equiv E-T S=E$, and we may use either notation for system's energy.

[^890]:    ${ }^{37}$ The fact that stable states always correspond to $\eta= \pm 1$, partly justifies the treatment of $\eta$ as a continuous variable in this crude approximation.
    ${ }^{38}$ For me, it was always surprising how little physics students knew about this fascinating field of modern engineering, which involves so much interesting physics and fantastic electromechanical technology. For getting acquainted with it, I may recommend, for example, the monograph by C. Mee and E. Daniel, Magnetic Recording Technology, $2^{\text {nd }}$ ed., McGraw-Hill, 1996.

[^891]:    ${ }^{39}$ Actually, the thermal stability of many real ferromagnets, with longer-range interaction between spins, is higher than that predicted by the Ising model.
    ${ }^{40}$ In some texts, this approximation is called the mean-field theory. This terminology may lead to confusion, because the molecular-field theory is on a completely different level of phenomenology than, say, Landau's mean-field theory. For example, the molecular-field approach may used for the calculation of parameters $a, b$, and $T_{c}$ participating Eq. (46) - the starting point of Landau's theory.

[^892]:    ${ }^{41}$ This fact may be readily verified by using Eqs. (64) and (68) to calculate $F$. Now condition $\partial F / \partial \eta_{h=0}=0$ returns us to Eq. (71), and calculating the second derivative, for $T<T_{c}$ we get $\partial^{2} F / \partial \eta^{2}>0$ at $\eta= \pm \eta_{0}$ (indicating two stable minima of $F$ ), and $\partial^{2} F / \partial \eta^{2}<0$ at $\eta=0$ (the unstable maximum of $F$ ).

[^893]:    42 It was developed in 1941 by H. Kramers and G. Wannier. Note that the approach is very close to the one used in 1D quantum mechanics - see, e.g., QM Sec. 2.5.

[^894]:    ${ }^{43}$ This is of course a result of the "translational" (or rather rotational) symmetry of the system, i.e. its invariance to the index replacement $j \rightarrow j+1$ in all terms of the energy $E_{m}$ (besides index $N$ which should be replaced with 1 ).

[^895]:    ${ }^{44}$ If the reader is still uncomfortable with this core result of thermodynamics, he or she is strongly encouraged to revisit Eq. (1.42) and its discussion.

[^896]:    ${ }^{45}$ For that, the reader is referred to either Sec. 151 in the textbook by Landau and Lifshitz or Chapter 15 in the text by Huang, both cited above.

[^897]:    ${ }^{46}$ Discussion of such laws in the task of physical kinetics, which will be briefly reviewed in Chapter 6.
    ${ }^{47}$ The calculation of these rates for several particular cases is described in QM Secs. 6.6, 6.7, and 7.6.

[^898]:    ${ }^{48}$ See, e.g., QM Eq. (7.196) for a quantum system bilinearly coupled to an environment in thermal equilibrium. By the way, that formula (as well as results for all realistic physical systems) does not feature the unphysical cusp of function $\Gamma(\Delta)$ at $\Delta=0$, assumed by the popular model (104).
    ${ }^{49}$ Note that the flip changes signs of only $(2 d+1)$ terms in sum (23), i.e. does not require re-calculation of all ( $2 d$ $+1) N$ terms of the sum, so that the computation of $\Delta$ takes just a few add-multiply operations even at $N \gg 1$.

[^899]:    ${ }^{50}$ Developed first in the quantum field theory in the 1950s, it was adapted to statistics by L. Kadanoff in 1966, with a spectacular solution of the so-called Kubo problem by K. Wilson in 1972, later awarded by a Nobel Prize. ${ }^{51}$ This might be expected, because physically $C$ is just a certain constant addition to system's energy. However, the introduction of that constant is mathematically necessary, because Eqs. (107) and (108) may be reconciled only if $C^{\prime} \neq C$.

[^900]:    52 This equation of state, suggested in 1948, describes most real gases better than not only the original van der Waals model, but also its later 2-parameter alternatives, such as the Berthelot, modified-Berthelot, and Dieterici models, though approximations with more fitting parameters (such as the Soave-Redlich-Kwong model) work even better.
    ${ }^{53}$ For real liquids, the model is reasonable only within certain parameter ranges.

[^901]:    ${ }^{54} \mathrm{~A}$ brief discussion of these parameters, as well as of the difference between the type-I and type-II superconductivity, may be found in EM Secs. 6.3-6.4.
    ${ }^{55}$ This model is formally similar to the genuine (quantum) Heisenberg model - see Eq. (21).

