THE CALCULATION OF STELLAR OPACITY

Helen M. Hollingsworth

A Thesis Submitted for the Degree of PhD
at the
University of St Andrews

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THE CALCULATION OF STELLAR OPACITY

by

Helen M. Hollingsworth

A Thesis presented for the Degree of Doctor of Philosophy

in the University of St Andrews

December, 1966

DECLARATION

I hereby declare that the following Thesis is based upon the results of experiments carried out by me, that the Thesis is my own composition, and that it has not previously been presented for a Higher Degree. The research was carried out in the University Observatory, St Andrews.

[redacted]

CERTIFICATE

I certify that Helen M. Hollingsworth has spent nine terms at Research Work in the University Observatory, St Andrews, that she has fulfilled the conditions of Ordinance No. 88 (St Andrews) and that she is qualified to submit the accompanying Thesis in application for the degree of Ph.D.

[redacted]

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CHAPTER I

INTRODUCTION

The structure and evolution of stars depends very sensitively on the rate at which radiation is transferred outwards through the stellar material. For stars of the sun's mass and greater the bulk of the material is at temperatures above a million degrees, and an accurate knowledge of opacities under these conditions is important for calculating the time scales of various phases of stellar development. At these high temperatures the pressures are correspondingly large, ranging from the order of a hundred megobars and upwards. As a star evolves the composition of the material varies from almost pure hydrogen with a few per cent by mass of the heavier elements like carbon, nitrogen, oxygen, neon, sodium, magnesium, aluminium, silicon, argon, and iron, to a mixture of almost pure helium with the same heavy element mixture.

At the very high temperatures right in the centre of the star, thermonuclear reactions occur, providing the source of the stellar energy. However at these temperatures all the elements that can ever attain appreciable abundance are completely ionized, and the calculations for the absorption and emission of radiation are simplified when there are no bound electrons. It is in the intermediate temperature range that the problem becomes more difficult. This text is concerned with the absorption and emission processes for stellar material in these conditions, and the calculation of opacity coefficients as the appropriately weighted averages over frequency of the resulting absorption coefficients.

The mean free path of the average photon in the hot stellar interior is usually of the order of a few centimetres or less, and particle mean free paths are also very small, so that collisions maintain the matter in a steady state of ionisation and excitation. Temperature gradients can be estimated by considering the drop of about 10^{7} °K over a radius of 10^{11} cm. in a typical star. This implies that the temperature changes by only about 10^{-4} °K per centimetre, so that in travelling along a mean free path a photon moves through a region whose temperature varies by only a fraction of a degree. Thus the photon is absorbed by material that is at the same temperature as the emitting material. The matter and radiation temperatures are almost equal, and we have local thermodynamic equilibrium and can apply Boltzmann statistics.

The macroscopic variations in T however, produce a net outward flux of radiative energy and a consequent variation in the radiation pressure with depth which is important in maintaining hydrostatic equilibrium in stars.

THE EQUATION OF RADIATIVE TRANSFER AND THE PLANCK AND ROSSELAND MEANS

The change in specific intensity, I_v, of a beam of radiation of frequency v, per unit path length through a material of density , $\frac{dI}{ds}v$, can be considered as follows. The beam will lose intensity by an amount $k_v I_v$ due to absorption by the medium with absorption coefficient k_v per gram of the material. It will also gain intensity by the induced emission into the beam. The induced emission is proportional to the intensity of the original beam, and is of the same direction, frequency, polarisation and phase. By the principle of detailed balance, and with the Boltzmann distribution for local thermodynamic equilibrium, the induced emission at temperature T contributes an amount $k_\nu e^{-h\nu/kT} I_\nu$ per unit path length. In addition the spontaneous emission contributes an amount j_ν. Then

$$\frac{dI_\nu}{ds} = \underbrace{-\rho\kappa_\nu I_\nu}_{\text{absorption}} + \underbrace{\rho\kappa_\nu e^{-u} I_\nu}_{\text{induced emission}} + \underbrace{j_\nu(s)}_{\text{spontaneous emission}} \qquad (11)$$

The spontaneous emission depends only on the states of the matter and not upon the radiation field, so that for L.T.E. the spontaneous emission is exactly the same as for the thermodynamic equilibrium when $\frac{dI_\nu}{ds}$ is zero, and the intensity is the Planck black body distribution. Thus

$$I_\nu = B_\nu - \frac{1}{\rho\kappa_\nu'}\frac{dI_\nu}{ds} \qquad (12)$$

where $$\kappa_\nu' = \kappa_\nu(1-e^{-u}) \qquad (13)$$

If we assume that the actual radiation field at each point, I_ν, does not differ greatly from the black body field B_ν, and carry out a perturbation expansion then the flux is given by

$$F_{\nu,s} = -\frac{4\pi}{3}\frac{1}{\rho\kappa_\nu'}\frac{dB_\nu}{ds} \qquad (14)$$

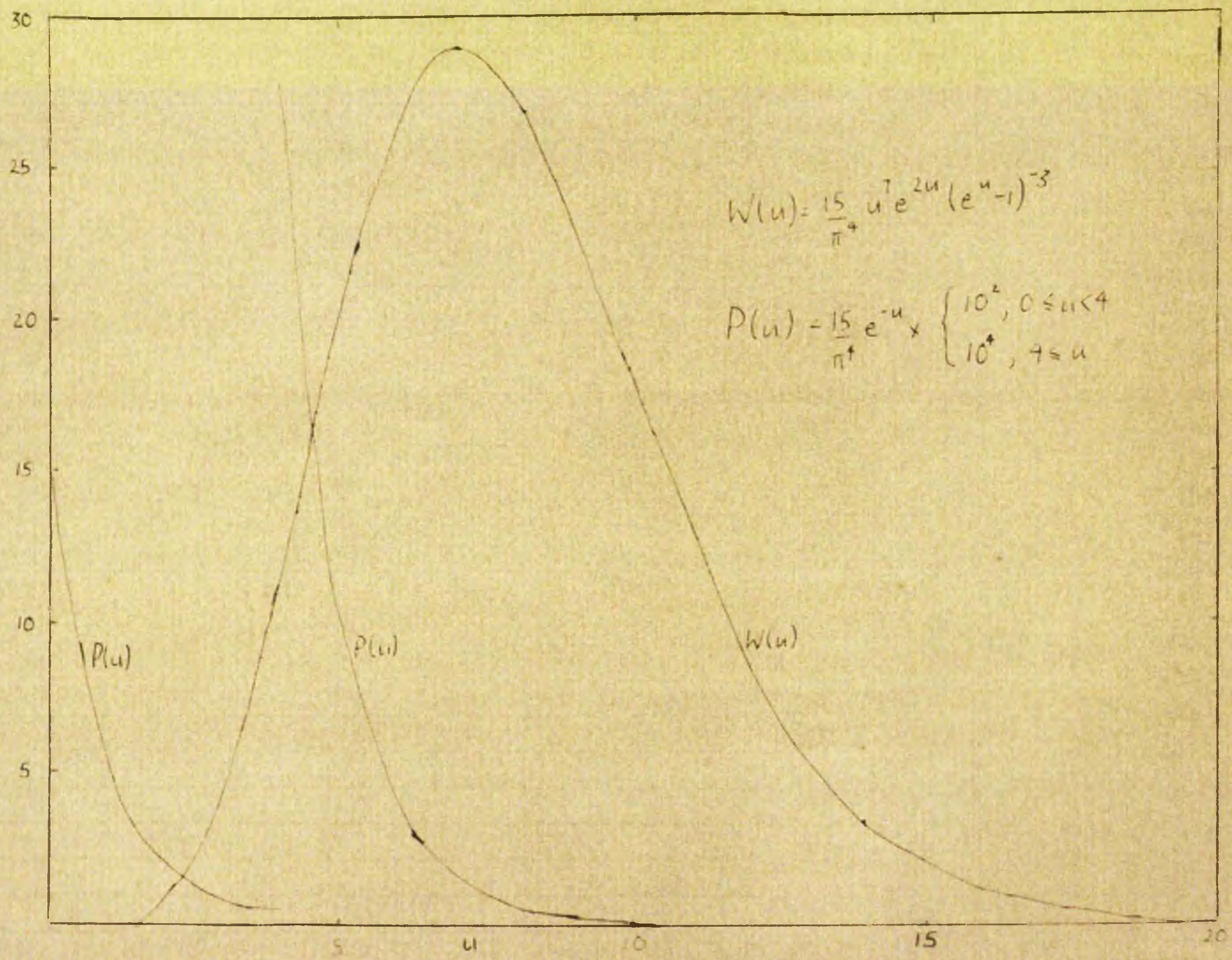

Fig 1A. Weighting Functions for Planck and Rosseland Mean Opacities.

Hence the total flux of radiation over all frequencies across a layer of stellar material may be expressed in terms of the Rosseland mean of the absorption coefficient $\bar{k}_R$

$$\frac{1}{\bar{\kappa}_R} = \frac{\int \frac{1}{\kappa_{\nu'}} \frac{dB_\nu}{dT} d\nu}{\int \frac{dB_\nu}{dT} d\nu} = \int \frac{W(u)\,du}{u^3 \kappa_\nu} \qquad (15)$$

with.

$$W(u) = \frac{15}{4\pi^4} \frac{u^7 e^{2u}}{(e^u - 1)^3} \quad ; \quad u = \frac{h\nu}{kT} \qquad (16)$$

The weighting fuction W(u) is shown in the graph 1A.

If on the other hand we were interested in the total flux of radiation emitted at a free surface then the appropriate mean over frequency would be the Planck mean, $\bar{k}_p$;

$$\bar{\kappa}_p = \frac{\int \kappa_{\nu'} B_\nu d\nu}{\int B_\nu d\nu} = \frac{15}{\pi^4} \int u^3 \kappa_\nu e^{-u} du \qquad (17)$$

THE ABSORPTION COEFFICIENT K_ν, AND THE PROCESSES CONTRIBUTING TO IT

Any process capable of removing quanta from an incident beam or emitting quanta into it, must be considered in the opacity problem. The ability of a particle to absorb radiation depends on such parameters as its charge, velocity, and energy, and upon its interaction with the surrounding potential field. Consequently, in calculating the opacity per gram of the mixture, we have to decide the possible states or classes of particles we can have to absorb the radiation, and find the number of particles per gram we expect to have in each class. Then for each particular class and frequency, we have to calculate the probability of absorption when an interaction takes place between a photon of that frequency and a member of the class. We can then sum the contributions from all the particles to obtain the absorption coefficient per gram of the absorbing material as a function of frequency, v.

The fraction of the flux of radiation of frequency v absorbed per gram is

$$\kappa_\nu = \sum_i N_i \sigma_i(\nu) \qquad (18)$$

where N_i is the number of absorbers of type i per gram of the mixture, and $\sigma_i(\nu)$ is the cross-section at frequency v for one of these particles.

Since the material is so highly excited that even the individual atoms are almost ionised, all molecules will be dissociated and absorbing particles such as negative ions will certainly not appear. On the other hand, processes such as pair production and annihilation occur only at much higher temperatures. To produce a free electron-positron pair requires an incident quantum of energy at least $2mc^2$, while even the production of a bound electron and positron requires energies greater than mc^2. Thus the absorption coefficient is the result of a multitude of atomic and free electron interactions involving many elements and many stages of ionisation.

The most important process is simple absorption and its inverse when a quantum is absorbed by an atomic system, its energy being transferred to excitation of the electrons. There are three different types of this absorption. Firstly we can have an electron in a bound state of an atom excited to another bound state, the familiar line absorption. It has been argued that although the individual lines are of great strength compared with other absorption processes, they will simply make a very small region of the spectrum opaque to radiation, and since the opacity is a weighted average over frequency of the absorption coefficient, the blackness of these small regions will not appreciably alter the opacity. However under the extreme temperature and density conditions of the stellar interior the individual lines are much broader than under normal terrestial conditions, and there will be an enormous number of lines of comparable strength arising from the various ionic configurations. Among the factors contributing to the line breadth are natural breadth, collision effects, both elastic and inelastic, and Doppler breadth, all of which are much more important in hot dense plasmas. Furthermore the Rosseland mean, being a harmonic mean, is very sensitive to the "windows" in the spectrum, and the shape of the line many half-breadths from the centre may be significant.

Secondly a bound state electron may interact with a quantum of higher energy, and make a transition into the continuum of free states available - the photoelectric effect. In contrast to line absorption this process is possible for any energy of the incident quantum greater than the ionisation energy of the electron, and there is an absorption edge at the threshold frequency.

Finally there may be transitions from one free state to another, and since there is a continuum of free states any amount of energy may be absorbed by this process. Since the ability of a particle to absorb radiation depends on its binding to the nucleus to conserve momentum, a bound electron has a much larger photo-electric cross section than a loosely bound one at the same frequency, and the free-free cross sections will be even smaller. On the other hand a very large proportion of the electrons are free, and also at large frequencies below the ionisation edges, free-free absorption may be the only pure absorption process possible.

All these processes differ only in the nature of the initial and final states of the atom. The radiation in each case affects the stability of an atom through the interaction of the atom's charge distribution with the electric and magnetic fields perpendicular to the direction of propagation of the radiation. Besides being absorbed, incident quanta may interact with atoms or electrons and emerge scattered from their original paths. Here the scattering is mainly Compton scattering by free electrons, and there is no inverse process corresponding to stimulated emission. Scattering becomes relatively more important at the higher temperatures or lower densities. The diagram 1B indicates the dominant processes under different conditions.

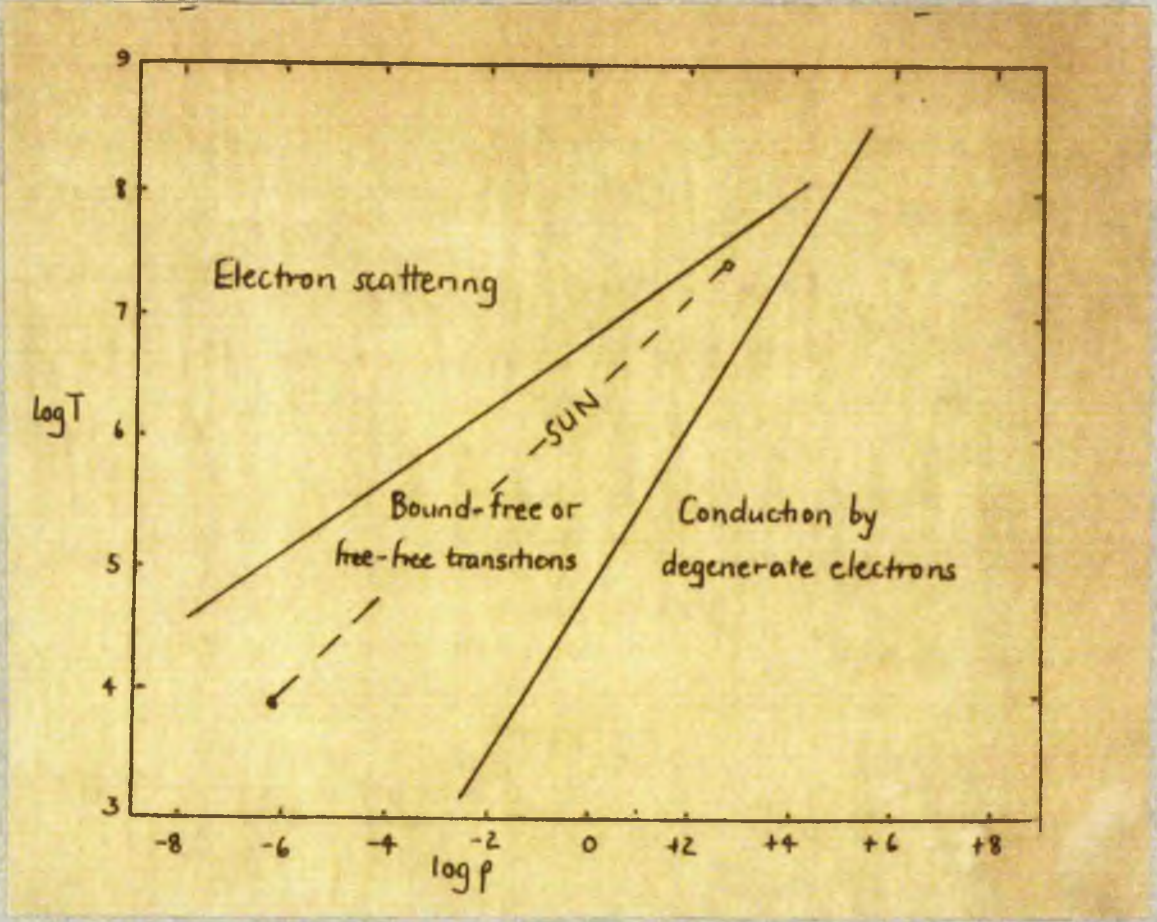

Fig 1B. Temperature-density diagram for the opacity. (Schwarzchild P72)

STEPS IN COMPUTING OPACITIES

The steps necessary to calculate opacities may therefore be summarised as follows:-

(1) Calculation of the occupation numbers N_i

Statistical mechanics predict the relative probabilities of the various possible electron states given their energy levels and associated multiplicities. These have to be calculated according to quantum mechanical principles by adopting a feasible model for the atom and the surrounding potential field.

(2) Calculation of frequencies of absorption lines and edges

This is necessary to determine what particles contribute in the summation of (1.8) at each frequency, and is again a quantum mechanical problem in finding energy levels and intercombination rules for the various atomic configurations.

(3) Calculations of the cross sections for the various atomic processes

These require the transition matrix elements requiring knowledge of the quantum mechanical wave functions describing the possible initial and final electron states. Usually only dipole matrix elements are required.

(4) Line profiles

In order to discover how the strength of an absorption line is distributed as a function of frequency, it is necessary to consider all the various ways in which an atom evolves when perturbed by the various surrounding particles. This involves a time dependent perturbation approach and again requires knowledge of the transition matrix elements.

(5) The absorption coefficient and opacity

Having obtained the information listed in 1 - 4 the absorption coefficient for each element in the mixture may be tabulated as a function of frequency. Finally the opacity coefficient for the mixture may be found by forming the mixture spectrum from the element spectra according to their concentrations, and performing the appropriate integrals over frequency.

OUTLINE OF CHAPTERS

The following chapters 2 - 4 give details of how all this may be done. In chapter 2 a model for the atom will be discussed and a method given for finding energy levels. All the information required in steps 1 and 2 is then derived. In chapters 3 and 4 the cross sections are given enabling the spectra to be formed. Chapter 3 deals with the processes involving a continuum of photon frequencies, the bound-free, and free-free absorption and scattering. Chapter 4 pays attention to the development of the electron wave functions in time, and the contribution of line absorption.

In chapter 5 the numerical procedures and approximations taken in adapting these methods to a form suitable for use on a computer, are given, and the results already obtained with such programs are listed and discussed.

Before embarking on the present methods, however, the progress of opacity calculations hitherto will be briefly reviewed.

HISTORICAL SURVEY

Although Scwarzschild had developed the equations of radiative equilibrium for the outer layers of a star in 1906, most of the work on stellar interiors before Eddington's investigations, was based on convective models. In fifteen papers written between 1916 and 1926, Eddington establsihed the importance of radiation transport in the inner regions of stars and examined the consequences in stellar models. In 1923 Kramers had produced absorption cross sections by calculating the radiation emitted from the acceleration of an electron moving classically along a hyperbolic path in the field of a central nuclear charge. In 1924 Rosseland emphasized the importance of working with a properly weighted mean of the coefficient of absorption. Eddington used the results of Kramers to estimate the opacity according to the Rosseland mean, but found that the theoretical results he obtained were far too small to be reconciled with the observational value he found for

Capella. The discrepancy could only be removed by allowing stars to have low mean molecular weights, that is, large hydrogen abundances.

