

MECHANICS AND OPTICS

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SPECIAL RELATIVITY

The later History of the Theory of the Aether.

The Lorentz Transformation

Einstein's Derivation of the Lorentz Transformation.

Views of Einstein on Space, Time and Simultaneity.

Minkowski's 4-dimensional analysis.

Invariance of Maxwell's Equations under a Lorentz Transformation

Mechanics in Special Relativity.

The Doppler Effect in Special Relativity.

Transformation of Tensors in Special Relativity.

QUANTUM THEORY

De Broglie Theory - Experimental verification.

Principles of Mechanics and Optics.

Germet - Hamilton

Comparison between the Development of Theory in Mechanics and Optics.

Schrodinger's Equation.

Solution of equation for the oscillator and the Hydrogen Atom.

Meaning of ψ .

Wave and Group Velocity.

Uncertainty Relation.

Relation between Heisenberg and Schrodinger.

Pauli's Inclusion of Spin.

Dirac's Equation.

Dirac Theory of the Electron in the Atom.

Invariance of the Dirac Equation.

Negative Energy States.

Mechanics and Optics

In these two branches of Physical Science, the phenomena, which in the course of time, first came to be studied, were those large scale or macroscopic effects which obtrude themselves upon the senses. This was so in Mechanics, the study of matter in motion and in equilibrium, where bodies at least comparable in size with the human body and moving slowly enough for their motion to be studied, first came under consideration, and in Light, where the study of the macroscopic qualities led to Geometrical Optics.

Laws were formulated which were in accord with the known phenomena until further study brought small scale phenomena under observation. Here difficulties were found, both where the bodies were extremely small and where motion was very great.

It seems understandable that if the behaviour of the very smallest portions of things is known, then by a kind of addition it may be possible to find the law for large effects and that the statistical law so obtained may not show the intricacies of the laws for the individual parts. Also we can imagine that various possible laws of behaviour for the individuals can lead to the same statistical law. In addition, it has begun to be understood that we cannot make exact measurement on all aspects of a physical problem at the same time, and that

though, if we are content with a roughly correct answer we may find a consistent formulation^{of} a law for the whole behaviour of a body, yet it now seems that if we concentrate upon one particular aspect and succeed in an explanation of that, it will not be possible to explain other aspects in the same terms. In both Mechanics and Optics we have a duality in that there is both a corpuscular and wave aspect of each to be considered.

The real development of both Mechanics and Optics as sciences in the systematic form in which we understand them, began in the 17th century, though long before that time there were theories of Matter and of Light, some of which bear distinct resemblance to views now held.

Of these we may note the Atomic theory due to Democritus of the 5th century B.C. according to which, all substances, solids, liquids, gases or light were corpuscular in nature and their behaviour became explicable by the motions and interactions of these 'atoms'. The corpuscles themselves were indivisible and were the ultimate units of nature. It is to be seen that a single underlying principle was postulated for the behaviour of both Matter and Light at this time.

In the 3rd century B.C. Archimedes, in his study of mechanics was mainly concerned with Statics and he was

familiar with the properties of the "burning glass" and the law of reflection of light, but it was not until the time of Galileo and Newton that the necessity of carefully devised observation and experiment for the verification of fundamental fact was realised.

Euclid published a book on Optics which commences with the assumption that objects are seen by rays emitted from the eye in straight lines, and adds "for if the light proceeded from the object we should not, as we often do, fail to perceive a needle on the floor".

In the first century B.C. Lucretius must especially be remembered for his theory of Light. He, like his predecessors held the general doctrine of the Atomic theory of natural phenomena and explained the formation of an image in the eye by the theory that bodies send forth, at tremendous speed, small particles which are replicas of the real body from which they come and which unite to form an exact image of the object seen. Lucretius found it necessary to ascribe a tremendous velocity to these particles in order for the effect to be possible.

In passing to the time of Newton it is worth noting that Leonardo da Vinci likened the phenomena of light to those of sound and ascribed a wave like character to it.

Newton (1642 - 1727) was the first to place mechanics on

Extension of the Variation Principles.

In the case of n independent variables $q_1, q_2, q_3 \dots q_n$

where $S = \int_{t_1}^{t_2} L (q_1, q_2, \dots, q_n, \dot{q}_1, \dot{q}_2, \dots, \dot{q}_n, t) dt$

and $\dot{q}_s = \frac{dq_s}{dt}$ the results given above must be

adjusted in the following manner.

1.a. $\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_s} \right) - \frac{\partial L}{\partial q_s} = 0$

2.a. $\sum \dot{q}_s \frac{\partial L}{\partial \dot{q}_s} - L = \text{constant.}$

3.a. $\frac{\partial L}{\partial \dot{q}_s} \delta \dot{q}_s = 0$

4.a. $(L - \sum \dot{q}_s \frac{\partial L}{\partial \dot{q}_s}) \Delta t + \sum \frac{\partial L}{\partial q_s} \Delta q_s = 0$

under the conditions given above. $s = 1, 2, \dots, n$

The Variation Principles as applied to Dynamics.

Newton's second Law states that " The rate of change of momentum is proportional to the impressed force and takes place in the direction in which that force acts."