[^902]:    ${ }^{1}$ Let me remind the reader that up to this point, the averaging signs $\langle\ldots\rangle$ were dropped in most formulas, for the sake of notation simplicity. In this chapter I have to restore these signs to avoid confusion. The only exception will be temperature whose average, following (bad :-) tradition, will be still call $T$ everywhere besides the last part of Sec. 3 where temperature fluctuations are discussed explicitly.

[^903]:    ${ }^{2}$ Unfortunately, even in some popular textbooks, a few formulas pertaining to fluctuations are either incorrect, or given without specifying the conditions of their applicability, so that reader's caution is advised.

[^904]:    ${ }^{3}$ See, e.g., MA Eq. (2.2).

[^905]:    ${ }^{4}$ Indeed, this is the most popular definition of this major mathematical constant - see, e.g., MA Eq. (1.2a) with $n$ replaced with $-1 / W$.

[^906]:    ${ }^{5}$ As a reminder, in geometry the term "cylinder" does not necessarily means the "circular cylinder"; the shape of base $A$ may be arbitrary; it just should not change with height.

[^907]:    ${ }^{6}$ As already was discussed in Sec. 4.1 in the context of the van der Waals equation, for mechanical stability of a gas (or liquid), derivative $\partial P / \partial V$ has to be negative, so that $\kappa$ is positive.
    ${ }^{7}$ One may meet statements that a similar formula,

    $$
    \left\langle\widetilde{P}^{2}\right\rangle=T\left(-\frac{\partial\langle P\rangle}{\partial\langle V\rangle}\right)_{X}, \quad \quad \text { WRONG! }
    $$

    is valid for pressure fluctuations. However, such statement does not take into account a different physical nature of pressure (Fig. 4), with its very broad frequency spectrum. This issue will be discussed later in this chapter.

[^908]:    ${ }^{8}$ Besides low internal electric noise, the sensor should have a sufficiently large temperature responsivity $d R / d T$, making the noise contribution by the pickup electronics insignificant - see below.

[^909]:    ${ }^{9}$ It was pioneered in the 1950 s by R. Dicke, so that the device is frequently called the Dicke radiometer.
    ${ }^{10}$ Clearly, this is a temporal analog of the spatial correlation function discussed in Sec. 4.2 - see Eq. (4.30).

[^910]:    ${ }^{14}$ See, e.g., MA Eq. (14.4a).
    ${ }^{15}$ The second form of Eq. (59) uses the fact that, according to Eq. (58), $S_{f}(\omega)$ is an even function of frequency just as $K_{f}(\tau)$ is an even function of time.
    ${ }^{16}$ Although Eqs. (58) and (59) look not much more than straightforward corollaries of the Fourier transform, they bear a special name of the Wiener-Khinchin theorem - after mathematicians N. Wiener and A. Khinchin who have proved that these relations are valid even for functions $f(t)$ which are not square-integrable, so that from the point of view of rigorous mathematics, their Fourier transforms are not well defined.

[^911]:    ${ }^{17}$ A popular alternative definition of the spectral density is $S_{f}(\nu) \equiv 4 \pi S_{f}(\omega)$, making average (61) equal to $S_{f}(v) \Delta v$. ${ }^{18}$ Such process is frequently called white noise, because it consists of all frequency components with equal amplitudes, reminding the white light, which consists of many monochromatic components.
    19 Just for one example, such description may be valid for the complex amplitude of an electromagnetic field mode weakly interacting with matter. To emphasize this generality, I will use letter $q$ rather than $x$ for "particle's" coordinate.

[^912]:    ${ }^{20}$ For a usual (ergodic) environment, the primary averaging may be interpreted as that over relatively short time intervals, $\tau_{c} \ll \Delta t \ll \tau$, where $\tau_{c}$ is the correlation time of the environment, while $\tau$ is the characteristic time scale of motion of our "heavy" system of interest.
    ${ }^{21}$ After P. Langevin whose 1908 work was the first systematic development of A. Einstein's ideas on Brownian motion (see below) using this formalism. A detailed discussion of this approach, with numerical examples of its application, may be found, e.g., in the monograph by W. Coffey, Yu. Kalmykov, and J. Waldron, The Langevin Equation, World Scientific, 1996.
    ${ }^{22}$ See, e.g., CM Sec. 4.1. In this and the next sections I assume that variable $f(t)$ is classical, with the discussion of the quantum case postponed until Sec. 6.