The next advance became possible when Gaunt calculated absorption cross sections for bound free transitions near the threshold according to quantum mechanics, expressing his results in terms of the ratios to the Kramers cross sections. The cross sections were subsequently extended to higher frequencies. Gaunt himself only calculated a straight mean of the opacity with his results.

Stromgren considered the effect of Gaunt's results but then used an average constant value of the Gaunt factor to retain the simple v^{-3} dependence of the Kramers cross sections. This simplification enabled him to perform the mean over the Rosseland weighting function as a simple sum of terms corresponding to each absorption edge. He considered free-free absorption and bound-free absorption processes with pure unscreened Coulomb energy levels, and calculated opacities for various proportions of hydrogen and the Russell mixture. He assumed that the hydrogen affected the opacity by supplying extra electrons, but did not include the free-free absorption in the regions of the hydrogen nuclei themselves. Stromgren also investigated the effects of scattering and showed that it was important at high temperatures, although the different frequency dependence and the harmonic nature of the Rosseland mean made it impossible to combine scattering effects with pure absorption accurately, using Stromgren's function and summation methods.

Morse (1940) proposed an iterative scheme for finding more accurate average energy levels for the discrete states and better occupation numbers, based on the use of Slater integrals and depression of the continuum according to zero temperature Thomas-Fermi potentials. He carried out opacity calculations on four mextures using Gaunt factors for bound-free and free-free absorption calculated by Menzel and Pekeris (1935). The Morse results could not be improved until better Gaunt factors and more efficient computing methods were available, although several advances were made relevant to the lower temperatures and densities of the outer stellar layers.

In 1947 Mayer presented detailed calculations obtaining the opacity of iron. He introduced the model for the atoms adopted in this thesis, in which it is assumed that the positively charged cores of the nuclei and attendant bound electrons are screened from each other by a uniform time-averaged distribution of free electrons. On the basis of this model he calculated average occupation numbers according to the "independent electron approximation". Scattering processes were discussed and account taken of the fact that scattering of induced radiation out of the beam is compensated exactly by induced scattering into the beam.

Mayer also paid much attention to including line absorption in his opacity calculations, and studied the effect of both single lines and statistical treatment of large numbers of overlapping lines, on the Rosseland opacity. In the case of pure iron at a density of 7.83gm/cc and a temperature of 1000 electron volts, he found that the line absorption increased the opacity by a factor three over the continuous opacity.

In 1955 Keller and Meyerott published opacities for 13 mixtures at temperatures ranging from 10^5 to $2x10^7$ degrees with refinements for electron screening and pressure ionization in elements heavier than helium, but they did not include line absorption.

Recently Cox at Los Alamos has given opacities over a wide range of pressures and temperatures. He includes all the processes of pure absorption and scattering following the principles established by Mayer. The results clearly emphasize the importance of line absorption.

The present work aims to calculate opacities with special investigation of the optimum use of hydrogenic Gaunt factors, and the seriousness of the deformation of the potential field from the Coulomb shape in the neighbourhood of the core electrons. The problem of line absorption and the various line broadening mechanisms will also be considered in detail. This involves calculating the probability of all significant ionic configurations and the splitting of lines. In view of the sensitivity of a harmonic mean to the less opaque regions of the spectrum and the positions of the absorption edges, the splitting of the edges may also be important and this effect will be taken into account.

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CHAPTER II

ENERGY LEVELS AND OCCUPATION NUMBERS

In order to obtain wave functions and energy levels to describe the possible electron orbits it is necessary to decide upon the form of the potential field in which the electron moves; this field will be a rapidly fluctuating function depending on the positions of all the surrounding particles. It is necessary to simplify the situation and obtain average energy levels by considering the time-averaged or statistical picture over many configurations. Having found the energy levels we can then proceed to consider the statistical mechanics of highly ionised material and to calculate the occupation numbers. Fortunately at high temperatures these do not depend critically on the energy levels so that the simplifications are justified.

THE AVERAGE POTENTIAL IN WHICH AN ELECTRON MOVES

When an electron penetrates very close to an atomic nucleus then the potential will tend to the unscreened Coulomb form Ze/r: that is, the interaction with the nucleus will dominate all other interactions. In these regions we shall expect to find possible negative energy states, representing electrons with insufficient kinetic energy to overcome the potential barrier and break away from the nucleus without stimulation from some external source. The nuclei with their attendant bound electrons will be embedded in a sea of high energy electrons moving freely from one ion to the next. These electrons may have any total energy above that required to climb the potential barrier between ions, giving rise to a continuous spectrum.

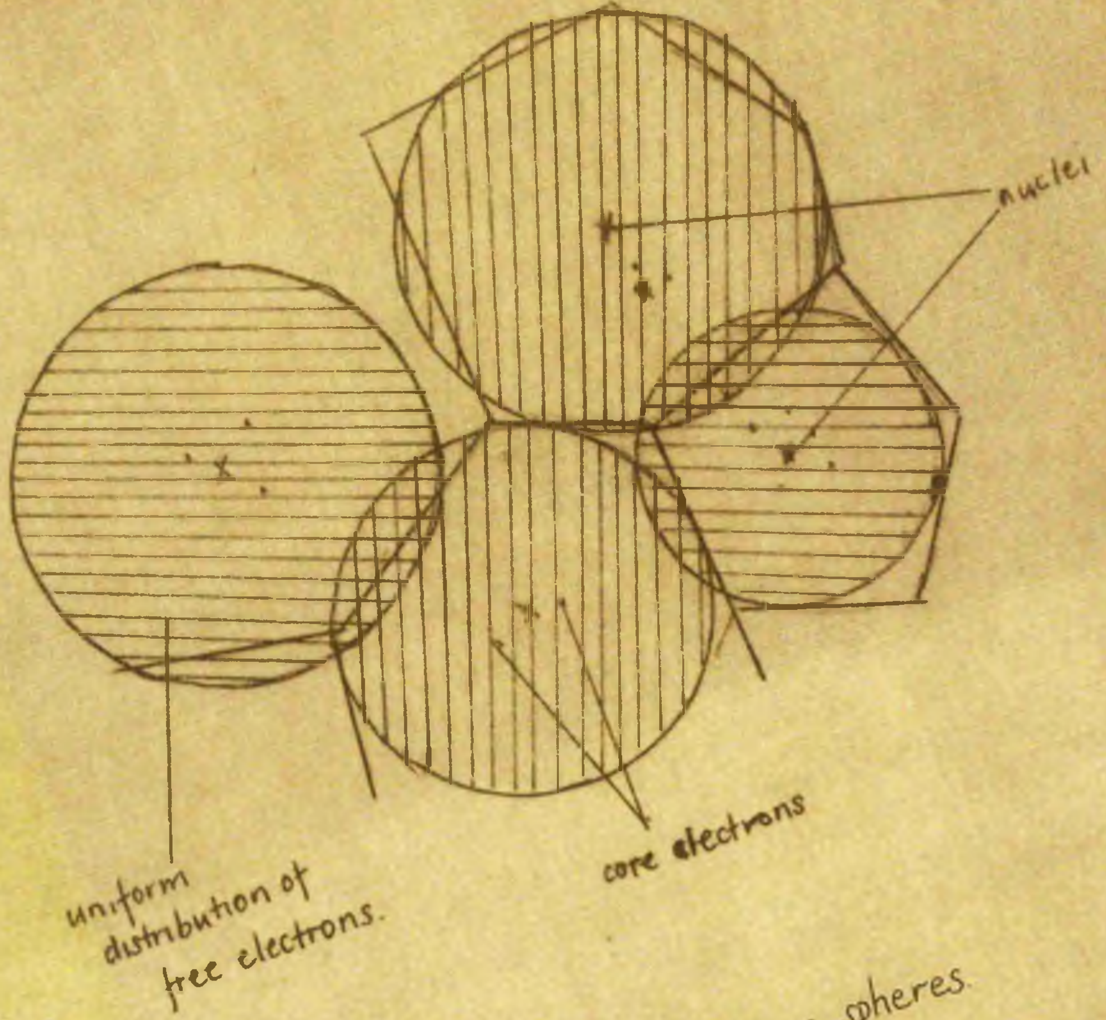

Fig. 2A. Model of overlapping atomic spheres.

Since the ions will have net positive charges they will tend to stand apart, when the intervening electrons will screen them from each other. We expect therefore that for the bound electrons the wave functions will be determined primarily by the nearest nucleus, secondarily by the nearest neighbours, and are scarcely affected by more distant nuclei. The fast moving free electrons will tend to accumulate very slightly round the nuclei according to the magnitude of their charge, but at high temperatures this effect is smaller, and we may assume that the time averaged distribution of free electrons is approximately constant throughout space. We thus have the picture, similar to that of a crystal lattice, with the ions at their average lattice positions and a uniform smeared out charge density due to the free electrons.

Supposing we divide up the volume V' into polyhedral cells centred on the lattice positions of the nuclei, of such a volume that the time-averaged number of conducting electrons inside just neutralizes the ionic charge, and then deform these polyhedra slightly so that they become sperical (see Fig. 2A). Then there is no contribution to the potential outside any sphere from the charge within it. On the other hand the time averaged contribution to the potential inside the sphere from all the other ionic spheres will also be negligible. We thus assume that we can approximate the conditions by such a set of spheres since the slight redistribution of charge involved should only distort the value of the potential near the boundaries of the spheres. The radius a_Z, of a sphere enveloping a nucleus of charge Z is determined by the condition that the average charge on such an ion $\bar{Z}'$, shall be just equal to the number of free electrons enclosed.

$$\bar{Z}' = \frac{4}{3}\pi a_{z'}^{3} \rho_e \tag{21}$$

where ρ_e is the density of free electrons. If N_Z is the number of atoms of charge Z in V, then the total number of free electrons in V' is $\sum_Z N_z \bar{Z}'$, and since the density is uniform

$$\rho_e = \frac{\sum_Z N_z \bar{Z}'}{V'} \tag{22}$$

The average potential due to Z' free electrons within a sphere S containing a nucleus of charge Z is then V_f,

$$V_f = -\frac{Z'e}{2a_{z'}}\left(3 - \frac{r^2}{a_{z'}^2}\right) \tag{23}$$

at distance r from the centre.

Now consider the potential field experienced by an electron well within the sphere S which also has (n_j) other electrons in the bound levels j. Then on an average there will also be Z' free electrons within S interacting with the electron where

$$Z^* + \sum_j n_j = Z - 1 \qquad (2.4)$$

and the average potential due to the electrons and ions outside the sphere will be negligible. Hence the time-averaged potential energy of the electron at a position r will be

$$V(r) = -\frac{Ze^2}{r} + \sum_j n_j V_j(r) + \frac{Z^* e^2}{2 a_{Z'}} \left(3 - \frac{r^2}{a_{Z'}^2}\right) \qquad (2.5)$$

where $V_j(r)$ is the average potential at position r due to an electron in the orbit j, and $Z^* = Z'$.

Because the form of the potential at the boundaries of the atomic spheres is rather arbitrary, it is impossible to impose precise boundary conditions on the individual electron potentials, and furthermore we are considering only a time-averaged potential. Moreover we can only solve the Schrodinger equation and obtain exact energy levels by simple analytic means for a very restricted set of potential functions. However electrons restricted well within a sphere moving mainly in the field of the ion core are not seriously affected by the boundary behaviour, and bearing in mind the asymptotic form of the potential near the nucleus, we are justified in applying perturbation theory, using the Coulomb case as the unperturbed solution. The discrete levels we obtain from the discrete Coulomb levels will actually be widened into bands by the periodic nature of the potential and by fluctuations in time. The band width is greater the higher the level so that above a certain band, all the bands may overlap and the upper states form a continuum. The depression of the onset of the continuum in this way due to broadening of discrete levels with pressure effects, is to be distinguished from the depression of the continuum due to the fact that the potential in which an electron moves never reaches zero, as in the case of the infinite atom. In many calculations the electron's potential function is artificially adjusted everywhere by a constant amount so that its minimum value does become zero, and the onset of the continuum of the spectrum conveniently coincides with electron energy zero. Mayer rather arbitrarily takes the relevant constant from the average value of the potential within the atomic sphere. Morse estimates the effect by considering the value of the Thomas Fermi potential for zero temperature according to Slater and Krutter. He regards the atoms as spheres with radii determined for each nuclear charge so that the potential at the boundary is the same for all atoms. The magnitude of the boundary potential is them taken as the minimum potential corresponding to the maximum potential energy of an electron.

There is however another effect which has not been considered, the role of electron correlation. The electrons are discrete charges and not smeared out charge distributions. Just as electrons can not escape unaided from an ion if they have insufficient kinetic energy to use up in penetrating the potential barrier between ions, so is the close approach of two electrons limited by the energy available to overcome the repulsive forces between them. Each electron repels those around it in such a way that it tends to form a hole around it unpenetrated by other electrons.

When an electron moves towards the boundary of an atomic sphere another electron tends to replace it in the sphere increasing Z^*, and we can no longer consider interactions with the electrons and nucleus in that sphere alone as in (2.5). Imagine the electron moving in a region between nuclear lattice points; then as before free electrons will intervene to screen the ionic charges from the electron, but they will not approach close to the electron itself. The average charge distribution outside this forbidden region will remain the same. Hence the average potential may be simulated by considering the uniform distribution of free electrons to extend throughout space with the ions at their lattice positions, and then deducting the potential due to the offending overestimate of the electron density in the vicinity of the electron. The average maximum value of the potential energy in the region between ions is then of equal magnitude and of opposite sign to the energy deducted for the "hole effect".

However the free electrons will tend to avoid close interactions with other electrons everywhere and not just at the boundary of the atomic spheres, so that a comparable deduction should also be made to the potential energy in (2.5) for this effect, say V_H. Hence if we adjust the potential energy by adding V_H so that the maximum value between atoms is zero, then this quantity should also be deducted to allow

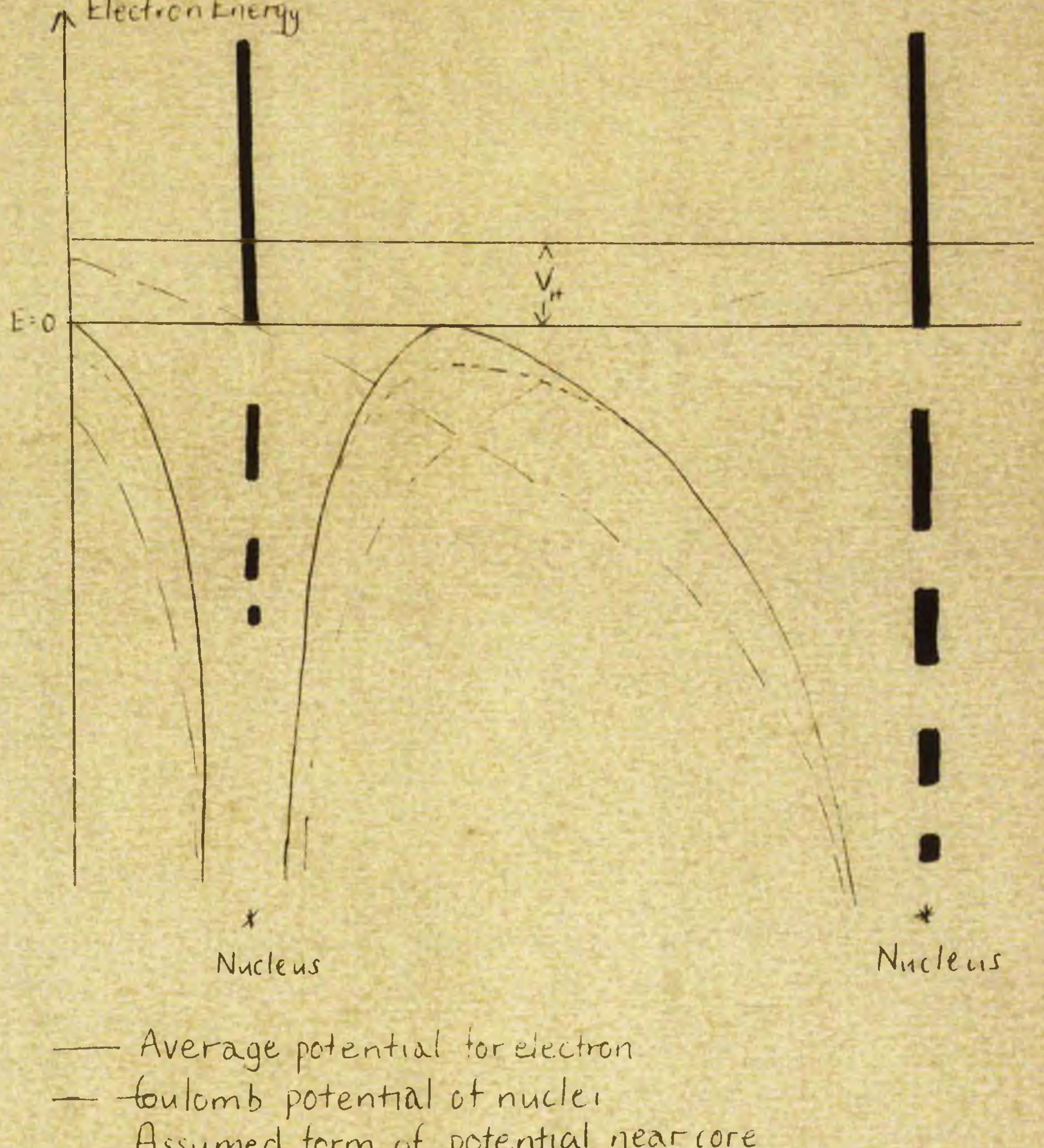

Fig 2B THE AVERAGE POTENTIAL FUNCTION

for the electron correlations (see Fig. 2B). The net result is that the average potential will take the form (2.5) with $Z^* = Z'$ for orbits close to the nucleus and tend to zero between ions as though Z^* increased to $Z'+1$ for more distant orbits, and we may calculate bound energy levels by perturbation theory using (2.5) and consider a continuous spectrum above the value zero. The treatment of electrons with total energy around and just below the average threshold of the continuum according to this scheme will be only approximate. Fortunately the statistical probability of these states is very low and they will have a small overall effect on the occupation numbers. The series of Coulomb bound wave functions we need to consider is terminated as soon as the perturbed energy becomes positive.