This may be written as $\frac{d(mv)}{dt} = F$
 where v is the velocity, m the mass and F , the force acting.
 Keeping, for simplicity, to one dimension in space, (since the results may be extended to three dimensions and to generalised

coordinates in the way shown) we may write

$$\frac{d(mx\dot{x})}{dt} = X$$

where X is the force in the x direction. If in addition we have $X dx = -dV$ where V is a function of position (the potential) and define a function K such that

$$\frac{\partial K}{\partial \dot{x}} = m\dot{x} = p, \text{ the momentum which}$$

does not contain x explicitly, then it can be seen that

$$\frac{d}{dt} \frac{\partial}{\partial \dot{x}} (K - V) - \frac{\partial}{\partial x} (K - V) = 0$$

since V does not contain \dot{x} explicitly and K does not contain x explicitly. This is of the Lagrange form where

$$L = K - V$$

We therefore obtain the results that

$$\frac{\partial L}{\partial \dot{x}} = p$$

$$\frac{\partial L}{\partial x} = \dot{p}$$

These results, in this form, are valid both for the Newtonian Dynamics and also for the later Relativistic Dynamics, though the exact form of K must be adjusted for relativity effects.

With m constant as in Newtonian Dynamics

$$\begin{aligned} K &= \int m\dot{x} dx \\ &= \frac{1}{2}m\dot{x}^2 \\ &= T \text{ the kinetic energy,} \end{aligned}$$

and the result $x \frac{\partial L}{\partial \dot{x}} - L = \text{constant.}$

becomes $x \cdot m\dot{x} - \frac{1}{2} m\dot{x}^2 + V = \text{constant}$.

or $T + V = \text{constant} = W$ the total energy and expresses the principle of the Conservation of Energy.

The expression $\delta S = \delta \int_{t_1}^{t_2} L \cdot dt = 0$ is known as Hamilton's Principle and S is Hamilton's Principle Function. The addition of the constant $T + V$ to L will not invalidate the equation (5) and it may be written

$$\begin{aligned} \delta A &= \delta \int_{t_1}^{t_2} (L + T + V) \cdot dt \\ &= \delta \int_{t_1}^{t_2} 2T \cdot dt \\ &= \delta \int_{t_1}^{t_2} p \cdot dx \end{aligned}$$

A being known as the Action or Hamilton's Characteristic Function.

In its three dimensional form this becomes

$$\delta \int_{t_1}^{t_2} p_x dx + p_y dy + p_z dz = 0$$

or $\delta \int_{t_1}^{t_2} \sum_{x,y,z} p_x \cdot dx = 0$

which is the Principle of Least Action or Mauvertuis' Principle.

$H = \sum_s p_s \dot{q}_s - L$ in its general form is known as the Hamiltonian, H being a function of the p 's, q 's, and t .

Hamilton (1805 - 1865) was aware of the formal analogy between Newtonian corpuscular dynamics and Geometrical Optics but was unable to see that it was more than formal. The principle of

least Action in the Newtonian form where m is constant, is reducible to $\delta \int v \cdot ds = 0$ for the trajectory of a corpuscle and the Fermat principle to $\delta \int \frac{ds}{u} = 0$ for the path of a light ray where u is the wave or phase velocity. The relation between these is made plain by the principles of Wave Mechanics where the relation between u and v is interpreted. Though Huyghens had shown that refraction and reflection could be explained by a wave theory of light, and that interference and diffraction received an adequate explanation on this theory, his view was not adopted until Fresnel (1788 - 1827) showed that it could give an explanation of rectilinear propagation. Then it seemed that the phenomena so far known could be explained by either the corpuscular or the wave theory and it remained for the decision between them to be made when Fizeau and Foucault measured the velocity of light in water. According to the corpuscular theory, the velocity should be greater in water than in air, but on the wave theory it would be less. From this period the study of Mechanics and that of Light became completely separated, that of Light proceeding by the study of waves, whereas that of Mechanics continued in the corpuscular form.

Wave Theories of Light.

If $S = f(t - \frac{s}{v})$ is the equation of a family of surfaces where s is the distance from the origin and t the time, then

Maxwell's equations however are not invariant for this type of transformation.

20th Century Theories

The new difficulties for the aether wave theories of light and for Newtonian relativity appeared when it became necessary to explain

1. The results of the Michelson-Morley experiment on the velocity of light, which failed to show any aether effect.
2. The behaviour of high speed particles.
3. The ultra-violet catastrophe in radiation, which led to the introduction of Planck's constant.
4. The photo-electric effect,

and between 1900 and 1905 the two new theories, the Quantum Theory and the Theory of Relativity came into being.

The Michelson Morley experiment of 1887 was designed to find the velocity of the earth relative to what was thought to be a stagnant aether. The negative results were explained by means of certain hypotheses, each of which led to what is known as the Lorentz transformation. The assumption made by both Lorentz and Fitzgerald, was that matter contracts in the direction of its motion by just that amount which would conceal its absolute velocity through the aether.

Einstein took the velocity of light as invariant for a change from one system of Cartesian coordinates to another moving with constant velocity with respect to it, and showed that

there is no absolute time, but that time has to be transformed in passing from the one system to the other.