[^913]:    ${ }^{23}$ At this stage we restrict our analysis to random, stationary processes $q(t)$, so that Eq. (57) is valid for this variable as well, if the averaging is understood in the $\langle\langle\ldots\rangle\rangle$ sense.
    ${ }^{24}$ See, e.g. MA Eq. (6.5a).

[^914]:    ${ }^{25}$ This means that the phenomenological description of dissipation by bare friction in classical mechanics (see, e.g., CM Sec. 4.1) is only valid approximately, when the energy scale of the process is much larger than $T$.
    ${ }^{26}$ It was published in one of the three papers of Einstein's celebrated 1905 "triad". As a reminder, another paper started the (special) relativity, and one more was the quantum description of photoelectric effect, essentially the prediction of light quanta - photons, which essentially started quantum mechanics. (Not too bad for one year!)

[^915]:    ${ }^{27}$ In solid-state physics and electronics, mobility is more frequently defined as $\left|\mathbf{v}_{\text {drift }} / \mathcal{E}\right|=e\left|\mathbf{v}_{\text {drift }} / \mathcal{Z}_{\text {det }}\right|$ (where $\mathcal{E}$ is the applied electric field), and is traditionally measured in $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$. In these units, the electron mobility in silicon wafers used for integrated circuit fabrication (i.e. the solid most important for engineering practice) at room temperature is close to $10^{3}$.
    ${ }^{28}$ The minus sign is due to the fact that in our notation, current through the resistor equals $(-I)$ - see Fig. 9 .
    ${ }^{29}$ Due to this fact, Eq. (64) is often called the Ohmic model of the environment response, even if the physical nature of variables $q$ and $\mathcal{F}$ is completely different from the electric charge and voltage.

[^916]:    ${ }^{30}$ Named after H. Nyquist who derived this formula in 1928 (independently of the prior work by A. Einstein, M. Smoluchowski, and P. Langevin) to describe the noise which had been just discovered experimentally by his Bell Labs' colleague J. B. Johnson. The derivation of Eq. (73) and hence Eq. (81) in these notes is essentially a twist of the derivation used by Nyquist.
    ${ }^{31}$ Another practically important type of fluctuations in electronic devices is the low-frequency $1 / f$ noise which was already mentioned in Sec. 3 above. I will briefly discuss it in Sec. 8 .

[^917]:    ${ }^{32}$ See, e.g., Y. Naveh et al., Phys. Rev. B 58, 15371 (1998). In practically used metals, $l_{e}$ is of the order of 30 nm even at liquid helium temperatures (and even shorter at ambient conditions), so that the usual "macroscopic" resistors do not exhibit the shot noise.
    ${ }^{33}$ For a review of this effect see, e.g., Ya. Blanter and M. Büttiker, Phys. Repts. 336, 1 (2000).

[^918]:    ${ }^{34}$ Reviewing the calculations leading to Eq. (73), we may see that if the possible real part $\chi^{\prime}(\omega)$ of the susceptibility just adds up to $\left(k-m \omega^{2}\right)$ in the denominator of Eq. (67), resulting in a change of oscillator's eigenfrequency. This renormalization is insignificant if the oscillator-to-environment coupling is weak, i.e. susceptibility $\chi(\omega)$ small, as had been assumed at the derivation of Eq. (69) and hence Eq. (73).
    ${ }^{35}$ It is sometimes called the Green-Kubo (or just "Kubo") formula. This is hardly fair, because, as the reader could see, Eq. (92) is just an elementary generalization of the Nyquist formula (81). Moreover, the corresponding works of M. Green and R. Kubo were published, respectively, in 1954 and 1957, i.e. after the 1950 paper by H. Callen and T. Welton, where a more general result (see below) had been derived. More adequately, the Green / Kubo names are associated with a related relation between the response function and the operator commutator see, e.g., QM Eq. (7.109).
    ${ }^{36}$ See, e.g., QM Sec. 4.6.

[^919]:    ${ }^{37}$ Please note that here (and to the end of this section) brackets $\langle\ldots\rangle$ mean quantum-statistical averaging (2.12). As was discussed in Sec. 2.1, for a classical-mixture state of the environment, this does not create any difference in either mathematical treatment of the averages or their physical interpretation.
    ${ }^{38}$ It was first derived in 1951 by H. Callen and T. Welton (in a somewhat different way). One more derivation of the FDT, which gives the Kubo formula as a by-product, may be found in QM Sec. 7.4.