COMPARISON WITH OTHER METHODS

Another method of finding the average potential round a nucleus in a surrounding sea of electrons is the Thomas Fermi approach. Application of Fermi-Dirac statistics gives the particle density in phase space, and hence the total electron density at each point, in terms of the potential energy, and using Laplace's equation a differentiel equation for the potential is obtained. A sophisticated numerical integration treatment requiring an iterative process to fit the desired boundary conditions, gives the solution for the potential function for any nuclear charge, temperature and electron density or pressure. The broken line graph in (2.c) shows $rV_T(r)/e^2$ where $V_T(r)$ is the Thomas Fermi potential energy of an electron at a distance r from the nucleus for the case of Neon at

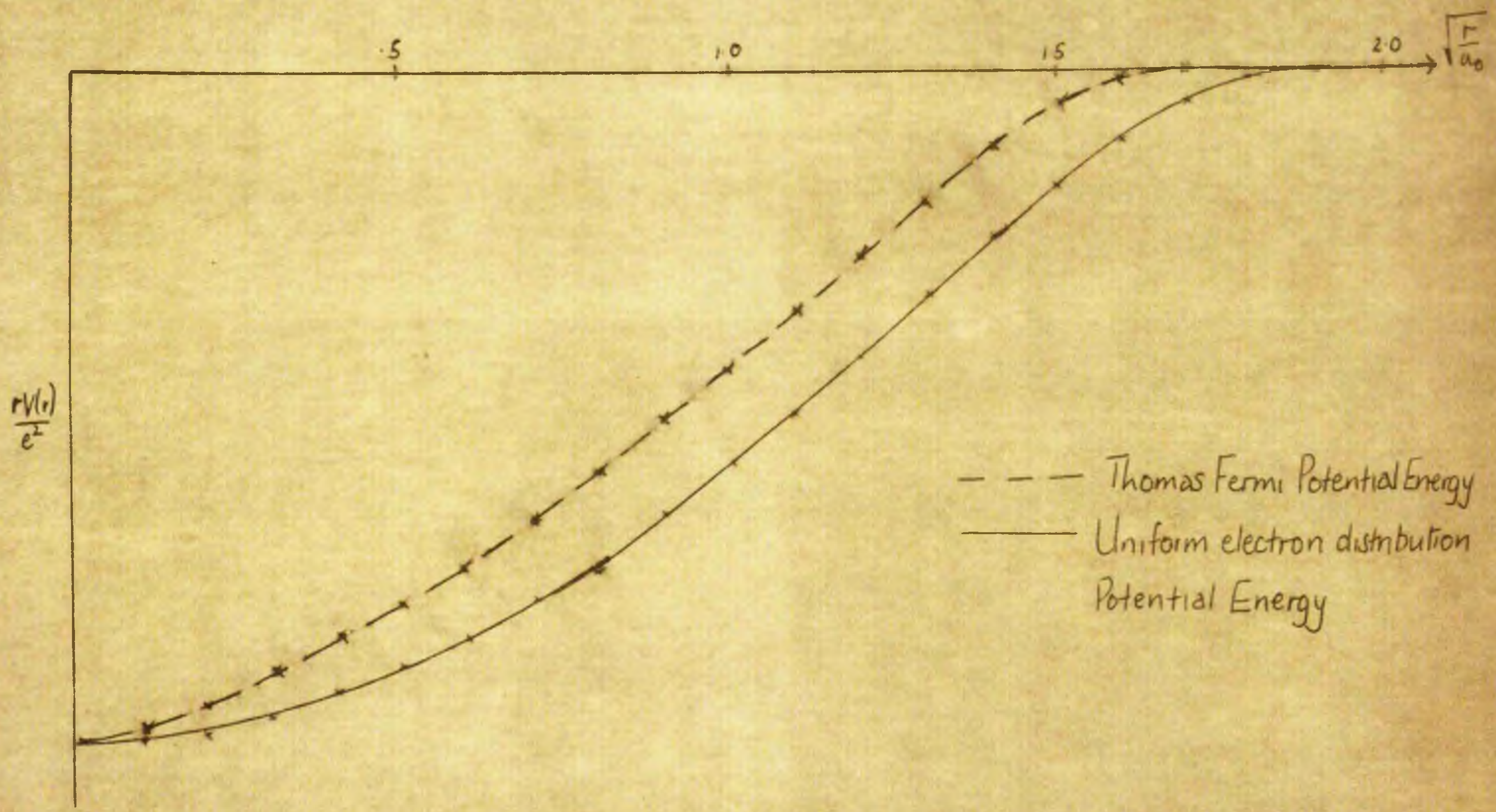

Fig 2C. Comparison of the potential energy of an electron as a function of $\sqrt{r/a_0}$ for the Thomas-Femi potential and the unifom electron distribution potential for Neon at $T = 10^{2.5}$ eV, $P = 10^{2.5}$ Mbars.

a temperature of $10^{2.5}$ electron volts, and a gas pressure of $10^{2.5}$ megobars. This is compared with the potential energy according to the previous sections averaged over the configurations according to their probability. The way in which the potential energy increases more sharply at short distances r in the first case shows the effect of the tendency of electrons to cluster round the nucleus, but this is overestimated in the Thomas-Fermi theory.

(N.B. The comparison is between the average potential energy which an extra electron inserted at any point would see due to all the particles as distinguished from the potential energy for any one electron in the neutral charge distribution whose own effect has been deducted). The comparison graph for the unscreened Coulomb potential of course, corresponds to the straight line $rV_C/e^2=10$.

PERTURBATION THEORY AND THE BOUND ENERGY LEVELS

We now have to calculate the perturbed energy levels of the electron states when the potential energy is given by (2.5) using the Coulomb wave functions in the bare field of the nucleus as the unperturbed solutions. These bound state wave functions are the solutions of

$$-\frac{\hbar^2}{2m}\nabla^2\psi_{nlm} - \frac{Ze^2}{r}\psi_{nlm} = E^C_{nl}\psi_{nlm} \qquad (2.6)$$

for the discrete values of $E^C_{nl}=-(Z^2/n^2)Ry$ where n may assume all positive integral values, and there are $(2l+1)$ possible solutions corresponding to values of m and two possible spin states, for each pair of quantum numbers n and l. The perturbing potential contributes the energy

$$V_p = \sum_j n_j V_j(r) + \frac{Z^* e^2}{2a_{z'}}\left(3 - \frac{r^2}{a_{z'}^2}\right) \tag{2.7}$$

and since it is spherically symmetric and does not act on the spin it will not remove this degeneracy, although it will split the energy levels according to the anguler momentum quantum number 1. To first order the change in energy from the Coulomb value will be the expectation value

$$\Delta E_{nl} = \langle \psi_{nlm} | V_p | \psi_{nlm} \rangle \tag{2.8}$$

$$= \sum_j n_j \langle \psi_{nlm} | V_j | \psi_{nlm} \rangle + \langle \psi_{nlm} | \frac{Z^* e^2}{2a_{z'}}\left(3 - \frac{r^2}{a_{z'}^2}\right) | \psi_{nlm} \rangle$$

The second term follows simply from the r^2 matrix element for the Coulomb states which is given by (Bethe and Salpeter P17)

$$\langle \psi_{nl} | \left(\frac{r}{a_0}\right)^2 | \psi_{nl} \rangle = \frac{n^2}{2Z^2}\left(5n^2 + 1 - 3l(l+1)\right) \tag{2.9}$$

and using the normalisation of the wave functions

$$\langle \psi_{nl} | \frac{Z^* e^2}{2a_{z'}}\left(3 - \frac{r^2}{a_{z'}^2}\right) | \psi_{nl} \rangle = Ry\, Z^* \frac{a_0}{a_{z'}}\left(3 - \frac{a_0^2}{a_{z'}^2}\frac{n^2}{2Z^2}\left(5n^2 + 1 - 3l(l+1)\right)\right) \tag{2.10}$$

The terms in $V_j(r)$ may be computed using Slater integrals. $V_j(r)$ is is the potential energy of an electron at the point r in an ion sphere due to an electron in the jth bound orbit in the ion, averaged over each possible position of that electron according to its probability. Hence

$$V_j(\underline{r}) = \frac{e^2}{a_0} \int \frac{\psi_j(\underline{r}_j) \cdot \psi_j^*(\underline{r}_j)}{\left| \frac{\underline{r} - \underline{r}_j}{a_0} \right|} \, d\underline{r}_j \qquad (2.11)$$

If the parameters nl correspond to the ith level then the expectation value of the interaction energy of electrons in the ith and jth levels $E_{nl,j}$, is $(e^2/a_0) x J_{ij}$;

$$J_{ij} = \iint |\psi_i(\underline{r}_i)|^2 \frac{1}{\left| \frac{\underline{r}_i - \underline{r}_j}{a_0} \right|} |\psi_j(\underline{r}_j)|^2 \, d\underline{r}_i \, d\underline{r}_j \qquad (2.12)$$

If we had taken into account exchange effects to allow for the indistinguishability of the bound electrons then we should also have had to consider integrals of the form

$$K_{ij} = \iint \psi_i^*(\underline{r}_i) \psi_j(\underline{r}_i) \frac{1}{\left| \frac{\underline{r}_i - \underline{r}_j}{a_0} \right|} \psi_i(\underline{r}_j) \psi_j^*(\underline{r}_j) \, d\underline{r}_i \, d\underline{r}_j \qquad (2.13)$$

(see for Example Hartree, Chapter 3)

Expanding $\frac{1}{|\underline{r}_i - \underline{r}_j|}$ in the usual form in terms of Legendre polynomials in μ, the cosine of the angle between the vectors $\underline{r}_i$ and $\underline{r}_j$

$$\frac{1}{|\underline{r}_i - \underline{r}_j|} = \sum_{k=0}^{\infty} U_k(\underline{r}_i, \underline{r}_j) P_k(\mu)$$

where

$$U_k(r_i, r_j) = \frac{r_i^{\,k}}{r_j^{\,k+1}} \qquad \text{for } r_i \leq r_j$$

$$= \frac{r_j^{\,k}}{r_i^{\,k+1}} \qquad \text{for } r_i > r_j$$

and performing the angular integrations, each integral can be expressed as the sum of a finite number of terms in k. Usually K_{ij} is very small compared with J_{ij} and we are justified in neglecting exchange effects, and the first term for J_{ij} dominates all the others. We obtain

$$J_{ij} \doteqdot F_0(ij) = \iint \frac{R_i(r_i)^2 R_j(r_j)^2 r_i^2 dr_i\, r_j^2 dr_j}{\frac{1}{a_0} \max(r_i, r_j)} \qquad (2.15)$$

where R_i and R_j are the radial wave functions. For Coulomb wave functions the result is conveniently expressed in terms of a Slater screening constant which is independent of the nuclear charge

$$\sigma_{ij} = \frac{n^2}{Z} F_0(i,j)$$

$$\Delta E_{n} = \frac{dE_n^c}{dZ} \sigma_{ij} \qquad (2.16)$$

The final perturbed energy level of the state nl in Rydbergs is thus

$$\frac{E_{nl}}{R_y} = -\frac{Z^2}{n^2} + \frac{2Z}{n^2}\sum_j n_j \sigma_{ij} + Z^* \frac{a_0}{a_{z1}}\left(3 - \frac{a_0^2}{a_{z1}^2}\frac{n^2}{2Z^2}\left(5n^2+1-3l(l+1)\right)\right) \quad (2.17)$$

and the bound states of the ion are limited to those for which this expression is negative.

COMPARISON WITH SELF-CONSISTENT FIELD APPROXIMATIONS

The interaction energies of bound level electrons are accurately given by the Slater integral method as long as there are not too many bound electrons simultaneously interacting in the same ion. In the conditions here where the atoms are almost ionised the results should be sufficiently accurate. Energy levels were calculated for isolated Neon ions with pairs of bound electrons in various states according to a Har Hartree (i.e. without exchange and non-relativistic) self consistent field treatment (SCF). This method takes into account the deformation of the electron wave functions due to the other electrons. As before each electron is assumed to move around the nucleus in a sperically symmetric statistical field of the others; starting with Coulomb wave functions a potential is calculated for each wave function giving a new radial wave function. The new radial functions give a new potential and so on iteratively, until consistency between wave functions and potentials is obtained.

In the table (2D) the Slater screening constants are compared with the corresponding quantities according to (2.19) calculated with the SCF wave functions. The closeness of the results shows the small effect of the deformations of the wave functions and justifies the sufficiency of first order perturbation theory only. It will be shown later that the free electrons deform the bound electron wave functions very little so that first order theory is sufficient in this case also.

Level of interacting electron, j	1s	2s
Level of perturbed electron, l		
1s	.6084 .6250	.1864 .2099
2s	.2031 .2099	.1474 .1504
2p	.2324 .2428	.1579 .1621

—— values given by SCF

━━ Slater integral values

TABLE 2D

COMPARISON OF VALUES OF $\sigma_{nl,n'l'}/n^2$

2p

.2218
.2428

.1586
.1621

.1760
.1816

BY SCF AND SLATER SCREENING APPROX

Comparison of energy levels from an isolated Carbon ion in the more complex configuration $1s^2 2s^2 2p^1$ is also given, showing the extent to which the theory deteriorates for the upper levels as the number of bound electrons increases relative to the charge on the nucleus. However even in this extreme configuration the 1s level agrees to 16% and it is usually this level which contributes most to the Rosseland mean of the absorption coefficient for carbon at temperatures of the order of a million degrees and greater.

COMPARISON OF ENERGY LEVELS BY SCF AND SLATER SCREENING APPROXIMATION FOR THE CONFIGURATION $1s^2 2s^2 2p^1$ IN CARBON

Level	Energy by SCF	Energy by Slater screening constants
1s	-23.81 Ry	-20. 65 Ry
2s	- 2.10 "	- .212 "
2p	- 1.56 "	- . 95 "

TABLE 2E.

As is to be expected the perturbation energy levels are consistently higher than the self consistent field calculations. However the average energy levels over the ionic configurations may be slightly lower than the Thomas-Fermi levels for the same pressures and temperature because of the clustering effect of the free electrons in the latter case. Neon at $T=10^{2.5}$ eV and $P=10^{2.5}$ mbars, where free electron interactions contribute more than bound-bound interactions to the average energy, was compared with the Thomas-Fermi energy levels for the same case.

COMPARISON OF ENERGY LEVELS IN THOMAS-FERMI FIELD WITH THE AVERAGE ENERGY LEVELS OBTAINED BY PERTURBATION THEORY AT THE SAME TEMPERATURE AND PRESSURE, $T=10^{2.5}$eV, $P=10^{2.5}$mbars, IN NEON

Level	Energy by Pert. theory		Energy in T-F field	
1s	-91.373	Ry	-80.887	Ry
2s	-14.115	"	-12.997	"
2p	-13.875	"	-12.592	"
3s	- 2.183	"	- 1.603	"
3p	- 2.038	"	- 1.426	"
3d	- 1.927	"	- 1.166	"

TABLE 2F

THE FERMI-DIRAC STATISTICS

The matter whose absorption properties we wish to find is prescribed by the pressure P, the temperature T, and the constituent elements with their relative concentrations. Supposing that the total number of atoms in the volume V' in a given case is N_a; then the number of atoms of charge Z is

$$N_z = \alpha_z N_a \qquad (2.18)$$

where α_Z , the fraction of atoms of charge Z, is determined by the concentration of the element. The total number of electrons in V' is

$$N_e = \sum_Z N_z Z \tag{2.19}$$

and we wish to determine how these are distributed among the various possible energy states discussed in the last section.

The Fermi-Dirac statistics predict that if each atom of charge Z has a group of states, i, of degeneracy g_{iZ}, then the most probable total number of electrons in these states averaged over the different possible configurations in the atom is

$$N_z \bar{n}_{iz} = \frac{N_z g_{iz}}{\exp(\alpha + \beta \bar{E}_{iz}) + 1} \tag{2.20}$$

where $\beta = 1/kT$ and k is the Boltzmann constant. α is a normalising constant such that the sum of electrons in all energy states is N_e. In this expression $\bar{E}_{iz}$ is the energy according to (2.17) averaged over all the possible ionic configurations which include an electron in one of the states i with quantum numbers n and l. Hence

$$\frac{\bar{E}_{iz}}{R_y} = -\frac{Z^2}{n^2} + \frac{2Z}{n^2}\sum_j n'_{ji}\sigma_{ij} + Z_i^* \frac{a_0}{a_{z'}}\left(3 - \frac{r_i^2}{a_{z'}^2}\right) \tag{2.21}$$

where n'_{ji} is the average number of electrons in the jth level which interact with an ith level electron and Z_i^* is the average of Z^* for the level i.

Mayer assumes an independent electron approximation in which the number of electrons in the ith level is uncorrelated with the number of electrons in any other level j. Green investigated the problem of interdependent electrons and showed that the error introduced by the independent electron approximation is small at the higher temperatures considered here: the effect of correlation is to alter the value of slightly by an amount proportional to βZ and the correction to the exponential term is then of order β^2. This means that for levels other than i, n'_{ji} is independent of i and equal to $\bar{n}_j$ the average number of electrons in the level j. However to find the average number of electrons which accompany an electron in the state i, both Mayer and Green regard the problem as though the degenerate level could be divided up into an undegenerate state corresponding to that occupied by the electron, interacting with a group of $g_{iZ}-1$ degenerate states so that $n'_{ii}=\bar{n}_i(1-1/g_{iZ})$: this seems to ignore the fact that the occupied state can be any one of the g_{iZ} states. If $P_i(m)$ is the probability of m electrons in the level i then n'_{ii} should be given by

$$n'_{ii} = \sum_{m=1}^{g_{iZ}} (m-1)\, P_i(m)$$

$$= \bar{n}_i - 1 + P_i(0) \qquad (222)$$

If $\bar{n}_i$ is large, then $P_i(0)$ is small, so that n'_{ii} is approximately $\bar{n}_i-1$. If $\bar{n}_i$ is small then the probability of having more than one electron in the level is negligible so that n'_{ii} is zero. If $\bar{n}_{ii}$ is greater than one then it will be sufficient to take n'_{ii} as $\bar{n}_i-1$, and if $\bar{n}_i$ is less than or equal to unity $n'_{ii}=0$.

$$n'_{ji} = \bar{n}_j \quad \text{if } j \neq i \tag{2.23}$$

$$n'_{ii} = \max(0, \bar{n}_i - 1)$$

Z_i^* may also be taken independently of the level i, as the average number of free electrons $\bar{Z}'$ associated with the nucleus Z. This has the desired property that for electrons in close lying orbits

$$Z_i^* = \left(Z - \sum_j n'_{ji}\right) - 1 \tag{2.24}$$

whereas for electrons lying nearer the boundaries of the ion spheres in less probable orbits $Z_i^* \rightarrow Z - \sum_j n'_{ji}$.

$$Z_i^* = \bar{Z}' = Z - \sum_j \bar{n}_j \tag{2.25}$$

Mayer and Green both ignore the possibility that the existence of an ith level is dependent on the particular ionic configurations. They assume that the ith level either exists to accommodate electrons for all ionic configurations of deeper electrons, or that there is never a bound ith level for any configuration, for an element at a fixed temperature and pressure in a mixture. This implies that the partition function varies discontinuously with the conditions and leads to inconsistencies between equations (2.20) and (2.21). A low occupation number in an upper state may indicate that the energy according to (2.21) is negative and the state is able to take this number of electrons. On the other hand the occupation number predicted by (2.20) may be so high that according to (2.21) the state does not exist! Obviously the possibility of obtaining a state does not vanish suddenly in this manner, and as the temperature and pressure increase the level will pass through a transition region where the probability of it existing gradually decreases. In this region the state will exist in those atoms with few core electrons and will not exist in the ions with more bound electrons. For example the average number of electrons in the 1s state, $\bar{n}_1$, will in general be non-integral (unless the binding energy is so large that $\alpha < -\beta \bar{E}_{1s,Z}$) representing an average of the possible integral occupation numbers; if n_1 and n_2 are the integers on either side of $\bar{n}_1$ then these will be the most probable numbers in any particular atom. If $E_{1s,Z}$ alters sign when $\bar{n}_1$ is replaced by n_1 or n_2 then the state is obviously sensitive to changes in the occupation numbers of the 1s state in which electrons have the greatest screening effect, and must depend on the configuration.