If to an observer at rest at the origin of coordinates of the first system, an observer at rest at the origin of the second moves with constant velocity along the x axis, then an event specified by the coordinates x, y, z, and t in the first system becomes x', y', z', t' in the second, where

$$\begin{aligned}
 x' &= \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} \\
 y' &= y \\
 z' &= z \\
 t' &= t - \frac{vx}{c^2} \\
 &\quad \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}
 \end{aligned}$$

These equations define the Lorentz Transformation.

Minkowski showed that if we use a four dimensional space, coordinates x_1, x_2, x_3, x_4 then by analogy with three dimensions x_1, x_2, x_3 we could define the change in coordinates consequent on a 'rotation'. For three dimensions where the rotation is in the $x_1 x_2$ plane the new coordinates would be

$$\begin{aligned}
 x'_1 &= x_1 \cos \theta + x_2 \sin \theta \\
 x'_2 &= x_2 \cos \theta - x_1 \sin \theta \\
 x'_3 &= x_3 \quad \text{where } \theta \text{ is the angle of rotation}
 \end{aligned}$$

where $\beta = \frac{1}{KT}$, $K =$ Boltzmann's constant and $T =$ temp. absolute. This gives

$$u_{\nu} d\nu = \frac{8\pi\nu^2 d\nu}{3c^2} KT$$

where $u_{\nu} d\nu$ is the energy density of radiation for the frequency range ν to $\nu + d\nu$. This is the Rayleigh-Jeans formula, which, it can be seen, gives the energy as increasing with the square of the frequency. This is not actually true, as there is a maximum energy density for a particular wave length for each temperature. The total energy would, with the above formula be infinite.

Planck's revolutionary assumption was, that the energy of the oscillators did not form a continuous spectrum but that they had the values $nh\nu$ where n is an integer, so that instead of the integral form we get

$$\begin{aligned} \bar{\epsilon} &= \frac{\sum n \epsilon e^{-\beta n \epsilon_0}}{\sum e^{-\beta n \epsilon_0}} \\ &= \frac{d}{d\beta} \log \sum e^{-\beta n \epsilon_0} \\ &= \frac{\epsilon_0}{e^{\epsilon_0/KT} - 1} \end{aligned}$$

In order to conform with thermodynamical principle $\bar{\epsilon}$ must be a function of $\frac{\nu}{T}$ and therefore ϵ_0 must have the form of a

constant times frequency or $h\nu$, where h is 6.55×10^{-27} erg.sec. The curve obtained by putting this value of the mean energy of an oscillator into the expression for the energy density does fit experimental results. In this way Planck has introduced discrete energy states for the oscillator and quantum conditions for the absorption and emission of energy, by means of the quantum of action h . This he did in 1900.

Metals illuminated by ultra violet light or radiation of high frequency emit electrons and these show the following characteristics.

1. The velocity of the emitted electrons and therefore their energy, is dependent entirely on the frequency of the incident light and only the number emitted is dependent upon the intensity.
2. The electrons are emitted immediately the light falls upon the metal and there is not a time lag.

Neither of these results is in conformity with the continuous wave conception of the nature of light. Though Planck had shown that radiation must be absorbed in quanta, he did not assume that it was by nature corpuscular, and it still seemed, on the continuous wave conception, that light of greater intensity should eject electrons of greater energy and that the time taken for the absorption of the energy necessary to cause the expulsion, would be of the order of seconds.

Einstein showed that these results could be explained if

Substituting for E'_1 and p'_1 in equation (b) we get

$$\frac{(E_1 + E_2 - E'_2)^2}{c^2} - (p_1 + p_2 - p'_2)^2 = m_0^2 c^2$$

which simplifies to

$$\frac{E_1(E_2 - E'_2) - E_2 E'_2}{c^2} = p_1 \cdot p_2 - p_1 \cdot p'_2 - p_2 \cdot p'_2$$

Now if the electron is at rest before collision (a system of reference may be chosen in which this is so) then $p_1 = 0$

$p_2 \cdot p'_2 = |p_2| \cdot |p'_2| \cos \theta$ where θ is the angle between the original and final direction of the photon.

Putting $E_2 = h\nu$ and $E'_2 = h\nu'$ where ν and ν' are the initial and final frequencies, substitution from the original equations gives

$$\nu - \nu' = \frac{h\nu\nu'}{m_0 c^2} (1 - \cos \theta)$$

that is $\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_0 c^2} (1 - \cos \theta)$

or $\lambda' - \lambda = d\lambda = \frac{h}{m_0 c} (1 - \cos \theta)$ since $c = \nu\lambda = \nu'\lambda'$

for the photon. The quantity $\frac{h}{m_0 c}$ is known as the

Compton wave length.

The introduction of a similar duality into mechanics was not a consequence of an attempt to fit theory to a particular set of experimental data but began when De Broglie associated a wave length with a corpuscle of matter. It was Schrödinger to whom this suggested that the difficulties encountered in small scale dynamics, such as in the study of the atom, were

analogous to the difficulties of geometrical optics in the region of small scale effects such as interference, and that the solution might be sought, for mechanics, in the way in which physical optics sought a solution in these problems, by means of waves. The principle is known as the Schrödinger Principle.