[^920]:    ${ }^{39}$ K. Likharev and V. Semenov, JETP Lett. 15, 442 (1972).
    ${ }^{40}$ R. Koch et al., Phys. Rev. B 26, 74 (1982).
    ${ }^{41}$ Another one is the Casimir effect - see, e.g., QM Sec. 9.1.
    ${ }^{42}$ See, e.g., QM Sec. 7.4.

[^921]:    ${ }^{43}$ See, e.g., CM Sec. 4.1, part (ii).
    ${ }^{44}$ Only explicitly so, because the complex susceptibility of the environment may depend on temperature as well.
    ${ }^{45}$ See, e.g., CM Sec. 3.4-3.6.

[^922]:    ${ }^{46}$ The generalization of Eq. (107) to higher spatial dimensionality is also straightforward, with the scalar variable $q$ replaced by vector $\mathbf{q}$, and the scalar derivative $d U / d q$ replaced with vector $\nabla U$.
    ${ }^{47}$ See, e.g., CM Secs. 3.2, 4.2, and beyond.
    ${ }^{48}$ See, e.g., Chapters 5 and 6 in W. Coffey et al., The Langevin Equation, World Scientific, 1996.
    ${ }^{49}$ After H. Kramers who, besides solving this important problem in 1940, has made significant contributions to many other areas of physics, including the famous Kramers-Kronig dispersion relations - see, e.g., EM Sec. 7.4.

[^923]:    ${ }^{50}$ If $U_{0}$ is comparable with $T$, system's behavior also depends substantially on the initial probability distribution, i.e., do not follow the universal law (111).
    ${ }^{51}$ See, e.g., either R. Stratonovich, Topics in the Theory of Random Noise, vol. 1., Gordon and Breach, 1963, or Chapter 1 in the monograph by W. Coffey et al., cited above.
    ${ }^{52}$ By the way, the goal of the traditional coefficient 2 in Eq. (77) is exactly to have the fundamental Eq. (114) free of numerical coefficients.

[^924]:    ${ }^{53}$ As will be discussed in Chapter 6, the equation of diffusion also describes several other physical phenomena in particular, heat propagation in a uniform, isotropic solid, and in this context is called the heat conduction equation or (rather inappropriately) just the "heat equation".
    ${ }^{54}$ Both forms of Eq. (117) are similar to the mass conservation law in classical dynamics (see, e.g., CM Sec. 8.2), and the electric charge conservation law in electrodynamics (see, e.g., EM Sec. 4.1).
    ${ }^{55}$ See, e.g., MA Eq. (12.2),

[^925]:    ${ }^{56}$ Named after M. Smoluchowski who developed this formalism in 1906, apparently independently from the slightly earlier Einstein's work, and in much more detail. This equation has important applications in many fields of science, including such surprising topics as statistics of spikes in neural networks.

[^926]:    ${ }^{57}$ If necessary, see MA Eq. (6.9b) again.

[^927]:    ${ }^{58}$ Actually, $\tau_{2}$ describes the characteristic time of the exponential growth of small deviations from the unstable fixed point $q_{2}$ at the barrier top, rather than their decay, as near point $q_{1}$.

[^928]:    ${ }^{59}$ It was derived in 1913 in A. Fokker's PhD thesis work; M. Planck was his thesis adviser.
    ${ }^{60}$ The reader should remember that these solutions embody, as the particular case $T=0$, all classical dynamics of a particle.

[^929]:    ${ }^{61}$ See, e.g., QM Secs. 2.3-2.4.
    ${ }^{62}$ As a reminder, an absolutely similar approximation is used in Exercise Problem 4.3 for the $P(V)$ function, in order to analyze properties of the van der Waals model near the critical temperature.

[^930]:    ${ }^{63}$ The main, exponential factor in this result may be obtained simply by ignoring the difference between $E$ and $U\left(q_{1}\right)$, but the correct calculation of the pre-exponent requires to take this difference, $\hbar \omega_{0} / 2$, into account - see K. Likharev, Physica B 108, 1079 (1981).
    ${ }^{64}$ See, e.g., QM Sec. 2.4.