This effect may be represented by considering the degeneracy as a continuous function depending on the conditions through the n'_{ji}. When a state represents a tightly bound electron then it will exist for all ionic configurations and for each state in the level so that g_{iZ} will be $2x(21+1)$, a constant as before. When the conditions become such that the states corresponding to level i depend critically on the ionic configuration, then the degeneracy of the level should gradually be reduced until, when the probability that the states exist is negligible, the degeneracy function becomes zero.

Carrying out the formal analysis with a variable degeneracy function equation (2.20) becomes modified to

$$N_z \bar{n}_{iz} = \frac{N_z g_{iz}}{\exp(\alpha + \beta E_{iz} + C_i) + 1} \qquad (2.26)$$

where C_i depends on the partial derivatives of the degeneracy function

$$C_i = \sum_j \frac{\partial g_{jz}}{\partial \bar{n}_{iz}} \left[\log \left(1 - \frac{\bar{n}_{jz}}{g_{jz}} \right) \right] \qquad (2.27)$$

Since $\partial g_{jz}/\partial n_{iz}$ will be zero except for levels j in the transition region, we need only consider the terms in C_i due to these levels. Secondly it can be seen that the logarithmic part of these terms becomes infinitely large and negative as $\bar{n}_{jZ}$ tends to g_{jZ}, and if $\frac{\partial g_{iz}}{\partial n_{iz}}$ is always a negative quantity in the transition region, C_i will become infinite.

Strictly speaking we should consider the probability f_p, that an atom Z can accommodate just p bound electrons in the ith level for all possible values of p by considering all the various ionic configurations. The degeneracy could then be written as

$$g_{iz} = \sum_p f_p G_{iz}(p)$$

where G_{iZ} is a function of p only. $\overline{E}_{iz}$ would also be different from the independent electron $\overline{E}_{iz}$ since the n'_{ji} would change and the first order perturbation theory of (2.17) might be insufficiently accurate to determine the existence of the level in a given configuration.

Again the high temperatures help the situation for unless the conditions become degenerate and α is small the levels have to be very deep to become statistically important. The transition states are unlikely to have any electrons in them and hence do not affect the overall occupation numbers very much (although their existence may be important in other contexts), so that an approximate treatment is sufficient and detailed considerations of all the possible ionic configurations is not necessary. We can choose a degeneracy function for the ith level which has the right qualitative behaviour as follows.

Supposing the average energy level given by (2.21) with the term due to other electrons in the ith level itself excluded, that is with $n'_{ii}=0$, is E_{iz}°. If this bare level is such that it can accomodate all the electrons predicted by (2.20) with g_{iZ} taken to be the full degeneracy $2x(2l+1)$ and $\bar{E}_{iz}=E_{iz}^{\circ}$, then it will be assumed that the level has this full degeneracy, and C_i is zero. If E_{iz}° is itself positive then it will be assumed that the ith level can rarely accommodate electrons under these conditions, with the corresponding zero degeneracy. If the average bare level can take a maximum number of electrons, p_i, which is less than $\bar{n}_i$ given by (2.20), it will be supposed that on the whole ions with an i shell have p_i or p_{i-1} electrons in the ith level. If we find the number of ways of arranging these electrons in the N_Z atoms such that there is a fraction u of unfilled i-level atoms with p_i-1 electrons, and a fraction v filled in the ith level with p_i, then the formal methods of the Grand Ensemble can be carried through giving the most probable ratio of u and v.

The average number of electrons in the level i is then

$$\bar{n}_{iZ} = u(p_i - 1) + v p_i \qquad (2.28)$$

and a relation of the type (2.26) holds if the corresponding degeneracy function and $\bar{n}_{iZ}$ are related by

$$F(g_{iZ}) - F(g_{iZ} - n_{iZ}) = F(g_{iZ,max}) - F(p_i - \bar{n}_{iZ}) \qquad (2.29)$$

$$- (g_{iZ,max} - \bar{n}_{iZ}) \log (g_{iZ,max} + 1 - p_i)$$

where

$$g_{iZ,max} = 2.(2l+1)$$

and $\qquad F(x) = x \log x$

In the case $p = g_{iZ,\,max}$ this implies g_{iZ} is equal to $g_{iZ,\,max}$ as we should expect, and when $p=0$, $\bar{n}_{iZ}$ and g_{iZ} are also zero. If we put

then

$$F(y) - F(y-1) = F\left(\frac{g_{iZ,max}}{\bar{n}_{iZ}}\right) - F\left(\frac{p_i}{\bar{n}_{iZ}} - 1\right) + \left(\frac{g_{iZ,max} + 1 - p_i}{\bar{n}_{iZ}}\right) \log \bar{n}_{iZ}$$

$$- \left(\frac{g_{iZ,max}}{n_{iZ}} + 1\right) \log (g_{iZ,max} + 1 - p_i)$$

$$(2.30)$$

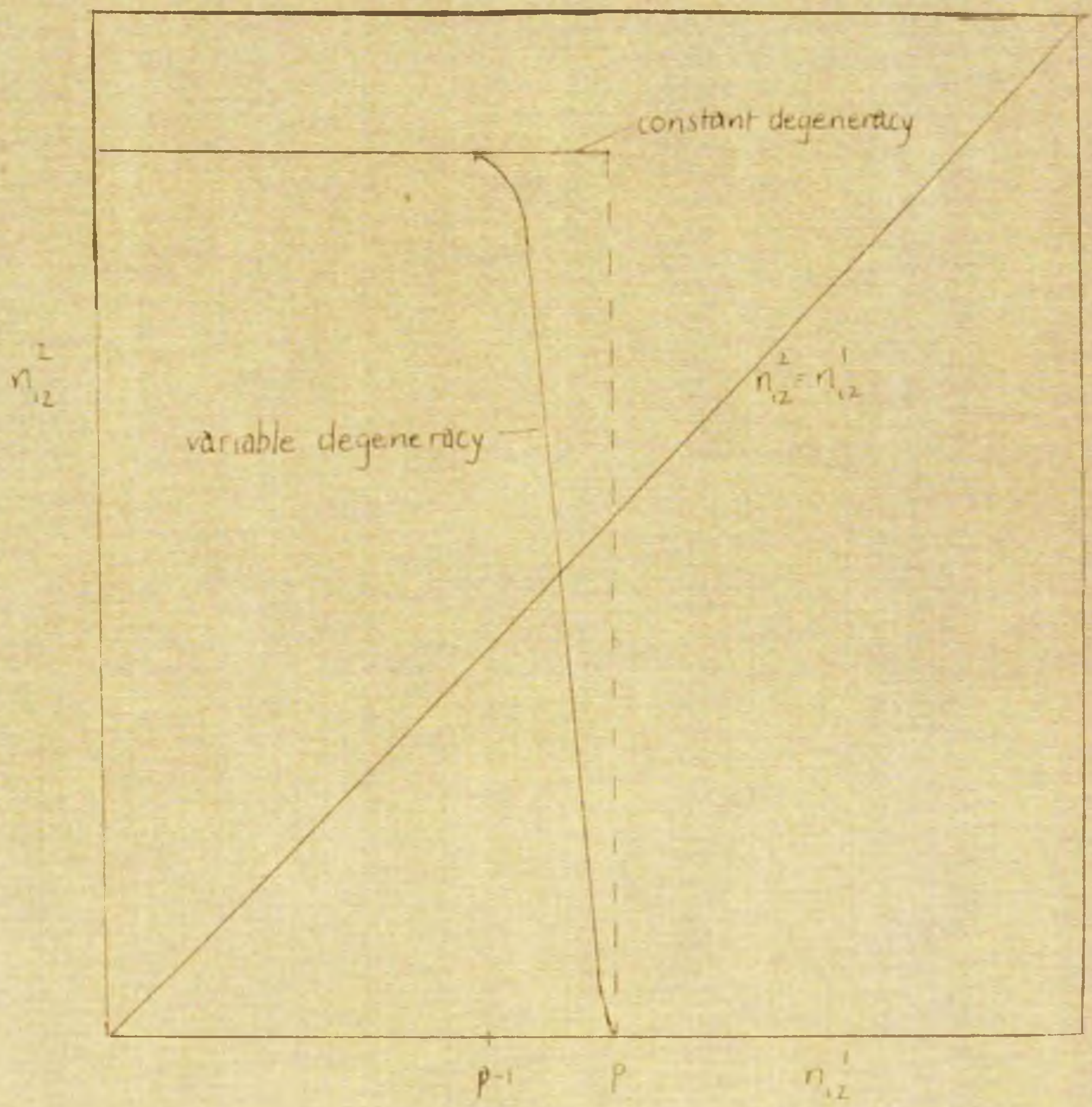

Fig. 2G Convergence of iterative method of solution for the occupation numbers.

and the right-hand-side depends only on $\bar{n}_{iZ}$ and p. We also have

$$\log\left(\frac{g_{iz}}{g_{iz}-\bar{n}_{iz}}\right)\frac{\partial g_{iz}}{\partial \bar{n}_{iz}} = C_i = \log\left[\frac{(p_i-\bar{n}_{iz})(g_{iz,max}+1-p_i)}{(g_{iz}-\bar{n}_{iz})}\right] \qquad 2.31$$

The degeneracy function is now defined as a continuous function of $\bar{n}_{iZ}$ for any given value of E_{iz}°, and we can obtain a solution of (2.26) consistent with (2.21) in all cases, by iteration. Supposing we assume a trial solution $\bar{n}_{iZ}$, say n^1_{iZ}; then this gives a value of $\bar{E}_{iz}$ and E_{iz}° using (2.20) and hence determines g_{iZ} and C_i. We can then find a new value, n^2_{iZ} from (2.26). The difficulty which arose with Mayers discontinuous degeneracy function does not occur now, as can be seen by comparing n^2_{iZ} with the trial value n^1_{iZ}. Formerly n^2_{iZ} took on an almost constant value up to the critical value of n^1_{iZ} at which $\bar{E}_{iz}$ changed sign, when it suddenly assumed the value zero. Hence if this critical value lay below that predicted by (2.20) there was no self consistent value of n^1_{iZ} such that n^1_{iZ} and n^2_{iZ} were equal. With the continuous degeneracy function as n^1_{iZ} tends to the maximum possible value, p_i, C_i tends to infinity so that n^2_{iZ} tends to zero. On the other hand when n^1_{iZ} is p_i-1, C_i is zero and $g_{iZ}=g_{iZ,\,max}$ so that n^2_{iZ} is equivalent to the value given by (2.20) with the full degeneracy. As n^1_{iZ} increases from p_i-1 to p_i, g_{iZ} decreases from $g_{iZ,\,max}$ and C_i increases monotonically. Hence a graph of n^2_{iZ} must cross the line $n^2_{iZ}=n^1_{iZ}$ at some point and hence a solution must exist. (see fig. 2G)

The free electrons also obey Fermi-Dirac statistics. The number of possible energy states in the interval E to E+dE per unit volume including spin, follows from the usual box normalisation

$$g(E)\,dE = \frac{8\pi\sqrt{2}}{h^3}\,m^{3/2}\sqrt{E+U^*}\,dE \qquad (2.32)$$

U^* is a small correction term which allows for the fact that the mean momentum of an electron increases as it moves into a region of negative potential energy. U^* is given by

$$\sqrt{U^*} = \frac{\int_{V'}\sqrt{-V_f}\,d\tau}{V'} \qquad (2.33)$$

where V_f is the average potential energy function of a free electron, and the integration extends throughout the volume V'. Except in the ion core regions the average potential energy due to the bound electrons is almost as though they were at the ion centre, and V_f is approximately given by

$$V_f = -\frac{Z'e^2}{2a_{z'}}\left(\frac{2a_{z'}}{r} - 3 + \frac{r^2}{a_{z'}^2}\right) \qquad (2.34)$$

in each ionic sphere. Hence summing over the atoms we have

$$\begin{aligned}\sqrt{U^*} &= \frac{1}{V'}\sum_Z N_Z\,4\pi\int_0^{a_{z'}}\sqrt{\frac{Z'e^2}{2a_{z'}}\left(\frac{2a_{z'}}{r}-3+\frac{r^2}{a_{z'}^2}\right)}\,r^2\,dr\\ &= \frac{1}{V'}\sum_Z N_Z\,4\pi\sqrt{\frac{Z'e^2a_{z'}^5}{2}}\times\int_0^1\sqrt{2/y-3+y^2}\,y^2\,dy\\ &= \frac{1}{V'}\left(\sum_Z N_Z\,4\pi\sqrt{\frac{Z'e^2a_{z'}^5}{2}}\right)\times .182588\end{aligned} \qquad (2.35)$$

Hence the number of free electrons per unit volume in V' with energies between E and E+dE is

$$n(E)\,dE = \frac{8\pi\sqrt{2}}{h^3}\,\frac{m^{3/2}\sqrt{E+U^*}\,dE}{\exp(\alpha+\beta E)+1} \qquad (2.36)$$

and the total number in V', N_r, is given by integrating over the energy and multiplying by the volume. Integrals of the form

$$\int_0^\infty (E+U^*)^n/[\exp(\alpha+\beta E)+1]\,dE$$

may be written in terms of the Fermi-Dirac functions

$$F_n(\alpha^*,\eta) = \int_\eta^\infty \frac{x^n}{\exp(\alpha^*+x)+1}\,dx$$

$$= \beta^{n+1}\int_0^\infty \frac{(E+U^*)^n\,dE}{\exp(\alpha+\beta E)+1}$$

where

$$x = \beta E$$

$$\eta = \beta U^*$$

$$\alpha^* = \alpha - \beta U^*$$

For sufficiently large electron energies $\exp(\alpha+\beta E)$ is large compared with 1 and the distribution (2.36) is almost the same as the plain Boltzmann distribution. As U* increases at higher densities the temperatures of interest increase and η remains small unless the matter becomes degenerate. The total number of free electrons is also given by adding up the Z' free electrons in each ionic sphere, and hence

$$N_f = \frac{8\pi\sqrt{2}}{h^3}\left(\frac{m}{\beta}\right)^{3/2} V' F_{\frac{1}{2}}(\alpha^*, \eta) = \sum N_Z \bar{Z}' \qquad (2.37)$$

and this equation may be used to determine α^*.

The equations given above determine the most probable distribution of electrons among the energy levels for a given mixture and temperature and density. It remains to find how the density depends on the pressure P. The virial theorem implies that the pressure is equal to two thirds of the kinetic energy plus one third of the potential energy of the particles, per unit volume

$$PV' = \frac{2}{3} K.E + \frac{1}{3} P.E \qquad (2.38)$$

In the case of an ideal gas the potential energy is negligible and the mean kinetic energy of each independent particle is $\frac{3}{2}kT$ so that this reduces to the form

$$PV' = N_p kT$$

However the following table gives the average interaction energies for each type of particle in an atom of charge Z as well as the expected average number and the average kinetic energy.

Particle	Ave no.	$\frac{1}{2}$intn. with nucleus	$\frac{1}{2}$intn. with bd. e^- in atom	$\frac{1}{2}$intn. with free e^- in atom	intn. with part. outside	mean KE
Nucleus	1	- - -	$\frac{1}{2}\sum_j \bar{n}_j \frac{2Z}{n^2} R_y$	$\frac{1}{2}\frac{3\bar{Z}'e^2}{2a_{z'}}$	0	$\frac{3kT}{2}$
Bound e^- in orbit i	$\bar{n}_i$	$\frac{1}{2}\frac{2Z}{n^2} R_y$	$\frac{1}{2}\sum_j n'_{ji}\frac{2Z}{n^2}\sigma_j R_y$	$\frac{3}{2}\frac{\bar{Z}'e^2}{2a_{z'}}$	0	$\frac{Z^2}{n^2} R_y$
Free electrons	$\bar{Z}'$	$\frac{1}{2}\frac{3Ze^2}{2a_{z'}}$	$\frac{1}{2}\sum_j \bar{n}_j \frac{3e^2}{2a_{z'}}$	$\frac{1}{2}\frac{12}{5}\frac{\bar{Z}'e^2}{2a_{z'}}$	0	$\bar{E}_f = \frac{\int n(E)(E+U^*)dE}{\int n(E)dE}$ $= \frac{1}{\beta}\frac{F_{3/2}(\alpha^*,\eta)}{F_{1/2}(\alpha^*,\eta)}$

TABLE 2G

AVERAGE ENERGY CONTRIBUTIONS TO THE PRESSURE FOR EACH TYPE OF PARTICLE IN AN ATOM

On adding the contributions from all the N_a atoms in V' we have

$$PV' = N_a\left(kT + \sum_z \alpha_z \bar{Z}' \tfrac{2}{3} \bar{E}_f\right) - \tfrac{1}{5} N_a \sum_z \alpha_z \bar{Z}'^2 \frac{a_0}{a_{z'}} R_y + \frac{N_a}{6} \sum \alpha_z \sum_i \bar{n}_{iz} \sum_j n'_{ji} \frac{2Z}{n^2} \sigma_{ij} R_y \quad (2.39)$$

We now have a set of equations which can be solved iteratively. If we guess a set of average occupation numbers and a value of α, then this gives us $\bar{Z}'$ by (2.25). The radii of the atoms can then be determined in terms of N_a/V' from (2.1) and (2.2), and (2.39) becomes a quartic in N_a/V', and hence we can find the number of atoms of each element in V'. The number of free electrons, N_f, follows from the $\bar{Z}'$, and we can find a new value of α by (2.37). Calculating new energy levels with the n'_{ji} defined by (2.23) and Z^* by (2.25), in (2.21), as given by the trial occupation numbers, we can find a new set of occupation numbers by (2.26) with the degeneracy function defined as in the paragraph preceding equation (2.29). The process may be repeated until the trial and calculated occupation numbers are equal and a consistent solution is obtained.

PROBABILITY OF EACH IONIC CONFIGURATION

The ability of an electron in a given level to absorb radiation frequently depends on the ionic configuration containing it. However it has already been shown that the probability of any state being occupied is almost independent of the configuration, in that deviations from the average energy levels are small in comparison with the characteristic energy kT. That is, the probability that any particular state in the group of levels g_{iz} is occupied is

$$p_{iz} = \bar{n}_{iz}/g_{iz}$$

and

$$q_{iz} = 1 - p_{iz}$$

is the probability that it is empty. The probability of any ionic configuration in which specific numbers of the degenerate states in each bound level are occupied, is thus equal to the product of the probabilities that these states are occupied times the product of the probabilities that all the other states are not. If we wish to know the probability $P(\{n_{iz}\})$ that $\{n_{iz}\}$ of the $\{g_{iz}\}$ states in the levels i are bound, irrespective of which particular states they are in each degenerate group, then there are

$$\prod_i \frac{g_{iz}!}{n_{iz}!\,(g_{iz}-n_{iz})!}$$

equivalent configurations corresponding to the various permutations and combinations. Hence

$$P(\{n_{iz}\}) = \prod_i \frac{g_{iz}!}{n_{iz}!\,(g_{iz}-n_{iz})!}\, p^{n_{iz}}\, q^{(g_{iz}-n_{iz})} \qquad (2.10)$$

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CHAPTER III

THE CONTINUOUS OPACITY

In this chapter the interaction between radiation and electrons will be discussed leading to the formulae for the absorption cross-sections, and these will be applied to the bound-free and free-free transitions. The bound-bound transitions require extra considerations to determine the line profiles, that is, the way in which the total absorption strength for each pair of levels is distributed as a function of frequency. This will be discussed in a later chapter.