In assuming that there is a periodicity connected with a particle De Broglie found it most natural to associate a stationary wave with a stationary particle. The equation for the stationary wave may be assumed to be of the form

$$\psi = A \sin 2\pi \nu' t' \sin \left(\frac{2\pi x'}{\lambda} + \delta \right)$$

which depends upon the time through the term $2\pi \nu' t'$. In the system of reference, this particle is at rest. To an observer stationary in another system, this particle is moving with velocity v . Let t be the time in this system, then

$$t' = \beta \left(t - \frac{vx}{c^2} \right)$$

for a relativity change of axes, so that the expression $2\pi \nu' t'$ becomes $2\pi \nu \left(t - \frac{vx}{c^2} \right)$. If $\nu = \beta \nu'$ then $\sin 2\pi \nu' t'$ becomes $\sin 2\pi \nu \left(t - \frac{vx}{c^2} \right)$ which is the form of a progressive wave with phase velocity $\frac{c^2}{v}$ and frequency ν . The particle with which this wave is associated has the velocity v for the observer, which the wave, which has been associated with it has the velocity V , such that $v \cdot V = c^2$. In addition the wave length to be associated with this wave is

$$\frac{V}{\nu} \quad \text{or} \quad \frac{c^2}{\nu v}$$

The De Broglie Wave Length

For a Lorentz transformation the scalar product of two, four vectors is invariant. The phase of a wave of the form

$$\Psi = \Psi_0 e^{-2\pi i \left(\frac{t}{T} - \frac{lx + my + nz}{\lambda} \right)}$$

travelling with the velocity of light is invariant, and we find it to be the scalar product of two vectors whose components are (x, y, z, ict) and $\left(-\frac{l}{\lambda}, -\frac{m}{\lambda}, -\frac{n}{\lambda}, -\frac{i}{cT} \right)$.

We have also shown that (p_x, p_y, p_z, p_4) is a four vector where p_4 is icm . Comparing p_4 with $-\frac{i}{cT}$ which may also be written $-\frac{i\nu}{c}$ we see that using the relation $W = mc^2 = h\nu$

p_4 may be written $h \cdot \frac{i\nu}{c}$ so that it is $-h$ times the fourth component of the vector $\left(-\frac{l}{\lambda}, -\frac{m}{\lambda}, -\frac{n}{\lambda}, -\frac{i}{cT} \right)$. This suggests that the vector (p_x, p_y, p_z, p_4) may reasonably be

put as $h \left(\frac{l}{\lambda}, \frac{m}{\lambda}, \frac{n}{\lambda}, \frac{i}{cT} \right)$ so that $p_x = \frac{hl}{\lambda}$, $p_y = \frac{hm}{\lambda}$
 $p_z = \frac{hn}{\lambda}$ so that $p = \frac{h}{\lambda}$.

$\lambda = \frac{h}{p}$ is the expression for the De Broglie wave length to be associated with a moving particle.

Returning to Fermat's principle and instead of $\delta \int \frac{ds}{v}$ write $\delta \int v \cdot \frac{ds}{v}$ or $\delta \int \frac{ds}{\lambda}$ and the principle becomes $\delta \int \frac{p \cdot ds}{h} = 0$, the link between the Fermat principle and the principle of Least Action now having been provided, since h is constant.

The Heisenberg relations may be written $\Delta p \Delta q \sim h$ where Δp is the uncertainty in p and Δq that in q .

The Wave Equation for a Particle

We have already seen by examination of the equation of a light wave in the form

$$\Psi = \Psi_0 e^{-2\pi i \left(\frac{t}{T} - \frac{lx+my+nz}{\lambda} \right)}$$

that the elements of the vector $\left(-\frac{l}{\lambda}, -\frac{m}{\lambda}, -\frac{n}{\lambda}, -\frac{i}{cT} \right)$ may be considered proportional to those of (p_x, p_y, p_z, iem) and given the relationship as $p_x = \frac{hl}{\lambda}$, $p_y = \frac{hm}{\lambda}$, $p_z = \frac{hn}{\lambda}$ for a particle. This therefore suggests the equation for a particle

$$\Psi = \Psi_0 e^{-2\pi i (Wt - p_x \cdot x - p_y \cdot y - p_z \cdot z)}$$

the phase velocity of which is $\frac{W}{P}$ and which is a solution of the wave equation

$$\nabla^2 \Psi = \left(\frac{P}{W} \right)^2 \frac{\partial^2 \Psi}{\partial t^2}$$

We may however, commence with the Hamilton principle function

$$S = \int L \cdot dt \quad \text{and using Cartesian coordinates put}$$

$$S_0 = \int_{xyz} p_x \cdot dx \cdot dt = \int_{xyz} p_x \cdot dx$$

$$H = \sum_{xyz} p_x \dot{x} - L = W, \text{ which is constant and}$$

equal to the total energy.

Then $S = S_0 - Wt$, where t is the time over which the integration is made.