[^931]:    ${ }^{65}$ The transition from the first line of Eq. (174) to its second one uses the fact that the system is stationary, so that $\langle E(t+\tau)\rangle=\langle E(t)\rangle=\langle E\rangle=$ const.

[^932]:    ${ }^{66}$ Regardless of the physical sense of such function of $\omega$, and of whether its maximum is situated at either zero as in Eq. (177), or at a finite frequency $\omega_{0}$ as in Eq. (68), it is often referred to as the Lorentzian (or "Breit-Wigner") line.

[^933]:    ${ }^{67}$ See, e.g., MA Eq. (6.9c).

[^934]:    ${ }^{68}$ This fact is not in any contradiction with the nonvanishing result (183) which is only valid for a sub-ensemble with a certain (deterministic) initial condition $q_{0}$.
    ${ }^{69}$ The involved table integral may be found, e.g., in MA Eq. (6.11).
    ${ }^{70}$ See, e.g., QM Sec. 7.6.
    ${ }^{71}$ See, e.g., the solutions of the 1D Kramers problem for quantum systems with low damping by A. Caldeira and A. Leggett, Phys. Rev. Lett. 46, 211 (1981), and with high damping by A. Larkin and Yu. Ovchinnikov, JETP Lett. 37, 382 (1983).

[^935]:    ${ }^{72}$ See, e.g., CM Sec. 4.3.
    ${ }^{73}$ See, e.g., EM Sec. 7.6.

[^936]:    ${ }^{1}$ See, e.g., CM Sec. 10.1.
    ${ }^{2}$ Actually, this is just one of several theorems bearing the name of J. Liouville (1809-1882).

[^937]:    ${ }^{3}$ See, e.g., CM Sec. 9.3.
    ${ }^{4}$ From this point on, I return to using the index-free symbol

[^938]:    ${ }^{5}$ Note that the master equations ignores possible quantum coherence of different scattering events, described by off-diagonal elements of the density matrix, because $w$ represents only the diagonal elements of the matrix. However, for ensembles close to thermal equilibrium, this is a reasonable approximation - see Sec. 2.1.
    ${ }^{6}$ One may wonder whether this approximation may work for Fermi particles, for whom the Pauli principle forbids scattering into the already occupied state, so that for scattering $\mathbf{p} \rightarrow \mathbf{p}$ ', the factor $w(\mathbf{r}, \mathbf{p}, t)$ in Eq. (12) has to be multiplied by the probability $\left[1-w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)\right]$ that the final state is available. Generally, this is a valid argument, but one should notice that if this modification has been done with both terms of Eq. (12), it yields

    $$
    \left.\frac{\partial w}{\partial t}\right|_{\text {scatteering }}=\int d^{3} p^{\prime} \Gamma_{\mathbf{p} \rightarrow \mathbf{p}^{\prime}}\left\{w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)[\mathbf{1}-w(\mathbf{r}, \mathbf{p}, t)]-w(\mathbf{r}, \mathbf{p}, t)\left[\mathbf{1}-w\left(\mathbf{r}, \mathbf{p}^{\prime}, t\right)\right]\right\} .
    $$

    Opening both square brackets, we see that the probability density products cancel, bringing us back to Eq. (12).

[^939]:    ${ }^{7}$ This was the approximation used by L. Boltzmann to prove the famous H-theorem, stating that entropy of the gas described by Eq. (13) may only grow (or stay constant) in time, $d S / d t \geq 0$. Since the model is very approximate, that result does not seem too fundamental nowadays, despite all its historic significance.
    ${ }^{8}$ Sometimes this approximation is called the "BGK model", after P. Bhatnager, E. Gross, and M. Krook who suggested it in 1954. (The same year, a similar model was considered by P. Welander.)
    ${ }^{9}$ See, e.g., CM Sec. 3.7.

[^940]:    ${ }^{10}$ See, e.g., QM Sec. 2.1.

[^941]:    ${ }^{11}$ First obtained by A. Sommerfeld in 1927.
    ${ }^{12}$ See, e.g., QM Secs. 2.7, 2.8, and 3.4. In this case, $\mathbf{p}$ should be understood as the quasi-momentum rather than genuine momentum.
    ${ }^{13}$ As Eq. (27) shows, if the dispersion law $\varepsilon(\mathbf{p})$ is anisotropic, the direction of current density may be different from that of the electric field. In this case, conductivity should be described by a tensor $\sigma_{i j}$, rather than a scalar.