For the free electrons the pure absorption cross sections are relatively small and their scattering cross sections may be of comparable magnitude. The classical absorption cross sections for bound-free transitions (which usually dominate the opacity) from any given level, vary as v^{-3} and hence the resulting spectrum of the absorbed radiation for each element is presented as the function

$$D(u) = C u^3 \kappa(u)$$

where C is a suitably chosen constant. The opacity of a mixture can then be found by adding the individual spectra together according to their concentrations, and carrying out the appropriate integrations over u.

ON THE INTERACTION BETWEEN RADIATION AND ELECTRONS

In the preceding chapter the distribution of electrons in the various energy levels was considered on the basis of the nuclei and their attendant bound electrons floating in a sea of weakly interacting free electrons. It is now necessary to consider how an electron in a given energy state absorbs or emits radiation.

A beam of radiation affects an electron through its interaction with the electric and magnetic fields perpendicular to the direction of propagation of the beam. In order to consider the problem quantum mechanically the radiation field has to be quantised, and the whole system of particles and radiation oscillators considered together with the electromagnetic fields as small perturbations. The radiation is then represented by an ensemble of normal modes λ each characterised by a frequency v, the direction of propagation $\Omega = (\theta, \phi)$ and the polarisation $\underline{e}_\lambda$. The energy of radiation of frequency v can only change by multiples of hv corresponding to absorption or emission of integral numbers of photons, and each normal mode is treated as a vibrating system with wave functions appropriate to the simple harmonic oscillator.

The atoms are randomly orientated with respect to the radiation flux so we may average over the directions of propagation and polarisation relative to the coordinate axes, and since the wave number, $\kappa = 2\pi/\lambda$, of the radiation is much smaller than 10^8 cm^{-1} so that exp($\underline{k}.\underline{r}$) remains almost constant for values of r up to several Bohr radii, the dipole approximation is justified. First order perturbation theory then predicts that the transition probability from a given state of the radiation and electron to another is zero except for absorption or emission of a single photon.

Suppose that at some given starting time an electron i is in a state s of energy E_s described by a stationary wave function ψ_{is}. The probability that this electron subsequently makes a transition to another available state a, with energy E_a and wave-function ψ_{ia}, with absorption of a photon of frequency v, averaged over the spin of the states a and s, may be expressed in terms of the momentum operator p and the two one-electron wave functions.

$$P_{s,\lambda,\nu} = \frac{1}{3}\frac{e^2}{m^2\hbar c\nu}\frac{I(\nu)}{h\nu}\left|\langle\psi_{ia}|\underline{p}|\psi_{is}\rangle\right|^2\frac{1}{2\pi}\delta\left(\frac{E_s-E_a}{\hbar}+2\pi\nu_\lambda\right) \qquad (3.1)$$

I(ν) is the intensity of the incident radiation and the δ-function implies that the transition can only take place if energy is conserved.

The momentum operator $\underline{p}$ arises because the interaction of the electron with a radiation field giving a vector potential $\underline{A}$ is

$$\frac{e\,\underline{p}\cdot\underline{A}}{mc}$$

The derivation of this formula will be considered in more detail in the next chapter when the time dependence of the wave functions is considered. The present approximation in which ψ_{is} and ψ_{ia} are the stationary solutions of the time independent Schrodinger equation then follows as a particular case.

There are two alternative forms of the matrix element of the momentum operator $\underline{p}$ in terms of the coordinate operator $\underline{r}$ or the potential gradient operator ∇V. These relations follow from the commutation relations with the electron hamiltomian.

$$\frac{i\hbar\,\underline{p}_{as}}{m} = \left[\underline{r}, H\right]_{as} = (E_a - E_s)\,\underline{r}_{as}$$

and $$(E_a - E_s)\,\underline{p}_{as} = \left[\underline{p}, H\right]_{as} = \left[p, V\right]_{as} = -i\hbar(\nabla V)_{as} \qquad (3.2)$$

We have the three equivalent forms

$$M_{as}^2 = r_{as}^2 = |\langle \psi_{1a} | r | \psi_{1s} \rangle|^2$$

$$= \frac{1}{4\pi^2 m^2 \nu_{as}^2} |\langle \psi_{1a} | p | \psi_{1s} \rangle|^2 \qquad (3.3)$$

$$= \frac{1}{16\pi^4 m^2 \nu_{as}^4} |\langle \psi_{1a} | \nabla V | \psi_{1s} \rangle|^2$$

The wave functions ψ_{1a} and ψ_{1s} may be expanded in spherical harmonics

$$\psi_{1a} = \sum_{q'l'm'} c_{aq'l'm'} R_{q'l'm'}(r) Y_{l'm'}(\theta, \varphi) \qquad (3.4)$$

$$\psi_{1s} = \sum_{qlm} c_{sqlm} R_{qlm}(r) Y_{lm}(\theta, \varphi)$$

and using the spherical symmetry of the potential and the resulting independence of m of the radial wave functions,

$$M_{as} = \sum_{qq'l'm'} \overline{|\langle c_{sqlm} \rangle|^2}$$

$$\times \left\{ \frac{\left|\int r^2 R_{q'l+1} O(r) R_{ql} \, dr\right|^2}{(2l+1)(2l+3)} \begin{pmatrix} |\langle c_{aq'l+1,m} \rangle|^2 (l+m+1)(l-m+1) \\ +\frac{1}{2}|\langle c_{aq'l+1,m+1} \rangle|^2 (l+m+1)(l+m+2) \\ +\frac{1}{2}|\langle c_{aq'l+1,m-1} \rangle|^2 (l-m+1)(l-m+2) \end{pmatrix} \right.$$

$$\left. + \frac{\left|\int r^2 R_{q',l-1,} O(r) R_{ql} \, dr\right|^2}{(2l+1)(2l-1)} \begin{pmatrix} |\langle c_{aq'l-1\,m} \rangle|^2 (l+m)(l-m) \\ +\frac{1}{2}|\langle c_{aq'l-1,m+1} \rangle|^2 (l-m)(l-m-1) \\ +\frac{1}{2}|\langle c_{aq'l-1,m-1} \rangle|^2 (l+m)(l+m-1) \end{pmatrix} \right\}$$

$$(3.5)$$

where the operator O(r) takes the three forms

$$O(r) = r \qquad (3.6)$$

$$= \frac{1}{4\pi^2 m^2 \nu_{as}^2} \left\{ \frac{\partial}{\partial r} - \frac{2l+1-\min(l)}{r} \right\}$$

min(l) = minimum value of angular momenta at radial wave functions

$$= \frac{1}{16\pi^4 m^2 \nu_{as}^4} \frac{\partial V}{\partial r}$$

according to whether the dipole moment, momentum, or potential gradient formula is used for M_{as}.

In finding the electron distribution the electron states were conveniently divided into groups according to their pairs of quantum numbers n and l for the negative energy states, together with a continuum group. We can find the average cross section for an electron occupying any one of the states in a particular group S, giving the average fraction of an incident flux of radiation I(v) absorbed by such an electron in transitions to a group A, by averaging over the initial states in S and summing over a basis of possible final states in A. The result may be written in terms of a set of numbers f_{SA} for the groups

$$f_{SA} = \frac{1}{g_s} \sum_{a \in A} \sum_{s \in S} |\langle \psi_{ia} | p | \psi_{is} \rangle|^2 \times \frac{1}{3\pi m \hbar \nu_{as}} \quad ; \; \nu_{as} = \frac{E_a - E_s}{h}$$

$$= \frac{1}{g_s} \sum_{a \in A} \sum_{s \in S} \frac{4\pi m \nu_{as}}{3\hbar} M_{as} \qquad (3.7)$$

where the summations are over the states in A and S and g_S is the order of the group S.

For photon energies which are too low to put the electron into a continuum state after absorption the cross section is zero unless the energy is close to one of the discrete values corresponding to the average energy difference between two negative energy groups S and A. The cross sections may then be written (eliminating the δ-function)

$$\sigma_{\iota v s} = \frac{\pi e^2}{mc} f_{SA}\, b'(v) \qquad (3.8)$$

where b' (v) gives the fraction of the total absorption strength $\frac{\pi e^2}{mc} f_{SA}$ of the two groups which is effective at frequency v. f_{sA} is just the usual mean oscillator strength for the levels. The line profile requires more individual attention to the specific states in the groups and the way in which they evolve, and will be considered in a later chapter.

In the case of a photon leaving the electron in the continuum the absorption cross section becomes

$$\sigma_{\iota v s} = \frac{\pi e^2}{mc} \frac{df_{SC}}{dv} \qquad (3.9)$$

where the suffix C refers to the continuum. By (df_{SC}/dv), which will be referred to as the differential oscillator strength at frequency v by analogy with the bound-bound case, we mean the limit as $\Delta v \to 0$ of $\frac{1}{\Delta v}$ times the contribution to f_{SC} from final states such that

$$|v_{uJ} - v| < \Delta v/2$$

These transition probabilities have been derived without considering whether the final state is available to the electron; if a state is already occupied by another electron in the atom then the Pauli principle forbids a transition into it. All states within a given level or with the same continuum energy have the same probability and the cross section for a transition should therefore be multiplied by the availability factor

$$q_a = 1 - p_a$$

$$= \left(1 - \frac{1}{\exp(\alpha+\beta E_a)+1}\right) \qquad (3.10)$$

BOUND FREE ABSORPTION

Although the proportion of bound electrons is relatively small the large cross sections frequently make bound-free transitions the dominant source of absorption and this process will be considered first. In this case the initial states s in the group S are prescribed by quantum numbers n^*, l^*, m^*, and the wave functions are of the form

$$\psi_{is} = R_{n^* l^* m^*} Y_{l^* m^*}(\theta, \varphi) \qquad (3.11)$$

so that the coefficients in the expansion of the initial wave function (3.4) are just

$$c_{sqlm} = \delta(q-n^*)\,\delta(l-l^*)\,\delta(m-m^*) \qquad (3.12)$$

and m may vary from -l to l.

The possible final states for the electron represent the electron being ejected from the atom with some positive energy E_a in some direction $\Omega = (\theta_a, \varphi_a)$, and hence the wave functions ψ_{ia} behave asymptotically like outgoing plane waves plus scattered spherical waves. Such wave functions can easily be represented in the form (3.4) as a superposition of the spherical harmonic (partial wave) wave functions $Y_{l'}^{m'}(\theta,\varphi)R_{E_a,l'}(r)$ where the radial wave functions $R_{E_a,l'}(r)$ are the solutions of the radial wave equation for electrons of energy E_a in the atomic sphere. The $R_{E_a,l'}$ behave like $\sin\frac{(kr - \pi l'/2 + \delta_{l'})}{kr}$ at large distances where

$$E_a = \frac{\hbar^2 k^2}{2m}$$

and the phase shift $\delta_{l'}$ also depends on E_a.

Bethe and Salpeter (p33) give the expansion of the continuum wave function normalised to represent a unit density of outgoing free electrons travelling in the direction $\Omega = (\theta_a, \varphi_a)$ relative to the coordinate axes in terms of the radial wave functions,

$$\psi_{1a}(r,\theta,\varphi) = \sum_{l'=0}^{\infty} (2l+1) i^{l'} e^{i\delta_{l'}} P_{l'}(\cos\alpha) R_{E_a,l'}(r)$$

where α is the angle between (θ,φ) and (θ_a,φ_a). The required expansion (3.4) may then be written

$$\psi_{1a}(r,\theta,\varphi) = \sum_{m=-l'}^{m=+l'} 4\pi i^{l'} e^{i\delta_{l'}} Y_{l'}^{m*}(\theta_a,\varphi_a) Y_{l'}^{m}(\theta,\varphi) R_{E_a,l'}(r) \qquad (3.13)$$

This enables us to find the matrix elements M_{as} in terms of the radial wave functions $R_{n''l''}$ and $R_{E_a,l'}$ using (3.5). These may vary slightly with the ionic configuration in which the absorption takes place and the effective contribution to f_{sc} from pairs of states requires a further averaging over the different possible configurations I according to the probability of their occurrence. The contribution to f_{SC}^{-I} from transitions to continuum states with energies E_a to E_a+dE_a is

$$\overline{\Delta f_{sc}}^{I} = \sum_{I} P_{I} \left\{ \frac{1}{2l+1} \sum_{m=-l}^{m=+l} g'(E_a) \int \frac{\pi e^2}{mc} \frac{4\pi m \nu_{as}}{3\hbar} M_{as_I} \frac{d\Omega}{4\pi} \right. \tag{3.14}$$

where $M_{as,I}$ is calculated for wave functions in the configuration I, and $g'(E_a)dE_a$ is the number of independent wave functions of the form $e^{i\underline{k}\cdot\underline{r}}$ in the energy interval E_a to E_a+dE_a with random direction of propagation $\Omega = (\theta_a, \varphi_a)$

$$g'(E_a) = \frac{4\pi m}{h^3} \sqrt{2mE_a}$$

We obtain

$$\overline{\sigma_{1s,\nu}}^{I} = \frac{\pi e^2}{mc} \overline{\frac{df_{sc}}{d\nu}}^{I} = \sum_{I} P_{I} \left\{ \frac{16\pi^2}{3} \frac{e^2}{\hbar c} \frac{mk\nu}{\hbar} \frac{g_a}{(2l+1)} \left[(l+1) \left| \int r^2 R_{E_a,l+1} O(r) R_{E_s,l} \, dr \right|^2 + l \left| \int r^2 R_{E_a,l-1} O(r) R_{E_s,l} \, dr \right|^2 \right] \right\} \tag{3.15}$$

where O(r) is defined by one of the three forms (3.6).

Kramers treated the problem of absorption in the field of a nucleus of charge Z semi-classically and obtained the cross section

$$\sigma_{1s,\nu}^{K} = \frac{64\pi^4}{3\sqrt{3}} \frac{Z^4 m e^{10}}{ch^6} \frac{1}{n^5} \frac{1}{\nu^3} \tag{3.16}$$

The ratio of the quantum mechanical cross section to the Kramers value is a slowly varying function of frequency, the so called Gaunt factor $G_{sa}(\nu)$ (N.B. This definition has often been taken with a variable effective charge instead of Z to improve the classical cross section but since this is an arbitrary quantity we shall keep to the above simple definition and keep the entire quantum mechanical dependence in the Gaunt factor).

Then

$$\mathcal{G}_{sa}(\nu) = \frac{3\sqrt{3}\, a_0 h^7 n^5 \nu^3}{128\, \pi^4 m^2 e^{10} Z^4} \frac{df_{sc}}{d\nu}$$

$$(3.17)$$

and

$$\sigma_{\iota\nu s} = \sigma_{\iota\nu s}^{K} \mathcal{G}_{sa}\, g_a$$

The Gaunt factors for the hydrogenic wave functions in the potential due to a central charge Z_{eff} for a state s with quantum numbers n and l and with energy $E_s = -\left(Z_{eff}^{*2}/n^2\right) R_y$ and a continuum state of energy $E_a' = E_s' + h\nu_H$ can be readily expressed analytically as a function of $\eta = E_a'/Z_{eff}^{*2}$. Values have been tabulated as for example given by Karzas and Latter (ref 7). If we can find a simple correspondence between matrix elements for our non-hydrogenic potential and such a hydrogenic case then the cross section may readily be defined in terms of the relevant hydrogenic Gaunt factor, $\mathcal{G}_{sa}^{H}(Z_{eff}^{*}, E_{a'})$

$$\mathcal{G}_{sa}(\nu) = \mathcal{G}_{sa}^{H}(Z_{eff}^{*}, E_{a'}) \times \frac{\nu^3 \dfrac{df_{sa}}{d\nu}}{\nu_H^3 \dfrac{df_{sa}^{H}(Z_{eff}^{*}, \nu_H)}{d\nu_H} \dfrac{d\nu_H}{d\nu}} \times \frac{Z_{eff}^{*4}}{Z^4} \qquad (3.18)$$

where $\dfrac{df_{sa}^{H}}{d\nu_H}$ is the differential oscillator strength for the hydrogenic case.

For a given level n, l there are essentially two independent variables which may be varied in order to obtain such a simple relation, Z_{eff}^* and the continuum energy E_a'. In order to consider the problem thoroughly we need to consider the deformations of the wave functions in the average non-hydrogenic fields of a given ionic configuration.

Many calculations, including those of Mayer and Cox, have assumed that a perturbed bound energy level E_{nl} implies that the wave functions for absorption from that level may be approximated by hydrogenic ones for an effective charge Z_{eff}^* such that

$$-\frac{Z_{eff}^{*2}}{n^2} R_y = E_{nl} \qquad (3.19)$$

and the continuum energy E_a' chosen equal to E_a so that v_H is the same as v. This gives the simple result that

$$G_{sa}(v) = G_{sa}^{H,Z^*}(v) \frac{Z_{eff}^{*4}}{Z^4} \qquad (3.20)$$

This was presumed to take account of electron screening but as we shall show a perturbation to an energy level does not necessarily imply screening. For example when an electron charge is confined in a sphere and then surrounded by a uniform shell of charge outside this sphere, the potential energy is raised uniformly everywhere inside but no fields are exerted. Hence in a quantum mechanical description the energy of the electron would increase but the wave function would remain the same shape. The way in which an electron orbit disturbs another depends on its position relative to the perturbed electron and the parent nucleus.

We have shown that the potential function for an electron near an atomic nucleus differs from the hydrogenic potential chiefly due to the other electrons in bound orbits and also due to bombarding free electrons within the atomic sphere. The different character of the electron effects can be seen qualitatively by applying the Rits variational principle to Coulomb wave functions with a variable charge parameter.

The potential energy function for an electron in the n'l' level of an ion which has $\{n_{nl}\}$ electrons in the levels $\{nl\}$ is

$$V = -\frac{Ze^2}{r} + \frac{Z^* e^2}{2 a_{z'}}\left(3-\left(\frac{r}{a_{z'}}\right)^2\right) + \sum_{nl \neq n'l'} n_{nl} V_{nl}(r) + \left\{\max\begin{pmatrix} n_{n'l'}-1 \\ 0 \end{pmatrix}\right\} V_{n'l'}(r) \qquad (3.21)$$

Using the Coulomb wave function with charge Z_v as the variable parameter the expectation value for the energy is

$$\frac{\langle E_{n'l'}\rangle}{R_y} = \frac{-2ZZ_v}{n'^2} + \frac{Z_v^2}{n'^2} + \sum_{nl \neq n'l'} \frac{n_{nl}\,\sigma_{n'l',nl} \times 2Z_v}{n'^2}$$

$$+ \max\begin{Bmatrix} n_{n'l'}-1 \\ 0 \end{Bmatrix} \frac{\sigma_{n'l',n'l'}}{n'^2} 2Z_v + \frac{Z^* a_0}{a_{z'}}\left\{3 - \frac{n'^2}{2Z_v^2}\left(5n'^2+1-3l'(l'+1)\right)\frac{a_0^2}{a_{z'}^2}\right\} \qquad (3.22)$$

That is

$$\frac{1}{R_y}\frac{dE_{n'l'}}{dZ_v} = \frac{-2Z+2Z_v}{n'^2} + 2\sum_{nl \neq n'l'} \frac{n_{nl}\,\sigma_{n'l',n'l'}}{n'^2} + 2\max\begin{Bmatrix} n_{n'l'}-1 \\ 0 \end{Bmatrix} \frac{\sigma_{n'l',n'l'}}{n'^2}$$

$$+ \frac{Z^*}{Z_v^3}\frac{n'^2 a_0^3}{a_{z'}^3}\left\{5n'^2+1-3l'(l'+1)\right\} \qquad (3.23)$$

The Ritz variational principle implies that the best wave function corresponds to the value of Z_v which makes the energy a minimum, that is

$$dE_{n'l'}/dZ_v = 0$$

The term involving $(Z_v)^{-3}$ due to the free electrons is proportional to the density of free electrons. For levels which are deep enough to be statistically important it is always very small by comparison with the other terms, showing that the density of free electrons has to become very large before Z_{eff}^* is very much affected by them. Hence

$$Z_{eff}^* \sim Z - \sum_{nl \neq n'l'} n_{nl}\, \sigma_{n'l',nl} - \max\left\{ \begin{matrix} n_{n'l'} - 1 \\ 0 \end{matrix} \right\} \sigma_{n'l',n'l'} \qquad (3.24)$$

implying that the bound electrons may screen the nuclear charge significantly but the free electrons very little. As we should expect those electrons readily penetrating inside the orbit n'l' screen significantly whereas those lying outside have little effect. At higher temperatures and densities the perturbations to the energy levels may be largely due to free electrons and in this case the error of choosing an effective charge from the energy level is clear.