The variation in S , that is δS may be written

$$\frac{\partial S}{\partial x} \delta x + \frac{\partial S}{\partial y} \delta y + \frac{\partial S}{\partial z} \delta z + \frac{\partial S}{\partial t} \delta t$$

$$\text{or } \frac{\partial S_0}{\partial x} \delta x + \frac{\partial S_0}{\partial y} \delta y + \frac{\partial S_0}{\partial z} \delta z - W \cdot \delta t$$

S_0 does not contain the time explicitly and W is constant.

From the expression for S_0

$$\frac{\partial S_0}{\partial x} = p_x ; \quad \frac{\partial S_0}{\partial y} = p_y ; \quad \frac{\partial S_0}{\partial z} = p_z \quad \text{and so}$$

comparing coefficients we have

$$\frac{\partial S}{\partial x} = p_x ; \quad \frac{\partial S}{\partial y} = p_y ; \quad \frac{\partial S}{\partial z} = p_z ; \quad \frac{\partial S}{\partial t} = -W$$

The velocity with which $S = \text{constant}$ moves outwards is given

by $p \cdot \delta n = W \delta t$ where $\delta n = (\delta x, \delta y, \delta z)$ and is $\frac{dn}{dt}$ and

therefore $\frac{W}{p}$

A suitable form of wave therefore appears to be $\Psi = \psi_0 e^{kS}$

or
$$\Psi = \psi_0 e^{k(S_0 - Wt)}$$

The quantity S has the dimensions of action and since the phase of a light wave is of zero dimensions, k must be of the dimensions of the reciprocal of action. Therefore putting

$k = \frac{2\pi i}{h}$ gives the form

$$\Psi = \psi_0 e^{-\frac{2\pi i}{h}(Wt - p_x x - p_y y - p_z z)}$$

from which the wave equation in the form

$$\nabla^2 \Psi = - \frac{4\pi^2 p^2}{h^2} \Psi \quad \text{can be obtained.}$$

In classical mechanics

$$p^2 = m^2 v^2$$

$$= 2m \times \text{kinetic energy.}$$

$$= 2m (E - V) \quad \text{where } E \text{ is the total energy}$$

and V the potential energy. If W is the relativistic total

energy then $E = W - m_0 c^2$

therefore writing the wave equation with the substitution for p we get

$$\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

which is the Schrodinger Wave Equation.

Since $\frac{\partial \psi}{\partial t} = -\frac{2\pi i}{h} W \psi$; $\frac{\partial \psi}{\partial x} = \frac{2\pi i}{h} p_x \psi$ etc.

the equation may be written

$$\nabla^2 \psi - \frac{8\pi^2 m}{h^2} (V + m_0 c^2) \psi + \frac{4\pi i m}{h} \frac{\partial \psi}{\partial t} = 0$$

which is a time dependent form which does not contain the energy explicitly. The value obtained above for $\frac{\partial \psi}{\partial x}$ suggests that p_x, p_y , etc may be replaced by the operators in the following way,

$$p_x = +\frac{h}{2\pi i} \frac{\partial}{\partial x}; \quad p_y = +\frac{h}{2\pi i} \frac{\partial}{\partial y}; \quad p_z = +\frac{h}{2\pi i} \frac{\partial}{\partial z}; \quad W = +\frac{h}{2\pi i} \frac{\partial}{\partial t}$$

and the Schrodinger equation then takes the form

$$\left[\frac{1}{2m} \left(\frac{h}{2\pi i} \frac{\partial}{\partial x} \right)^2 + \frac{1}{2m} \left(\frac{h}{2\pi i} \frac{\partial}{\partial y} \right)^2 + \frac{1}{2m} \left(\frac{h}{2\pi i} \frac{\partial}{\partial z} \right)^2 + V \right] \psi = E \psi$$

where the left hand side may be considered the operator form of $\frac{p^2}{2m} + V$. Either sign for p_x etc gives the same equation.

For classical mechanics the Hamiltonian $H = \sum_{x,y,z} p_x^2 - L$ becomes $\frac{p^2}{2m} + V = E$ giving the form

$$H \psi = E \psi$$

for the Schrodinger equation. The problem now becomes one of finding values of the energy E for which ψ is a well-behaved function, that is, finite from $-\infty$ to $+\infty$ continuous and

and real. The Schrodinger equation succeeded the Bohr theory of the atom (1912) and was able, without imposing additional quantum conditions to give the energy states of the atoms, the results being those obtained on the Bohr theory.

Calculation of the Energy levels on the Bohr Theory.

The calculation is based on classical dynamics and the orbits are supposed circular.