[^942]:    Drude
    formula

[^943]:    ${ }^{14}$ Calculations for a classical gas (which are important, in particular, for most plasmas and non-degenerate semiconductors) are left for the reader - see the first assignment of Problem 5.
    ${ }^{15}$ At least explicitly, because in some particle collision models, $\tau$ may be a function of temperature, which levels out only at some temperature much lower than $\varepsilon_{\mathrm{F}}$.
    ${ }^{16}$ Its was derived in 1900 by P. Drude. Note that Drude also used the same arguments to derive a very simple (and very reasonable) approximation for the complex electric conductivity in the ac field of frequency $\omega$ : $\sigma(\omega)=$ $\sigma(0) /(1-i \omega \tau)$, with $\sigma(0)$ given by Eq. (32); sometimes the name "Drude formula" is used for this expression rather than for Eq. (32) - see Problem 1.

[^944]:    ${ }^{17}$ As a reminder, here it is (see also EM Sec. 4.2): Let $\tau$ be the average time at which scattering causes a particle to loose all the deterministic component of its velocity, $\mathbf{v}_{\text {drift }}$, provided by electric field $\boldsymbol{\mathcal { E }}$, on the top of electron's random thermal motion (which does not contribute to the net current). Using the $2^{\text {nd }}$ Newton law to describe particle's acceleration by the field, $d \mathbf{v}_{\text {drift }} / d t=q \boldsymbol{\mathcal { L }} / \mathrm{m}$, we get $\left\langle\mathbf{v}_{\text {drift }}\right\rangle=\tau q \boldsymbol{\mathcal { E }} / \mathrm{m}$. Multiplying this result by the particle charge $q$ and density $n=N / V$, we get the Ohm law $\mathbf{j}=\sigma \boldsymbol{\varepsilon}$, with $\sigma$ given by Eq. (32).
    ${ }^{18}$ By the way, since the scale of the fastest change of $w_{0}$ in the momentum space is of the order of $\partial w_{0} / \partial p=$ $\left(\partial w_{0} / \partial \varepsilon\right)(d \varepsilon / d p) \sim(1 / T) v_{\mathrm{F}}$, the linear approximation (34) is valid if $e \mathcal{E} \tau<T / v_{\mathrm{F}}$, i.e. if $e d \ll T$, where $l \equiv v_{\mathrm{F}} \tau$ is called the mean free path. This is the promised quantitative condition of the electric field smallness; since the lefthand part of the last inequality is just the average energy given to the particle by the electric field between two scattering events, the condition may be interpreted as the smallness of electron gas' "overheating" by the applied field. However, another condition is also necessary - see the last paragraph of this section.

[^945]:    ${ }^{19}$ So here, as it frequently happens in physics, formulas (or drawings, such as Fig. 4b) give a more clear and unambiguous description of the reality than words - the privilege lacked by many other scientific (and "scientific") disciplines, frequently leading in unending, shallow verbal debates.

[^946]:    ${ }^{20}$ Since we consider $w_{0}$ as a function of two independent arguments $\mathbf{r}$ and $\mathbf{p}$, taking its gradient, i.e. differentiation of this function over $\mathbf{r}$, does not involve its differentiation over the kinetic energy $\varepsilon$ - which is a function of $\mathbf{p}$ only.
    ${ }^{21}$ In electronic engineering literature, variable $q \Phi \equiv \mu+q \phi$, called the local Fermi level, is more frequently used.
    ${ }^{22}$ Relation (42) does not include the phenomenological parameter $\tau$ of the relaxation-time approximation, so that it is more general than the RTA. Indeed, Eq. (42) is based on the relation between the second and third terms in the left-hand part of the rather general Eq. (10).

[^947]:    ${ }^{23}$ Sometimes also called the "electron affinity", though the latter term is mostly used for atoms and molecules.
    ${ }^{24}$ In semiconductor physics and engineering, the situation shown in Fig. 5b is called the flat-band condition, because in semiconductors, any electric field at the surface leads to band bending - a gradual spatial change of the background potential $U_{0}$ and hence of all energy band/gap edges. For a discussion of the band bending and its effects on semiconductor device operation, see, e.g., either Chapter 6 in J. Hook and H. Hall, Solid State Physics, $2^{\text {nd }}$ ed. Wiley, 1991, or Chapter 3 in S. Sze, Semiconductor Devices, $2^{\text {nd }}$ ed., Wiley, 2001.
    ${ }^{25}$ As measured from a common reference value, for example from the vacuum level.
    ${ }^{26}$ In physics literature, it is usually called the contact potential difference, while in electrochemistry (for which it is one of the key notions), the term Volta potential is more common.