The Ritz variational principle only indicates the best overall bound level wave function of the specified parametric form giving the best approximation for the energy. In finding the bound-free cross sections we are evaluating matrix elements between a bound electron state and a free electron state which may lay stress on their behaviour in a particular region of the atom. The radius which is most important will vary according to which operator O(r) is used to evaluate the differential oscillator strength. The potential gradient weighting function lays stress on smaller radii than the momentum operator, whereas the dipole moment weighting function gives greater sensitivity to more distant regions.

The free and bound electron perturbations will now be considered separately in more detail in this context, the aim in each case being to find hydrogenic wave functions which match the distorted wave functions throughout a region contributing significantly to any one of the three alternative radial integrals. We shall retain the model of the crystal lattice already introduced in the last chapter.

FREE ELECTRON PERTURBATIONS

Imagine for the moment that we have a single bound electron in orbit round a nucleus of charge Z in a level n'l' interacting only with the free electrons which penetrate within the electron sphere. The behaviour of the average additional potential is

$$V_f = -\frac{Z^* e^2}{2a_{z'}}\left(3 - r^2/a_{z'}^2\right) \qquad (3.25)$$

where Z^* is such that it is equal to Z-1, the net charge of the enclosed ion, throughout the central regions of the sphere, and rises to Z near the boundary where the effects of other atoms are important. The radial wave function n'l' will then be a solution of

$$\left\{-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right) - E_{n'l'} + V(r) + \frac{\hbar^2}{2m}\frac{l'(l'+1)}{r^2}\right\} R_{n'l'}(r) = 0 \qquad (3.26)$$

where

$$V(r) = -\frac{Ze^2}{r} + \frac{Z^* e^2}{2a_{z'}}\left(3 - \frac{r^2}{a_{z'}^{2}}\right) \tag{3.27}$$

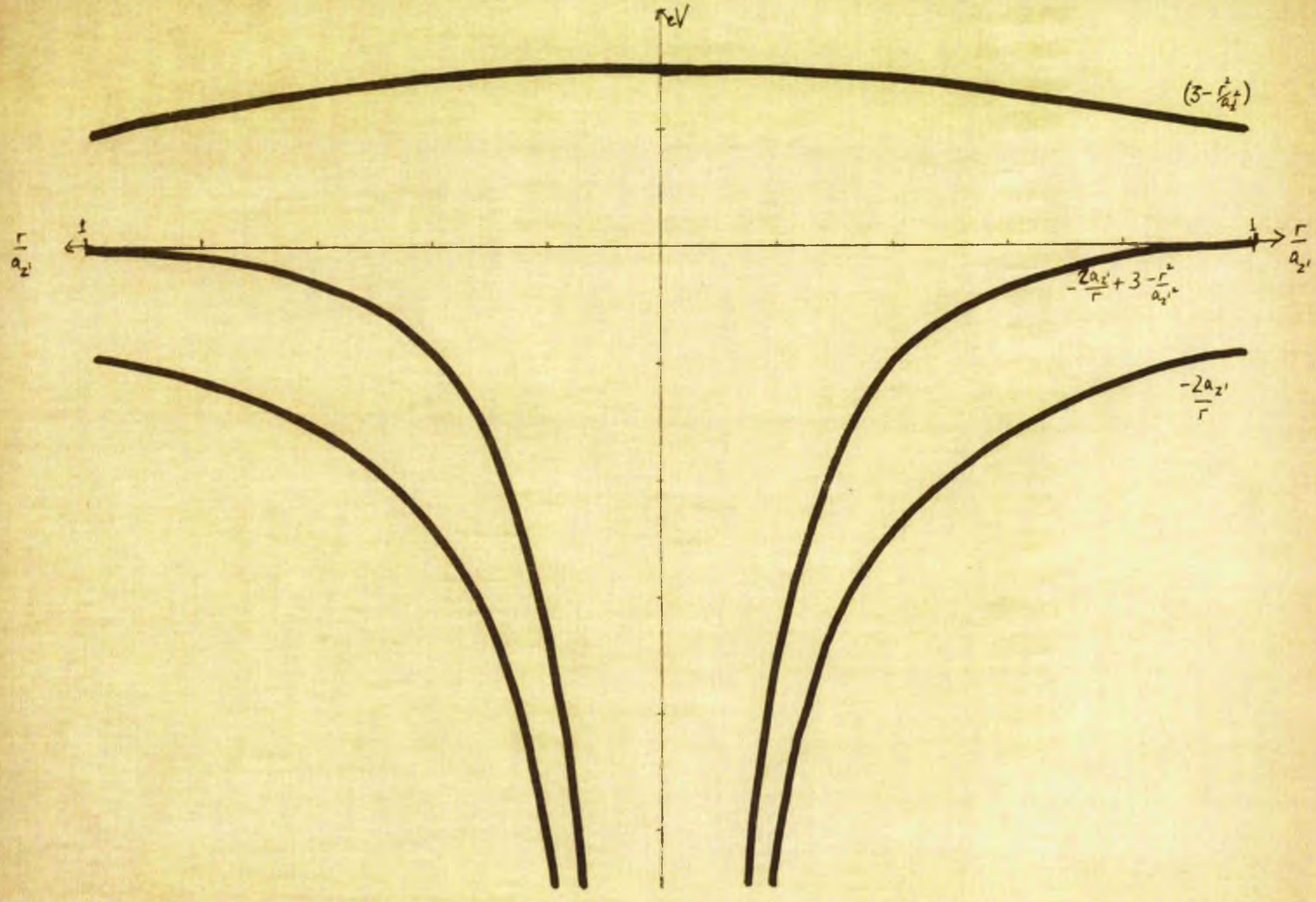
which satisfies the boundary condition that $r R_{n'l'}$ remains finite as r tends to zero. The boundary conditions at large radii are variable and difficult to define. However admissible solutions should be small where the value of the potential energy rises above the energy level $E_{n'l'}$, and will be a rapidly decreasing functions whenever they cross into such a region.

The fact that the Coulomb potential of the nucleus is large in comparison with the potential due to the free electrons at small radii, the normal condition for perturbation theory, coupled with the fact that the free electron potential fluctuates considerably about the average at large radii, suggests that we investigate the behaviour of the wave functions in the central regions with a view to using the potential gradient integrals to find the differential oscillator strengths. We may write the exact initial and final state wave functions R_1 and R_2 as $R_1^H + \delta R_1$ and $R_2^H + \delta R_2$ where R_1^H and R_2^H are hydrogenic wave functions and the potential energy function is

$$-\frac{Ze^2}{r} + \delta V(r)$$

The potential gradient formula to first order is then

$$\underline{I}(r) = \int r^2 R_1 \frac{dV}{dr} R_2\, dr = \int r^2 R_1^H \frac{Ze^2}{r^2} R_2^H\, dr + \int r^2 R_1^H \frac{d}{dr}\delta V(r) R_2^H\, dr$$
$$+ \int r^2 \delta R_1 \left(\frac{Ze^2}{r^2}\right) R_2^H\, dr + \int r^2 R_1^H \frac{Ze^2}{r^2} R_2^H\, dr \tag{3.28}$$



Diag. 3A. Perturbation Potential of the free electron distribution superimposed on Coulomb potential.

and we attempt to choose R_1^H and R_2^H so that the last two terms are negligible.

Towards the nucleus the potential energy, $-eV_f$, of the perturbation flattens off at a constant value $K = +\frac{3Z'a_0}{a_{Z'}} R_y$, where $Z'=Z-1$ in this case of a single bound electron. Now compare the solutions of (3.26) with V(r) given by

$$-\frac{Ze^2}{r} + K$$

and by (3.27) for the energy value

$$E_{n'l'} = -\frac{Z^2}{n'^2} R_y + K \qquad (3.29)$$

Integrating outwards from the nucleus the solutions are very similar until the radius becomes such that the difference between K and $-eV_f$ is no longer small in comparison with the functions V(r). If the two solutions are converging to small values in the classically forbidden regions by this time then they will differ markedly only in their exponentially decreasing tails where the second solution will decrease slightly faster than the first, and the normalisation to one electron in the atom will be the same.

However the first solution is identical with the usual Coulomb wave function for the potential function Ze/r and energy $E_{nl}^C = -(Z^2/n^2)Ry$. The solutions deform continuously with small changes in the energy $E_{n'l'}$ and hence the band of solutions for the perturbed potential with energies close to $E_{nl}^C + K$ will all be very similar to this wave function and have approximately the correct behaviour at the potential barrier between atoms. If the energy level $E_{n'l'}$ given by (2.17) is very close to $E_{nl}^C + K$ then the effect of the free electron potential varying as a function of r is negligible and the wave function is undistorted from the Coulomb one.

The same argument holds for the behaviour of the free-electron wave functions near the nucleus. The wave functions for energy E_a in the free electron potential will be very similar in shape to the hydrogenic wave functions with energy $E_{a'}=E_a-K$. Furthermore the W.K.B. approximation gives us that the amplitude of the wave varies as

$$\frac{1}{r}\,\frac{1}{\sqrt{m\,(E-V(r))}}$$

whenever the potential gradient is small. (The criterion is that

$$\frac{\hbar\, m\,\frac{dV}{dr}}{\left[2m\,(E-V)^{3/2}\right]} \ll 1 \qquad .)$$

The hydrogenic solution $R^{H}_{2,E_{a'}}$ for the radial wave function normalised to one electron per unit volume at energy $E_{a'}$ for an infinite Coulomb field has the asymptotic behaviour

$$\frac{\cos\,(k'r' + \delta')}{k'r}$$

where

$$k' = \sqrt{\frac{2mE_{a'}}{\hbar^2}}$$

Hence if the W.K.B. approximation holds by the time eV_r deviates significantly from K, then integrating out this solution in the free electron field it will behave like

$$\frac{\cos\,(kr+\delta)}{\sqrt{k'kr}}$$

at the boundary where δ is a different phase factor for this field and $k = \sqrt{E_a/E_{a'}}\,k'$. Hence the normalised wave function (one electron per unit volume) will be $\sqrt{k'/k}$ times the hydrogenic wave function of reduced energy E_a, near the origin.

This argument also implies that for continuum energies less than E_a, the wave functions are like hydrogenic bound wave functions of high quantum number n. It is interesting to see what happens to the energy spectrum and corresponding wave functions as we increase the density, effectively pressing in the Z' free electrons into a smaller sphere. As the electrons intrude the wave functions are gradually deformed in the outer regions and at the same time the energies may take on wider bands of values which overlap to form a continuum. In other words as the electrons penetrate a bound electron orbit and screen the nucleus the electron tends to move outwards particularly at large distances where it is more probable that it is completely screened, and can leak away altogether. The missing bound states are not really missing but joined on to the states at the onset of the continuum.

In order to justify the hydrogenic approximation and put $R_1=R_1^H$, $R_2=R_2^H$, we have to show that the potential gradient integral converges well within the regions in which these are good approximations. We can show that this is true when the energy difference between the initial and final levels is sufficiently large and we shall then have

$$\underline{I}(r) = \int r^2 R_1^H \frac{Ze^2}{r^2} R_2^H dr + \int r^2 R_1^H \frac{d}{dr} \delta V(r) R_2^H dr$$

$$= \int R_1^H \frac{Ze^2}{r^2} \left(1 - f(r)\right) R_2^H r^2 dr \qquad (3.30)$$

where
$$f(r) = \frac{Z' r^3}{Z a_{2'}^3}$$

representing the correction term for δV, is a monotonic increasing function of r. Supposing that at frequency ν, the ratio of the correction term to the uncorrected matrix element I(r) is F(ν). Now if we choose a value of r, say r', and we find that F(ν) is less than f(r') then we should expect that the matrix element I(r) must come largely from regions r less than r', for otherwise the matrix element would have shown a greater sensitivity to the tail of ∇V. But at any frequency ν using the commutation relations (3.2)

$$F(\nu) = \frac{Z'e^2}{Z a_{Z'}^3} \frac{1}{4\pi^2 \nu_{as}^2 m} \tag{3.31}$$

In general the important regions will be those for which F(ν) and f(r) are of the same order of magnitude or

$$\frac{Z'e^2}{a_{Z'}^3} \frac{1}{4\pi^2 \nu_{as}^2 m} \sim \frac{Z'r^3}{Z a_{Z'}^3}$$

Hence

$$\frac{r^3}{a_0^3} \sim \frac{Ze^2}{4\pi^2 a_0^3 \nu_{as}^2 m} \tag{3.32}$$

At these distances

$$\frac{|K - eV_f|}{V(r)} = \frac{\frac{Z'e^2r^2}{2a_{Z'}^3}}{\frac{Ze^2}{r}} = \frac{Z'r^3}{2Za_{Z'}^3} \sim \frac{1}{2}F(\nu) \tag{3.33}$$

Hence our approximation will be good when $F(v)$ is small. $F(v)$ is proportional to the density of free electrons ρ_e

$$F(v) = \frac{3\rho_e e^2}{2\pi m v_{as}^2} \qquad (3\ 34)$$

and hence is greatest at the higher densities and temperatures for any given frequency.

The Rosseland weighting function has a maximum about $u=h\nu/kT=7$ and is small at low and high values of u (see graph 1A) so we are particularly interested in obtaining good cross sections at intermediate frequencies. In the Coulomb case the absorption cross sections for the levels vary approximately as n^{-3} with the principal quantum number, so that they decrease rapidly with the binding energy to the nucleus as we should expect. Furthermore the deeper levels are statistically more probable so that at any frequency ν it will be the bound levels which have the greatest threshold frequencies below ν, which will dominate the bound-free absorption. At high temperatures the absorption edges of the deeper levels will occur at lower values of u and the absorption cross-sections of the lightly bound levels will be less important. For example at $T=10^{2.5}$eV the frequencies coinciding with the maximum of the weighting function $\nu=7kT/h$ correspond to electron transitions with an energy increase of about 175 Rydbergs. The ionization energies of 1s levels for elements up to about Silicon will fall below this value. The wave functions of the deeper levels converge well within the atomic spheres and hence they should be well represented by the wave functions R_1^H

associated with them.

Also at the frequencies $\nu \sim 7kT/h$ we find

$$F(\nu) \sim \frac{\pi}{2} \rho_e a_0^3 B^2$$

where $B = Ry/kT$. This expression is always small at the densities and temperatures considered here. In the example just considered $T = 10^{2.5}$ eV with the pressure $P = 10^{2.5}$ Mbars the density of free electrons is about $.3 \cdot 10^{24}$ per cc. and $F(7kT/h)$ is close to 10^{-4}. Hence the regions where the hydrogenic approximations for the wave functions do not hold will contribute little to the integrals we require.

Since the energy parameters of the hydrogenic wave functions vary by the same amount as the ones with which they are associated in the free electron potential, the frequency is invariant

and so

$$\frac{\nu^3 \dfrac{df_{sa}}{d\nu}}{\nu_H^3 \dfrac{df^H_{sa}(Z^*, E_{a'})}{d\nu_H} \dfrac{d\nu_H}{d\nu}} = \frac{k}{k'}\left(\sqrt{\frac{k'}{k}}\left(1 - \frac{3\rho_e e^2}{2\pi m v_{as}^2}\right)\right)^2$$

$$= \left(1 - \frac{3\rho_e e^2}{2\pi m v_{as}^2}\right)^2 \qquad (3.36)$$

so that

$$g_{as} = g^H_{as}(Z, E_{a'})\left(1 - \frac{3\rho_e e^2}{2\pi m v_{as}^2}\right)^2 \qquad (3.37)$$

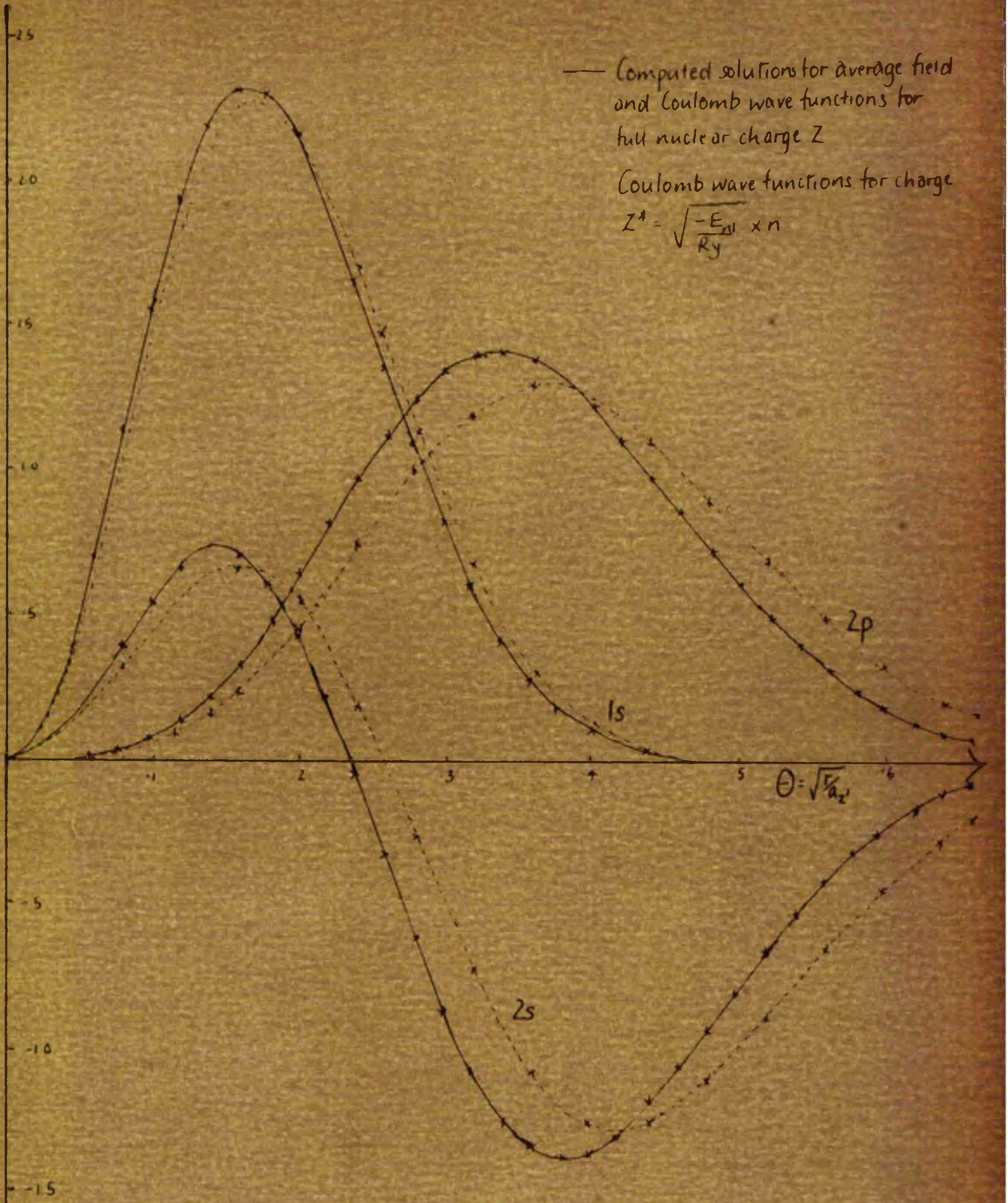


Fig 3A. Comparison of computed bound wave functions in the average field of the nucleus and free electrons with hydrogenic bound wave functions for full nuclear charge Z and for an effective charge taken from the energy level

At low frequencies where the approximation is not so good the correction term may be cut out conveniently by an exponential factor or else ignored altogether since it is small at high frequencies in any case.