The Principle of Least Action gives $\oint p_x dx = \text{constant}$ and the quantum theory gives the value of the constant as nh . For an orbit of radius r where ds is an element of the orbit this means $\oint mv \cdot ds = 2\pi mvr = nh$

For the hydrogen atom with the charge on the nucleus $+e$ and a single electron with charge $-e$, the total energy is

$$E = \frac{1}{2} mv^2 - \frac{e^2}{r}$$

and the force of attraction is

$$\frac{e^2}{r^2} = \frac{mv^2}{r}$$

This gives for E the value $\frac{2\pi^2 me^4}{n^2 h^2}$

Calculation of the Energy levels of the Hydrogen atom from the Schrodinger Equation

In this case the equation must be written

$$\nabla^2 \psi + \frac{8\pi^2 m_e}{h^2} \left(E + \frac{e^2}{r} \right) \psi = 0$$

where m_e is the mass of the electron.

$$(\ell + n + 1)(\ell + n)a_{n+1} + 2(\ell + n + 1)a_{n+1} - (\ell + n)a_n + (\lambda - 1)a_n - \ell(\ell + 1)a_{n+1} = 0$$

Therefore $a_{n+1} \{ (\ell + n + 1)(\ell + n + 2) - \ell(\ell + 1) \} = a_n(\ell + n + 1 - \lambda)$
 a_{n+1} is zero if $\lambda = \ell + n + 1$ which means that the series terminates, in this case.

$$\text{But } \alpha^2 = \left[\frac{4\pi^2 m_e e^2}{h^2(n + \ell + 1)} \right]^2 \quad \text{since } \lambda = \frac{4\pi^2 m_e e^2}{h^2 \alpha}$$

$$\text{that is, } \frac{-8\pi^2 m_e E_n}{h^2} = \frac{16\pi^4 m_e^2 e^4}{h^4(n + \ell + 1)^2}$$

Therefore

$$E_n = -\frac{2\pi^2 m_e e^4}{h^2(n + \ell + 1)^2} \quad \text{which since } n + \ell + 1$$

is an integer, is the Bohr form. The function ψ is

found to be of the form $P_l^m(\mu)$ where $\mu = \cos \theta$ and

$$R = F_{nl} \quad \text{where } F_{nl} = e^{-\frac{r}{a}} \sum_n a_n r^{l+n}$$

$$\text{so that } \psi_{n,l,m} = F_{nl} P_l^m(\mu) \cos m\phi$$

The energy levels found in a similar manner for a linear oscillator do not agree with those obtained in the classical way, for in this case, half quantum numbers, which had to be introduced into the early quantum mechanics are found to occur naturally.

The Schrodinger equation is not able to give the fine structure found in the spectra of the hydrogen atom any more

than the Bohr theory. For the latter, Sommerfeld, regarding the difficulty as due to the use of Newtonian instead of Relativistic dynamics worked out the following formula.

$$E_{nk} = - \frac{Rh}{n^2} \left\{ 1 + \frac{\alpha^2}{n^2} \left(\frac{n}{k} - \frac{3}{4} \right) \right\} \quad \alpha^2 = (5.2 \times 10^{-5} \text{ c.g.s})$$

$\alpha = \frac{2\pi e^2}{hc}$ and is the fine structure constant.
and $-\frac{Rh}{n^2}$ is the Bohr value of the energy.

Sommerfeld obtained his correction^{ion} by changing the idea of the circular orbit, and introducing relativistic mechanics. Using two variables r and θ so that the orbit is referred to polar coordinates, we get two independent equations

$$\oint_{2\pi} p_r dr = \oint_{2\pi} m \dot{r} dr = n_1 h$$

and $\int_0^{2\pi} p_\theta d\theta = \int_0^{2\pi} m r^2 \dot{\theta} d\theta = n_2 h$ since the quantum conditions are applied to each component of the momentum

and $m = \beta m_0$, $v = (\dot{r}^2 + r^2 \dot{\theta}^2)^{\frac{1}{2}}$

The total energy = W

$$\begin{aligned} &= mc^2 - \frac{e^2}{r} \\ &= c \sqrt{m_0^2 c^2 + p_r^2 + \frac{p_\theta^2}{r^2}} - \frac{e^2}{r} \\ &= E + m_0 c^2 \end{aligned}$$

$p_\theta = \frac{n_2 h}{2\pi}$ and with this value

$$p_r = \sqrt{A + \frac{B}{r} + \frac{C}{r^2}}$$

where

$$A = \frac{E^2}{c^2} + 2m_0 E$$

$$B = \frac{E e^2}{c^2} + m_0 e^2 E$$

$$C = \frac{e^4}{c^2} - p_\theta^2$$

$$= \frac{e^4}{c^2} - \frac{h^2}{4\pi^2}$$

Completion of the integration leads to the formula given,

$$\text{if } n = n_1 + n_2 \quad \text{and } k = n_1$$

Since relativity considerations led to this correction formula which gives the correct results in the case of the hydrogen spectra, attempts at a relativistic wave equation which would give the results without the need for correction were made.

Using Relativistic dynamics we get that for a free particle

$$W = \sqrt{m_0^2 c^4 + p^2 c^2}$$

but there is no operator to replace the right hand side as it stands. It may however be rewritten

$$\frac{W^2}{c^2} = m_0^2 c^2 + p^2$$

and now substituting the operators representing W and p we get the equation

$$\left[\nabla^2 + \left(\frac{2\pi i}{h} \right)^2 m_0^2 c^2 \right] \Psi = \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2}$$

which however, is of the second order in time. This requires that both Ψ and $\frac{d\Psi}{dt}$ be known at time $t = 0$ in order that for a solution for any other time may be obtained and constitutes a difficulty for the equation. This form of equation was due to Klein-Gordon and was the first attempt at a relativistic wave equation.