[^948]:    ${ }^{27}$ In particular, in physics of semiconductor devices, where electrons in the conduction band, and holes in the valence band, may be frequently treated as nearly-ideal classical gases.
    ${ }^{28}$ Sometimes this term is associated with Eq. (52).
    ${ }^{29}$ And hence, at negligible $\nabla U$, identical to the diffusion equation (5.116).

[^949]:    ${ }^{30}$ See, e.g., CM Sec. 3.7.

[^950]:    ${ }^{31}$ Named after T. Seebeck who experimentally discovered, in 1821 (independently of J. Peltier), the effect expressed by Eq. (62).
    ${ }^{32}$ Again, such independence infers that Eq. (60) should have a broader validity than in our simple model of an isotropic gas. This is indeed the case: at $T \ll \varepsilon_{\mathrm{F}}$, this result turns out to be valid for any form of the Fermi surface, and for any dispersion law $\varepsilon(\mathbf{p})$.

[^951]:    ${ }^{33}$ Both these materials are alloys, i.e. solid solutions: chromel is $10 \%$ chromium in $90 \%$ nickel, while constantan is $45 \%$ nickel and $55 \%$ copper.

[^952]:    ${ }^{34}$ One more way to look at Eq. (63) is as at the difference between the total energy flow density, $\mathbf{j}_{e}=\int_{\varepsilon v} w d^{3} p$, and the product of a constant ( $\mu$ ) by the particle flow density, $\mathbf{j}_{n}=\int_{\mathbf{v}} w d^{3} p=\mathbf{j} / q$.
    ${ }^{35}$ The expression given by the second term of this relation, $\mathbf{j}_{h}{ }^{\prime}=-\kappa \nabla T$, is much more general than our analysis: for small temperature gradients it is valid in virtually any medium - for example, in insulators, where the first term of Eq. (64) vanishes. (In the general case, the thermal conductivity $\kappa$ is of course different from that given by Eq. (66).) As a result, this relation has its own name - the Fourier law, because it has been first suggested by the same universal genius J.-B. J. Fourier - who has not only developed such a key mathematical tool as the Fourier series, but also discovered what is now called the greenhouse effect!
    ${ }^{36}$ The simplicity of this relation (first discovered experimentally in 1854 by W. Thompson, a.k.a. Lord Kelvin) is not occasional. This is one of fundamental Onsager reciprocal relations between kinetic coefficients (L. Onsager, 1931), which are model-independent, i.e. valid within very general assumptions. Unfortunately, I have no time left for a discussion of this interesting topic, and have to refer the interested reader, for example, to Sec. 120 in L . Landau and E. Lifshitz, Statistical Physics, $3^{\text {rd }}$ ed., Pergamon, 1980. Note, however, that the range of validity of the Onsager relations is still debated - see, e.g., K.-T. Chen and P. Lee, Phys. Rev. B 79, 18 (2009).

[^953]:    ${ }^{37}$ It was named after G. Wiedemann and R. Franz who noticed the constancy of ratio $\kappa / \sigma$ for various materials, at the same temperature, as early as in 1853 . The direct proportionality of the ratio to the absolute temperature was noticed by L. Lorenz in 1872. Due to this contribution, the Wiedemann-Franz law is frequently presented as $\kappa / \sigma=$ $L T$, where constant $L$, called the Lorenz number, in SI units is close to $2.45 \times 10^{-8} \mathrm{~W} \cdot \Omega / \mathrm{K}^{2}$. Theoretically, Eq. (69) was derived in 1928 by A. Sommerfeld.

[^954]:    ${ }^{38}$ See, e.g., D. Rowe (ed.), Thermoelectrics Handbook: Macro to Nano, CRC Press, 2005.
    ${ }^{39}$ A much more detailed coverage of this important part of physics may be found, for example, in the textbook by L. Pitaevskii and E. Lifshitz, Physical Kinetics, Butterworth-Heinemann, 1981. A detailed discussion of its applications to mechanical engineering may be found, e.g., in T. Bergman et al., Fundamentals of Heat and Mass Transfer, $7^{\text {th }}$ ed., Wiley, 2011.

[^955]:    ${ }^{1}$ Actually, this leading term was derived by A. de Moivre in 1733, before the J. Stirling’s work.