AGREEMENT WITH COMPUTED GAUNT FACTORS

Calculations were carried out on Neon in the mixture (5.A) which at $P=10^{2.5}$ mbars, $T=10^{2.5}$ eV has an average of one bound electron in each atom. The mean radius of the atom $a_{Z'}$ is $3.565a_0$ Bohr radii and there are up to six bound levels of which the last three are too lightly bound to be statistically important. Using the exact solutions for the wave functions in the average potential with nine free electrons computed numerically, Gaunt factors were calculated precisely for the first three levels and compared with various hydrogenic Gaunt factors. The convergence of the integrals was investigated in each case and the way in which the radius of convergence decreased with increasing frequency for each given initial bound level was clearly shown. The wave functions were tested where possible by comparing Gaunt factors calculated from the potential gradient, momentum and dipole-moment operators. However at low continuum energies the dipole-moment, and occasionally the momentum integrals, did not converge within the atomic sphere, another reason for considering the potential gradient integral at low frequencies. The graphs (3.A) show the bound wave functions for the 1s, 2s, and 2p states and the corresponding Coulomb functions for the full charge Z as the functions $f_{nl}(r)$,

$$f_{nl}(r) = r R_{nl}(r)$$

for values of $\theta = \sqrt{r/a_{Z'}}$ They are the same to within .01 and hence

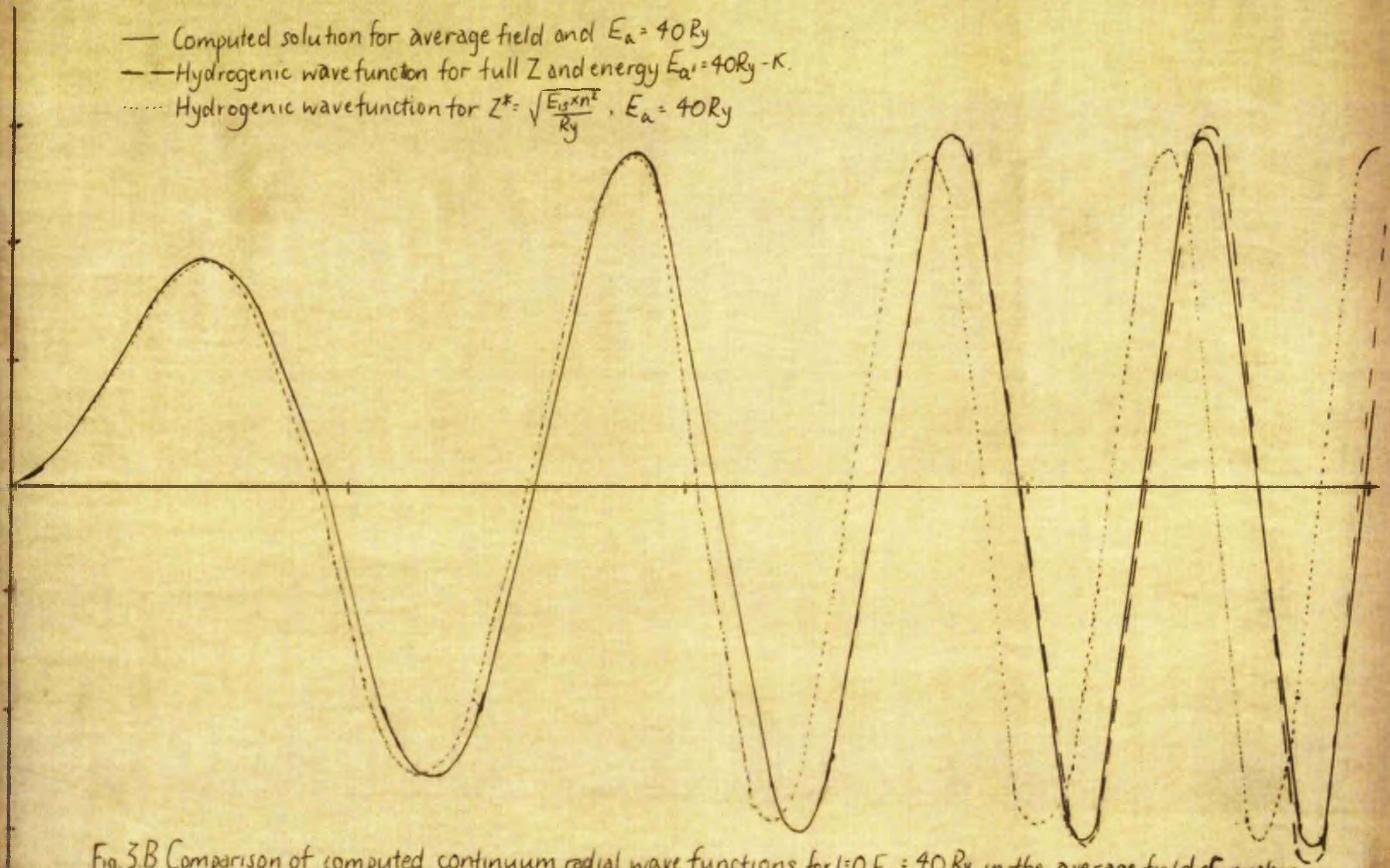


Fig. 3.B Comparison of computed continuum radial wave functions for $l=0$, $E_a = 40\,Ry$ in the average field of nucleus and free electrons with hydrogenic wave functions for the effective nuclear charge from the 1s energy level and the same energy of 40Ry and for full nuclear charge Z and reduced energy $E_{a'} = E_a - K$.

Continuum Energy in Rydbergs	Computed in average field of Z and 4 free e	Hydrogenic $\nu \neq \nu_H$ $Z_{eff}^* = Z$, $E_{a'} = E_a$	Hydrogenic $\nu = \nu_H$ $Z_{eff}^* = \sqrt{-E_{1s}/Ry}$, $E_{a'} = E_a$	Hydrogenic $\nu = \nu_H$ $Z_{eff}^* = Z$, $E_{a'} = E_a - K$
250.0	.994	.991	.849	.990
200.0	.994	.984	.844	.982
150.0	.979	.969	.832	.965
100.0	.926	.942	.810	.935
50.0	.866	.892	.766	.881
40.0	.865	.877	.755	.865
30.0	.848	.861	.740	.847
20.0	.827	.842	.723	.827
15.0	.815	.832	.714	.815
10.0	.803	.822	.704	.803
5.0	.794	.810	.693	.797
2.5	.766	.804	.688	.797
1.0	.820	.799	.684	.797

TABLE 3C BOUND FREE GAUNT FACTORS FOR 1S STATE AND 13 CONTINUUM ENERGIES.

Continuum Energy in Rydbergs	[illegible] field [illegible]	Hydrogenic [illegible] $Z_{eff}^4 = Z$ [illegible]	Hydrogenic [illegible]	Hydrogenic [illegible] $Z_{eff}^4 = Z$, [illegible] K
250.0	3.300	3.340	1.710	3.320
200.0	3.170	3.200	1.670	3.170
150.0	2.950	2.990	1.590	2.950
100.0	2.550	2.660	1.450	2.580
50.0	1.870	2.070	1.160	1.960
40.0	1.770	1.910	1.060	1.770
30.0	1.550	1.720	.965	1.560
20.0	1.300	1.500	.830	1.310
15.0	1.160	1.370	.753	1.170
10.0	1.000	1.240	.665	1.010
5.0	.842	1.090	.568	.934
2.5	.730	1.010	.516	.934
1.0	.726	.968	.481	.934

TABLE 3C. CONT BOUND-FREE GAUNT FACTORS FOR 2S STATE AND 13 CONTINUUM ENERGIES

Continuum Energy in Rydbergs	Computed in intermediate Z and 2 pure	Hydrogenic at v_a $Z_{eff}^{*} = Z$, $E_a = E_i$	Hydrogenic $v = v_a$ $Z_{eff}^{*} = \sqrt{\frac{E_a \times 4}{R_y}}$, $E_a' = E_a$	Hydrogenic $v = v_a$ $Z_{eff}^{*} = Z$, $E_a' = E_i - K$
250.0	.303	.300	.113	.307
200.0	.349	.347	.132	.357
150.0	.421	.415	.163	.428
100.0	.534	.510	.209	.530
50.0	.708	.659	.287	.686
40.0	.722	.696	.311	.727
30.0	.764	.738	.335	.769
20.0	.808	.780	.364	.813
15.0	.827	.802	.379	.832
10.0	.845	.823	.394	.850
5.0	.858	.842	.408	.856
2.5	.827	.850	.415	.856
1.0	.900	.854	.418	.856

TABLE 3C Cont BOUNDFREE GAUNT FACTORS FOR 2P STATE AND 13 CONTINUUM ENERGIES unresolved. The Coulomb states 1s, 2s, and 2p for an effective charge Z_{eff}^* taken from the energy are also given for comparison. In Fig. 3B the s-state free electron wave functions are similarly compared for the energy of 40 Rydbergs by plotting $r\sqrt{\frac{2k}{\pi}}\,R_E$ (this corresponds to normalising the wave functions per unit density per unit energy interval). The continuous line is the exact numerical solution, the dotted line the hydrogenic one for

$$Z_{eff}^*(1s) = \sqrt{\frac{-E_{1s}}{R_y}\times 11^2} \qquad (3.51)$$

with the same energy (k'=k), and the dashed line the curve for $r\sqrt{\frac{2k'}{\pi}}$ times the hydrogenic wave function for reduced energy $E' = k'k'/2m = E-K$

In the table (3C) the actual Gaunt factors are given for each level for a series of energies E_a in the continuum for the final state. In the first column are given the exact calculated Gaunt factors in the average potential of the nucleus and 9 free electrons; in the second the plain hydrogenic Gaunt factors for the full nuclear charge and same continuum energy are given. In the third column the Gaunt factors taking an effective charge from the bound energy level are shown and finally in the fourth column are the Gaunt factors obtained as explained here, using the full nuclear charge and a reduced continuum energy such that the frequency remains invariant.

BOUND ELECTRON EFFECTS

Many attempts have been made to account for the interaction of the other bound electrons on the oscillator strengths. The objection to using most of these methods again lies in the fact that they do not necessarily provide wave functions which are accurate throughout any of the regions where the matrix elements for the oscillator strengths lay emphasis. For example the quantum defect method is based on the dipole length form for the oscillator strength for which the major contribution comes from the outer regions, where the potential is assumed very close to a Coulomb one produced by an effective charge of the nucleus and bound electrons. The bound wave functions are approximated by hydrogenic wave functions with the same angular momentum parameters and an effective quantum number n_{nl}^*

$$n^*_{nl} = \left(\frac{Z_{nl}}{\sqrt{-E_{nl}/R_y}} \right) \tag{3.38}$$

where E_{nl} is the energy of the bound level. The difference between n and n_{nl}^* is the quantum defect for the level. The continuum radial wave functions are expressed by choosing a combination of the two Coulomb wave functions with the given energy E behaving as r^{l+1} at the origin, and with the correct asymptotic behaviour with phases given by $\delta = \pi\mu$ where μ is the extroplated quantum defect. The method is only applicable at low continuum energies

$$\left(\exp(-2\pi Z/\sqrt{E}\,)^{1/2} \ll 1 \text{ i.e. } E \ll Z^2 \right)$$

There is still the same difficulty in this method, of determining the effective charge Z_{nl} at large distances, especially when we may simultaneously have free electrons and surrounding atoms completely neutralising the potential at large radii. A serious result of the high densities and the non-isolated atoms is the fact that the dipole length integrals do not necessarily converge within the finite atomic boundaries, and the region in which we are most uncertain of the potential and wave functions is often critical.

The potential energy of an electron in the level n'l' is given by (3.21). The potential energy of the electron at the point r due to an electron in the state described by the wave function $\psi_{nl} = R_{nl} Y_l^m$ averaged over that electrons position is

$$V_{nl}(r) = e^2 \int_0^r \frac{|R_{nl}(a)|^2}{r} a^2 \, da + e^2 \int_r^{a_{zl}} |R_{nl}(a)|^2 a \, da \qquad (3.39)$$

The first term is due to the charge inside the sphere radius r and gives a potential just equivalent to a charge

$$e \int_0^r |R_{nl}(a)|^2 a^2 \, da$$

at the centre, that is, it effectively diminishes the nuclear charge by this amount. The second term is due to the probability that the nl shell electron lies outside the sphere of radius r. If then all the nl orbits lie almost completely outside the range of the n'l' orbit then the potential is raised uniformly throughout this region and the effect is very like that of the free electrons, when the wave functions are deformed little by the interaction although the energy associated with them is raised. We can again account for this by choosing the energy $E_{a'}$ in the Coulomb approximation such that the frequency remains the same, $v_{H=v}$, with the same full nuclear charge Z.

If some of the orbits nl lie within or overlap the n'l' orbit then the same argument no longer holds and the potential can not be approximated by the full Coulomb field of the nucleus for a sufficiently large radial interval. This suggests that we should now attempt to obtain a better hydrogenic approximation by varying the second available parameter Z_{eff},* to take account of screening by just these inner levels.

Moszkowski and Meyerott investigated the electron screening of bound electrons in K and L shells using Hartree wave functions and calculating the fractional change in the radial matrix element to order $1/Z^2$. They reduced their results to an effective charge form neglecting the splitting of the l degeneracy -

$$\frac{\nu^3 \frac{df_{sa}}{d\nu}}{\nu_H^3 \frac{df^H(Z,\nu_H)}{d\nu_H}} = \frac{Z_M^4}{Z^4} = \frac{\left(Z - \sum_{n \epsilon n'} N'_n \sigma^M_{n,n'}\right)^4}{Z^4}, \quad h\nu = \left(Z^2\eta - \frac{E_{n'}}{R_y}\right)R_y$$

$$h\nu_H = \left(Z^2\eta + \frac{Z^2}{n'^2}\right)R_y \qquad (3.40)$$

and the prime on $N_{n'}$ denotes that one electron is deducted from the number of electrons in the shell n'.

Retaining only terms of order 1/Z they expanded the screening constants $\sigma^M_{n,n'}$ in the form of the sum of a term due to the change in the dipole length and a term varying inversely as the frequency and depending on the Slater screening constant $\overline{\sigma}^{ll'}_{n'l',nl}$

$$\overrightarrow{\sigma}^M_{n,n'} = -b^{n'}_n + \frac{2}{n'^2}\frac{\overline{\sigma}_{n'l',nl}}{\eta + 1/n'^2}$$

Unfortunately the $b^{n'}_n$ also show considerable variation with frequency but the average total screening constants are about the magnitude of the Slater screening constants. Retaining higher order terms to $1/Z^2$ though not permitting a simple expansion equivalent to (3.41) improves agreement slightly between the Moszkowski and Slater screening values. The table

(3D) shows values of the effective charge computed to both orders $1/Z$ and $1/Z^2$, by Moszkowski and Meyerott for the elements and configurations stated. The quantity $Z-Z_s$ gives the value reducing Z as though the electrons screened of the charge for the n'l' electron path according to the probability that they lie nearer to the nucleus, and may be written approximately in terms of the Slater screening constants using (2.12) and (2.16), as

$$Z-Z_s = \sum_{nl<n'l'} n_{nl}\,\sigma_{n'l',nl} + \max\left\{\begin{matrix} n_{nl}-1 \\ 0 \end{matrix}\right\} \frac{\sigma_{n'l',n'l'}}{2} \qquad (342)$$

where we include half screening for electrons in the same orbit. (The Slater screening constants used by Moszkowski and Meyerott are the empirical values given by Slater in 1930 which are independent of l and differ slightly from those evaluated by the formula (2.16).)

	$(Z_M)_K$		$(Z_M)_L$		$(Z_M)_L$		$(Z_M)_L$	
	$Z=13, N_K=2, N_L=0$		$Z=29, N_K=2, N_L=1$		$Z=29, N_K=2, N_L=4$		$Z=29, N_K=2, N_L=8$	
	$1/Z^2$	$1/Z$	$1/Z^2$	$1/Z$	$1/Z^2$	$1/Z$	$1/Z^2$	$1/Z$
0.00	.295	.394	1.216	1.508	2.78	3.81	4.86	7.37
0.25	.318	.360	1.788	1.720	2.50	2.29	3.45	3.03
0.50	.321	.337	1.676	1.595	2.39	2.00	3.34	2.28
1.00	.314	.304	1.470	1.401	2.11	1.75	2.95	1.97
$Z-Z_s$	.30		1.70		2.75		4.15	

Table 3D Effective screening constants as evaluated by Moskowski and Meyerott. (Ap.J. 124, 1956, P540)

	Final Energy in Rydbergs	Perturbing electron in 1s State				Perturbing electron in 2p State			
		A	U	B	S	A		B	S
1s	100.0	0.837	[0.942]	0.832	(0.710)	0.950	AS COLUMN U	0.937	(0.835)
	60.0	0.780	[0.904]	0.795	(0.683)	0.895		0.896	(0.802)
	40.0	0.746	[0.877]	0.768	(0.662)	0.865		0.867	(0.778)
	30.0	0.727	[0.861]	0.752	(0.648)	0.848		0.850	(0.762)
	20.0	0.704	[0.842]	0.733	(0.633)	0.827		0.830	(0.746)
	15.0	0.692	[0.832]	0.723	(0.625)	0.816		0.819	(0.736)
	10.0	0.679	[0.821]	0.711	(0.616)	0.804		0.807	(0.726)
	5.0	0.664	[0.809]	0.706	(0.606)	0.791		0.797	(0.715)
	2.5	0.653	[0.803]	0.706	(0.609)	0.781		0.797	(0.709)
	1.0	0.649	[0.799]	0.706	(0.597)	0.777		0.797	(0.706)
		A	U	B	S	A		B	S
2s	100.0	2.21	[2.66]	1.97	(1.78)	2.44	AS COLUMN U	2.36	(1.91)
	60.0	1.80	[2.22]	1.67	(1.50)	1.99		1.96	(1.62)
	40.0	1.52	[1.91]	1.43	(1.30)	1.68		1.67	(1.39)
	30.0	1.35	[1.72]	1.27	(1.16)	1.49		1.49	(1.25)
	20.0	1.15	[1.50]	1.10	(1.01)	1.28		1.28	(1.09)
	15.0	1.04	[1.37]	0.996	(0.919)	1.15		1.16	(0.987)
	10.0	0.925	[1.24]	0.888	(0.820)	1.02		1.03	(0.885)
	5.0	0.755	[1.09]	0.763	(0.707)	0.640		0.888	(0.765)
	2.5	0.683	[1.01]	0.695	(0.647)	0.764		0.820	(0.702)
	1.0	0.638	[0.968]	0.660	(0.608)	0.715		0.830	(0.661)
		A	U	B	S	A		B	S
2P	100.0	0.331	[0.510]	0.310	(0.263)	0.455	AS COLUMN U	0.433	(0.300)
	50.0	0.439	[0.659]	0.415	(0.356)	0.581		0.567	(0.403)
	40.0	0.464	[0.696]	0.443	(0.382)	0.611		0.602	(0.431)
	30.0	0.494	[0.738]	0.476	(0.410)	0.641		[illegible]	(0.462)
	20.0	0.529	[0.780]	0.510	(0.442)	0.668		[illegible]	(0.496)
	15.0	0.543	[0.802]	0.527	(0.459)	0.680		0.700	(0.513)
	10.0	0.558	[0.823]	0.545	(0.475)	0.689		0.719	(0.531)
	5.0	0.572	[0.842]	0.561	(0.490)	0.688		[illegible]	[illegible]
	1.0	0.582	[0.854]	0.569	(0.500)	0.686		[illegible]	[illegible]

TABLE 3E BOUND FREE GAUNT FACTORS

It is evident that the Slater screening approximation breaks down as the number of electrons increases relative to the nuclear charge, but that it is better in ionic configurations with only a few bound electrons.