As with the first wave equations of optics, the Fresnel scalar waves, the first wave equations of mechanics, the Schrodinger equation with a single Ψ component, could not deal

with the problems of the effect of a magnetic field. Neither the Schrodinger equation nor the Sommerfeld fine structure corrections were effective in dealing with the Zeeman effect. The idea of a spinning electron was introduced by Uhlenbeck and Goudsmit and satisfactory results were obtained with this addition to the theory, but the equation, did not, of itself give the corrections. Pauli attempted to include spin by means of matrices with two rows and columns and had two Ψ components, and finally Dirac proposed a first order, relativistic equation for an electron, having four Ψ components, in which the spin numbers occur quite naturally. There is the difficulty of negative energy states here, but the equation predicts the energy levels for hydrogen and the fine structure and in addition terms appear when a field is introduced with the value of the Bohr magneton as a factor.

The Pauli attempt.

The Schrodinger equation may be written

$$\left(\frac{p^2}{2m} + V \right) \Psi = E \Psi$$

and in order to account for the spin Pauli suggested that it be written

$$\left(\frac{p^2}{2m} + V + S \right) \Psi = E \Psi$$

where S stands for the terms due to the magnetic field H.

In the operator form

$$S = \sigma_1 \mu_0 H_1 + \sigma_2 \mu_0 H_2 + \sigma_3 \mu_0 H_3$$

$$\begin{vmatrix} \mu_0 H_3 - \lambda & \mu_0 (H_1 + iH_2) & 0 & 0 \\ \mu_0 (H_1 - iH_2) & -\mu_0 H_3 - \lambda & 0 & 0 \\ 0 & 0 & \mu_0 H_3 - \lambda & \mu_0 (H_1 - iH_2) \\ 0 & 0 & \mu_0 (H_1 + iH_2) & \mu_0 H_3 - \lambda \end{vmatrix} = 0$$

and they are $\lambda = \pm \mu_0 H$ where $H = \sqrt{H_1^2 + H_2^2 + H_3^2}$

This result suggests that the energy arises from a magnetic moment whose components are represented by the matrices $\sigma_i \mu_0$ with the proper values $\pm \mu_0$. This result is obtained without any special hypotheses added to the equation and have arisen from the form of the equation itself.

The Invariance of the Dirac Equation

The Dirac equation is a relativistic equation and its properties under a Lorentz transformation are distinctive. Commencing with the equation in the form

$$[P_4 + \sum \alpha_i P_i + \alpha_4 m_0 c] \psi = 0$$

multiply from the front by $i\alpha_4$ to obtain the form

$$[i\alpha_4 P_4 + \sum_1^3 i\alpha_4 \alpha_i P_i + im_0 c] \psi = 0$$

Let $P_1 = \pi_1$, $\gamma_1 = i\alpha_4 \alpha_1$
 $P_2 = \pi_2$, $\gamma_2 = i\alpha_4 \alpha_2$
 $P_3 = \pi_3$, $\gamma_3 = i\alpha_4 \alpha_3$
 $iP_4 = \pi_4$, $\gamma_4 = \alpha_4$

and the equation may be written

$$\left(\sum_1^4 \gamma_i \pi_i + im_0 c \right) \psi = 0$$

For a Lorentz transformation, the following equation give the manner in which quantities may be transformed.

$$x'_i = o_{ij} x_j$$

$$x_j = o_{kj} x'_k \quad \text{where } o_{ij} o_{kj} = \delta_{ik}$$

Changing the π 's in this manner gives the equation

$$\left(\sum_i^4 \gamma_i o_{ji} \pi'_j + im_0 c \right) \Psi = 0$$

Let $\gamma'_j = o_{ji} \gamma_i$

Then $\left(\sum_j^4 \gamma'_j \pi'_j + im_0 c \right) \Psi = 0$ where Ψ is now a function of the new coordinates.

Assuming that γ'_j may be written $\Lambda^{-1} \gamma_j \Lambda$ where Λ is a matrix, and justifying this assumption by the calculation of the matrix for which it holds we therefore obtain

$$\left(\sum_j^4 \Lambda^{-1} \gamma_j \Lambda \pi'_j + im_0 c \right) \Psi = 0$$

and $\left(\sum_j^4 \gamma_j \Lambda \pi'_j + \Lambda im_0 c \right) \Psi = 0$

Λ permutes with π and therefore

$$\left(\sum_j^4 \gamma_j \pi'_j + im_0 c \right) \Lambda \Psi = 0$$

or $\left(\sum_j^4 \gamma_j \pi'_j + im_0 c \right) \Psi' = 0$ where $\Psi' = \Lambda \Psi$.