[^956]:    ${ }^{2}$ Note that definitions of $B_{k}$ (or rather their signs and indices) vary even in the most popular handbooks.
    ${ }^{3} \mathrm{I}$ am confident that the reader is quite capable of deriving relations (3.1) by representing exponent in the elementary relation $e^{i(a \pm b)}=e^{i a} e^{ \pm i b}$ as a sum of its real and imaginary parts, Eqs. (3.3) directly from Eqs. (3.1), and Eqs. (3.2) from Eqs. (3.3) by variable replacement; however, I am still providing these formulas to save his or her time. (Quite a few formulas below are included because of the same reason.)

[^957]:    ${ }^{4}$ Higher-order formulas (e.g., the Bode rule), and other guidance including ready-for-use codes for computer calculations may be found, for example, in the popular reference texts by W. H. Press et al., cited in Sec. 16 below. Besides that, some advanced codes are used as subroutines in the software packages listed in the same section. In some cases, the Euler-Maclaurin formula (2.12) also may be useful for numerical integration.

[^958]:    ${ }^{5}$ A powerful (and free :-) interactive online tool for working out indefinite 1D integrals is available at http://integrals.wolfram.com/index.jsp.
    ${ }^{6}$ Eq. (6.5a) follows immediately from Eq. (6.3d), and Eq. (6.5b) from Eq. (6.2b) - a couple more examples of the (intentional) redundancy of this list.

[^959]:    ${ }^{7}$ Other popular notations for this vector set are $\left\{\mathbf{e}_{j}\right\}$ and $\left\{\hat{\mathbf{r}}_{j}\right\}$.
    ${ }^{8}$ It is easy to use Eq. (7.3) to check that the direction of the product vector corresponds to the well-known "righthand rule" and to the even more convenient corkscrew rule: if we rotate a corkscrew's handle from the first operand toward the second one, its axis moves in the direction of the product.

[^960]:    ${ }^{9}$ One can run into the following notation: $\nabla \equiv \partial / \partial \mathbf{r}$, which is convenient is some cases, but may be misleading in quite a few others, so it will be not used in these notes.
    ${ }^{10}$ In this, and four next sections, all scalar and vector functions are assumed to be differentiable.

[^961]:    ${ }^{11}$ Some other orthogonal curvilinear coordinate systems are discussed in EM Sec. 2.3.
    ${ }^{12}$ In the 2D geometry with fixed coordinate $z$, these coordinates are called polar.

[^962]:    ${ }^{13}$ The coefficient in this equation may be readily recalled by considering its left-hand part as the Fourier-integral presentation of function $f(s) \equiv 1$, and applying Eq. (14.1) to the reciprocal Fourier transform

    $$
    f(s) \equiv 1=\frac{1}{2 \pi} \int_{-\infty}^{+\infty} e^{-i s \xi}[2 \pi \delta(\xi)] d \xi
    $$

[^963]:    ${ }^{14}$ On a personal note, perhaps $90 \%$ of all formula needs throughout my research career were satisfied by a tiny, wonderfully compiled old book: H. Dwight, Tables of Integrals and Other Mathematical Formulas, $4^{\text {th }}$ ed., Macmillan, 1961, whose used copies, rather amazingly, are still available on the Web.
    ${ }^{15}$ An updated version of this collection is now available online at http://dlmf.nist.gov/ .

[^964]:    1 The listed numerical values of the constants are from the most recent (2014) International CODATA recommendation (see, e.g., http://physics.nist.gov/cuu/Constants/index.html), besides a newer result for $k_{\mathrm{B}}$ - see C. Gaiser et al., Metrologia 52, 217 (2015). Please note the planned (but not yet official) adjustment of the SI values - see, e.g. https://www.nist.gov/si-redefinition/meet-constants. In particular, the Planck constant will also get a definite value (within the interval specified in the given table), enabling a new, fundamental standard of the kilogram.

[^965]:    ${ }^{2}$ Note that the selected value of $\mu_{0}$ may be changed (a bit) in a few years - see, e.g., D. Newell, Phys. Today 67, No. 7, pp. 35-41 (2014).

[^966]:    ${ }^{1}$ The list does not include the sources (mostly, recent original publications) cited in the lecture notes and problem solutions, the open-access materials mentioned in the Preface, and the mathematics textbooks and handbooks listed in MA Sec. 16.