To find the value of Λ

For a Lorentz transformation in which the 'rotation' takes place in the $x_1 x_4$ plane the matrix O giving the elements o_{ij} may be written

$$\begin{pmatrix} \text{ch } \theta & 0 & 0 & -\text{ish } \theta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \text{sh } \theta & 0 & 0 & \text{ch } \theta \end{pmatrix}$$

Returning to the original Dirac equation and making the change from P to P' in accordance with the Lorentz transformation it becomes

$$(P'_4 \text{ch } \theta + P'_1 \text{sh } \theta + \alpha_1 P'_1 \text{ch } \theta + \alpha_1 P'_4 \text{sh } \theta + \alpha_2 P'_2 + \alpha_3 P'_3 + \alpha_4 m_0 c) \Psi = 0$$

or

$$[P'_4 (\text{ch } \theta + \alpha_1 \text{sh } \theta) + \alpha_1 P'_1 (\text{ch } \theta + \alpha_1 \text{sh } \theta) + \alpha_2 P'_2 + \alpha_3 P'_3 + \alpha_4 m_0 c] \Psi = 0$$

This may be put

$$[P'_4 (\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2})^2 + \alpha_1 P'_1 (\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2})^2 + \alpha_2 P'_2 (\text{ch}^2 \frac{\theta}{2} - \text{sh}^2 \frac{\theta}{2}) + \alpha_3 P'_3 (\text{ch}^2 \frac{\theta}{2} - \text{sh}^2 \frac{\theta}{2}) + \alpha_4 m_0 c (\text{ch}^2 \frac{\theta}{2} - \text{sh}^2 \frac{\theta}{2})] \Psi = 0$$

$$\text{Since } (\text{ch}^2 \frac{\theta}{2} - \text{sh}^2 \frac{\theta}{2}) = 1 = (\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2})(\text{ch } \frac{\theta}{2} - \alpha_1 \text{sh } \frac{\theta}{2})$$

the permutation rules allow this to be written

$$(\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2})(P'_4 + \alpha_1 P'_1 + \alpha_2 P'_2 + \alpha_3 P'_3 + \alpha_4 m_0 c)(\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2}) \Psi = 0$$

Multiplying this from the front by $(\text{sh } \frac{\theta}{2} - \alpha_1 \text{ch } \frac{\theta}{2})$

$$\text{we have } (P'_4 + \alpha_1 P'_1 + \alpha_2 P'_2 + \alpha_3 P'_3 + \alpha_4 m_0 c)(\text{ch } \frac{\theta}{2} + \alpha_1 \text{sh } \frac{\theta}{2}) \Psi = 0$$

$$\text{so that } \Lambda \Psi = (\text{ch } \frac{\theta}{2} \cdot I + \alpha_1 \text{sh } \frac{\theta}{2}) \Psi = \Psi,$$

where I is the unit matrix.

Therefore

$$\Lambda = \begin{pmatrix} \text{ch } \frac{\theta}{2} & 0 & 0 & \text{sh } \frac{\theta}{2} \\ 0 & \text{ch } \frac{\theta}{2} & \text{sh } \frac{\theta}{2} & 0 \\ 0 & \text{sh } \frac{\theta}{2} & \text{ch } \frac{\theta}{2} & 0 \\ \text{sh } \frac{\theta}{2} & 0 & 0 & \text{ch } \frac{\theta}{2} \end{pmatrix}$$

This gives the transformation

$$\psi'_1 = \text{ch } \frac{\theta}{2} \psi_1 + \text{sh } \frac{\theta}{2} \psi_4$$

$$\psi'_2 = \text{ch } \frac{\theta}{2} \psi_2 + \text{sh } \frac{\theta}{2} \psi_3$$

$$\psi'_3 = \text{ch } \frac{\theta}{2} \psi_3 + \text{sh } \frac{\theta}{2} \psi_2$$

$$\psi'_4 = \text{ch } \frac{\theta}{2} \psi_4 + \text{sh } \frac{\theta}{2} \psi_1$$

which introduces half angles, so that the quantities ψ do not transform like a four vector under the Lorentz transformation. Functions which transform in the above manner are called spinors and were introduced into physics by Dirac.

$\psi^* \psi$ as in the Schrodinger theory is the probability density ρ . In the Dirac theory it is not invariant but transforms like the fourth component of a vector.

To demonstrate this we have

$$\begin{aligned} \gamma'_i &= o_{ij} \gamma_j \quad (o_{ij} \gamma_j) \\ &= o_{i1} \gamma_1 + o_{i2} \gamma_2 + o_{i3} \gamma_3 + o_{i4} \gamma_4 \end{aligned}$$

$$\gamma'^x_i = o^x_{i1} \gamma^x_1 + o^x_{i2} \gamma^x_2 + o^x_{i3} \gamma^x_3 + o^x_{i4} \gamma^x_4$$

$$\text{Since } (\gamma'^x_i)_{ln} = (\gamma'_i)^+_{nl}$$

$$(\gamma'_i)^+ = o_{i1} \gamma_1 + o_{i2} \gamma_2 + o_{i3} \gamma_3 - o_{i4} \gamma_4$$

since o_{i4} is imaginary.

$$\begin{aligned} \gamma_4 (\gamma'_i)^+ / \gamma_4 &= -o_{i1} \gamma_1 - o_{i2} \gamma_2 - o_{i3} \gamma_3 - o_{i4} \gamma_4 \\ &= -\gamma'_i \end{aligned}$$