Moskowski and Meyerott's expansion is based on the radial matrix element and since the wave functions are not true solutions the relations (3.2) do not hold exactly and the expansion of the potential gradient formula would differ in order $1/Z^2$. To investigate this sort of screening approximation further, calculations were carried out to find the exact electron wave functions for the typical cases of Neon in which one electron was assumed to be in one of the levels 1s, 2p in turn, and to determine the Gaunt factors from these exactly for each level 1s to 2p and several continuum energies. The results are shown in tables (3E). The figures in the columns B are the hydrogenic approximation for the Gaunt factors corresponding to frequency v, obtained using the effective charge $\cancel{Z-}Z_s = Z_{eff}$ to account for inner screening electrons, and a continuum energy $E_{a'}$,

$$E_{a'} = h\nu - \frac{(\cancel{Z-}Z_1)^2}{n^2} R_y$$

such that the hydrogenic frequency v_H remains the same as v, to take care of the perturbations from the outside electrons. For comparison the unscreened hydrogenic Gaunt factors are given in the square brackets and hydrogenic Gaunt factors screened according to the binding energy of the initial bound level are shown in ( ).

The arguments applied in the previous section to the superposition of the free electron field on a Coulomb field depend only on the constant nature of the perturbing field over the range of the bound level electron under consideration, and are independent of the unperturbed field. The

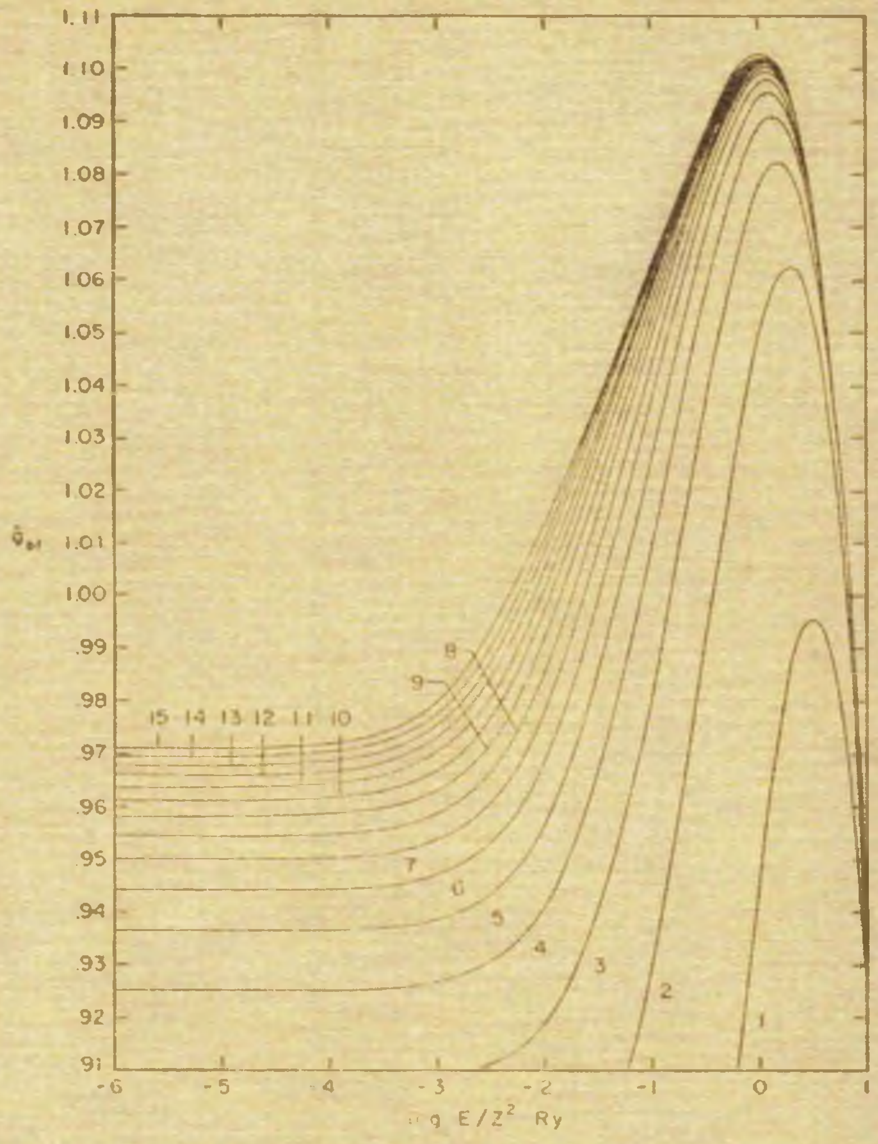


Fig 3F —Bound-free Gaunt factor averaged over a shell versus free electron energy for $n = 1$–15 effects of the free electrons and bound electrons outside the electron orbit are additive and the correspondence $T: E_a \rightarrow E_{a'}$ is defined by their combined contribution to the potential energy near the nucleus. Hence when the effect of all the electrons are considered together the above choice of Z_{eff}^* and continuum energy $E_{a'}$ will still be correct. We can then write for all cases

$$\begin{aligned} g_{sa}(\nu) &= g_{sa}^H(Z_{eff}^*, E_{a'}) \times \frac{Z_{eff}^{*4}}{Z^4} & E_{a'} > 0 \\ &= g_{sa}^H(Z, 0) \times \frac{Z_{eff}^{*4}}{Z^4} & E_{a'} \leq 0 \end{aligned} \qquad (3.43)$$

The complications of taking a frequency dependent formula to improve upon this screening approximation are considerable and such approximations are not necessarily consistent with the sum rule for the oscillator strengths which must always apply (Bethe and Salpeter P 260.) The frequency dependence is most important in the case of several electrons occupying the same shell and the probability of such configurations is small in most cases; if the error in the Gaunt factor in the case of more than one electron in the same orbit is 10% and the probability of this occurring is less then 1/10, then the percentage error on averaging over configurations is less than 1%.

Furthermore the Gaunt factors are slowly varying functions of frequency tending to values of the order of unity near the threshold edges, (see Fig. 3F), so that it is usually sufficient to average over the ionic configurations I at frequencies above the highest component edge by using the average value $\overline{Z}_{eff}^{\,4}$ of Z_{eff}^{*4} and the Gaunt factors

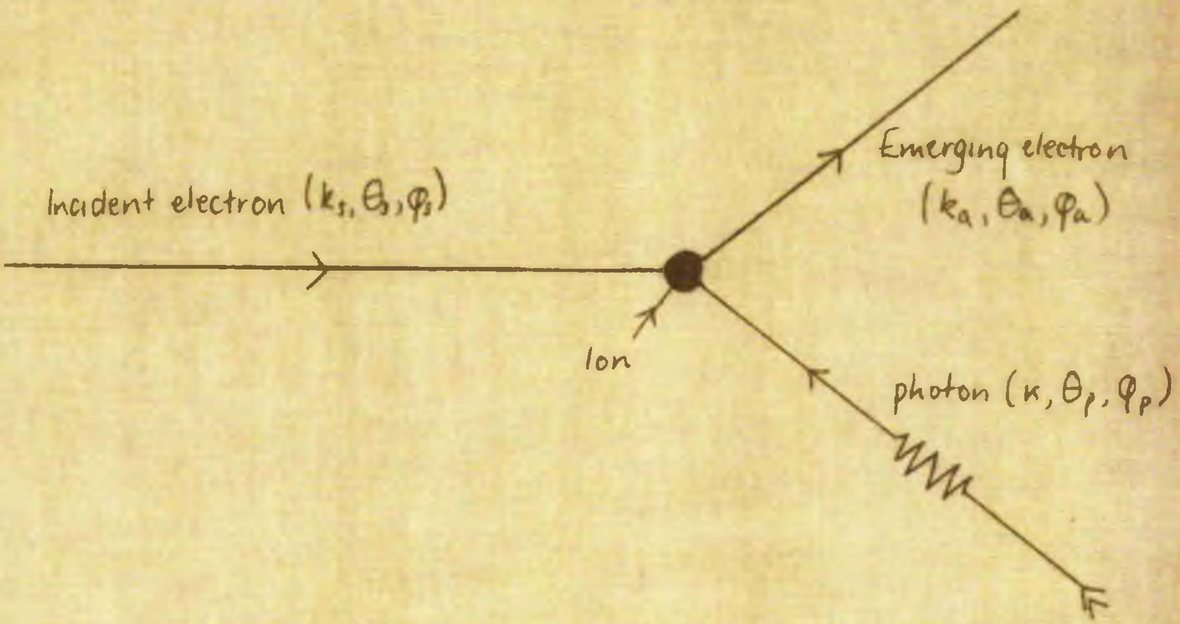


Fig. 39 Free-free absorption process. – $\frac{\hbar^2}{2m}(k_a^2 - k_s^2) = h\nu$

for the average parameters $\bar{Z}_{eff}$ and $E_{a'}$.

$$\overline{\sigma_{\iota\nu s}}^{I} = \sum_{I} P_{I} (\sigma_{\iota\nu s})_{I} = \sigma_{\iota\nu s}^{K} \left\{ \sum P_{I} \left(G_{sa}^{H}(Z_{eff}^{*}, E_{a'}) \frac{(Z_{eff}^{*4})_{I}}{Z^{4}} \right) \right\} \tag{3.44}$$

$$\simeq \sigma_{\iota\nu s}^{k}\, G_{sa}^{H}\left(\left[\sum_{I} P_{I} (Z_{eff}^{*})_{I}^{4}\right]^{1/4}, \sum P_{I} (E_{a'})_{I} \right) \sum \frac{P_{I} (Z_{eff}^{*})_{I}^{4}}{Z^{4}}$$

$$= \sigma_{\iota\nu s}^{K}\, G_{sa}^{H}(\bar{Z}_{eff}, E_{a'})\, \bar{Z}_{eff}^{4}/Z^{4} \quad ; \nu > \nu_{max}^{T}$$

However in the region between the lowest and highest configuration edges the average cross-section is

$$\overline{\sigma_{\iota\nu s}}^{I} = \sigma_{\iota\nu s}^{K}\, G_{sa}^{H}(Z,0) \times \sum_{\{I \,:\, \nu_{I,s}^{T} << \nu\}} P_{I} (Z_{eff}^{*})_{I}^{4} \quad ; \nu \leq \nu_{max}^{T} \tag{3.45}$$

where the summation is only over the configurations I of probability P_I for which the threshold frequency $\nu_{I,S}^{T}$ does not lie above ν.

FREE-FREE ABSORPTION

In the absorption problem here we have free electrons of all positive energies moving into the field of an atom from random directions. These electrons interact with the radiation field and may emerge with different energies and directions. (Fig. 3G)

We shall find the fraction of the flux of radiation of frequency ν absorbed per atom when there is a unit flux of electrons per unit area of energy E_s,

$$E_s = \frac{\hbar^2 k_s^2}{2m} \tag{3.46}$$

impinging on the nucleus from a direction (θ_s, φ_s). We can then find the average cross section per atom per unit density of free electrons by averaging over the flux as a function of the energy.

Accordingly the incident uniform flux of electrons is described by a wave function which behaves asymptotically like an incoming plane wave in the direction (θ_s, φ_s) plus a scattered sperical outgoing wave. This may be expressed in the form (3.4) as a superposition of partial waves just as the final state wave functions in the case of bound-free absorption

$$\psi_s = 4\pi\sqrt{\frac{m}{\hbar k_s}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} i^l e^{i\delta_l} Y_l^{m*}(\theta_s, \varphi_s) R_{E_s,l}(r) Y_l^m(\theta, \varphi) \tag{3.47}$$

where again the $R_{Es,l}$ are the solutions of the radial wave equation (3.26) for energy E_s and angular momentum parameter l, which behaves like $\frac{1}{k_s r}\sin(k_s r - \pi l/2 + \delta)$ for large r.

(N.B. This wave function is normalised to represent a unit flux of electrons with velocity v, not a unit density).

For the final states exactly as in the bound free absorption we have

$$\frac{4\pi m}{h^3}\sqrt{2mE_a}\,\frac{d\Omega_a}{4\pi} = \frac{m}{h^3}\hbar k_a\, d\Omega_a \tag{3.48}$$

wave functions per unit energy interval representing outgoing electrons travelling in directions within the sold angle $d\Omega_a$ about (θ_a, φ_a) and defined by

$$\psi_a = \sum_{l=0}^{\infty} \sum_{m=l}^{m=+l} 4\pi i^l e^{i\delta_l} Y_l^{m*}(\theta_a, \varphi_a) R_{E_a,l}(r) Y_l^m(\theta, \varphi) \tag{3.49}$$

Hence

$$M_{as} = \sum_{l,m} |\langle 4\pi i^l e^{i\sigma_l} Y_l^m(\theta_s,\varphi_s)\rangle|^2$$

$$\times \left\{ \frac{\left|\int r^2 R_{E_a',l+1}\,\alpha(r)\,R_{E_s,l}\,dr\right|^2}{(2l+1)(2l+3)} \begin{pmatrix} |\langle 4\pi i^{l+1} e^{i\sigma_{l+1}} Y_{l+1}^{m}(\theta_a,\varphi_a)\rangle|^2 (l+m+1)(l+m+2) \\ +\frac{1}{2}|\langle 4\pi i^{l+1} e^{i\sigma_{l+1}} Y_{l+1}^{m+1}(\theta_a,\varphi_a)\rangle|^2 (l+m+1)(l+m+2) \\ +\frac{1}{2}|\langle 4\pi i^{l-1} e^{i\sigma_{l-1}} Y_{l+1}^{m-1}(\theta_a,\varphi_a)\rangle|^2 (l-m+1)(l-m+2) \end{pmatrix} \right.$$

$$\left. + \frac{\left|\int r^2 R_{E_a,l-1}\,\alpha(r)\,R_{E_s,l}\,dr\right|^2}{(2l+1)(2l-1)} \begin{pmatrix} |\langle 4\pi i^l e^{i\sigma_{l-1}} Y_{l-1}^{m}(\theta_a,\varphi_a)\rangle|^2 (l+m)(l-m) \\ +\frac{1}{2}|\langle 4\pi i^l e^{i\sigma_{l-1}} Y_{l-1}^{m+1}(\theta_a,\varphi_a)\rangle|^2 (l-m)(l+m+1) \\ +\frac{1}{2}|\langle 4\pi i^l e^{i\sigma_{l-1}} Y_{l-1}^{m-1}(\theta_a,\varphi_a)\rangle|^2 (l+m)(l+m-1) \end{pmatrix} \right\} \qquad (3.50)$$

Bound free absorption normally dominates the free-free absorption in the mixture except in conditions where the degree of ionisation is almost complete; it is not really necessary to consider the effects of bound electron screening and as we have shown free electron screening is small. (This was confirmed by calculating oscillator strengths using the numerical solutions for the continuum wave functions in the average potential and comparing with the corresponding unscreened Coulomb values). Hence we can use the Coulomb wave functions and potential gradient formula. Integrating over Ω_a and averaging over Ω_s the resulting cross section becomes

$$\sigma(E_s,\nu) = \frac{m}{\hbar k_s}\,\frac{8Z^2}{3}\left(\frac{e^2}{\hbar c}\right)^3 \frac{\hbar^2 c^2}{m\nu^2}\,\frac{k_a}{h\nu}\,q_a \left\{ \sum_l \left[(l+1)\left|\int r^2 R_{E_a,l+1}\frac{1}{r^2}R_{E_s,l}\,dr\right|^2 + l\left|\int r^2 R_{E_a,l-1}\frac{1}{r^2}R_{E_s,l}\,dr\right|^2 \right] \right\} \qquad (3.51)$$

The Pauli exclusion principle makes little difference to the energy distribution of free electrons so that $q_a \sim 1$ and the velocity distribution is very nearly Maxwellian. The fraction of electrons with velocity V_s is then

$$f(V_s) = \frac{2}{\sqrt{\pi}}\left(\frac{2m}{\beta}\right)^{3/2} V_s^2 e^{-\beta V_s^2} \tag{3.52}$$

so that the total flux of electrons incident on the atom with this velocity is

$$\rho_e V_s f(V_s) \tag{3.53}$$

where ρ_e is the density of free electrons.

Hence the total cross section per atom per unit density of free electrons on averaging over the velocity is

$$\sigma_{AH}(\nu) = \int \sigma(E_s,\nu) V_s f(V_s) dV_s \tag{3.54}$$

This may be written in terms of the classical Kramers total cross section and a mean Gaunt factor

$$\sigma_{AH}(\nu) = \int dV_s \left[\frac{4\pi}{3\sqrt{3}} \frac{e^6 Z^2}{hcm^2} \frac{1}{\nu^3} \times \frac{f(V_s)}{V_s} \times \left(\frac{2}{\pi}\sqrt{3}\, k_a k_s \left\{\sum_l \left[(l+1)\left|\int r^2 R_{E_a,l+1} \frac{1}{r^2} R_{E_s,l}\, dr\right|^2 + l\left|\int r^2 R_{E_a,l-1} \frac{1}{r^2} R_{E_s,l}\, dr\right|\right]\right\}\right)\right]$$

$$= \frac{4\pi}{3\sqrt{3}} \frac{e^6}{hcm^2} Z^2 \frac{1}{\nu^3} \times \int \frac{f(V_s)}{V_s} dV_s \times \frac{\int \frac{f(V_s)}{V_s} g_H(\nu) dV_s}{\int \frac{f(V_s)}{V_s} dV_s}$$

$$= \overline{\sigma_{AH}}^{K} \times \bar{g}_H(\nu) \tag{3.55}$$

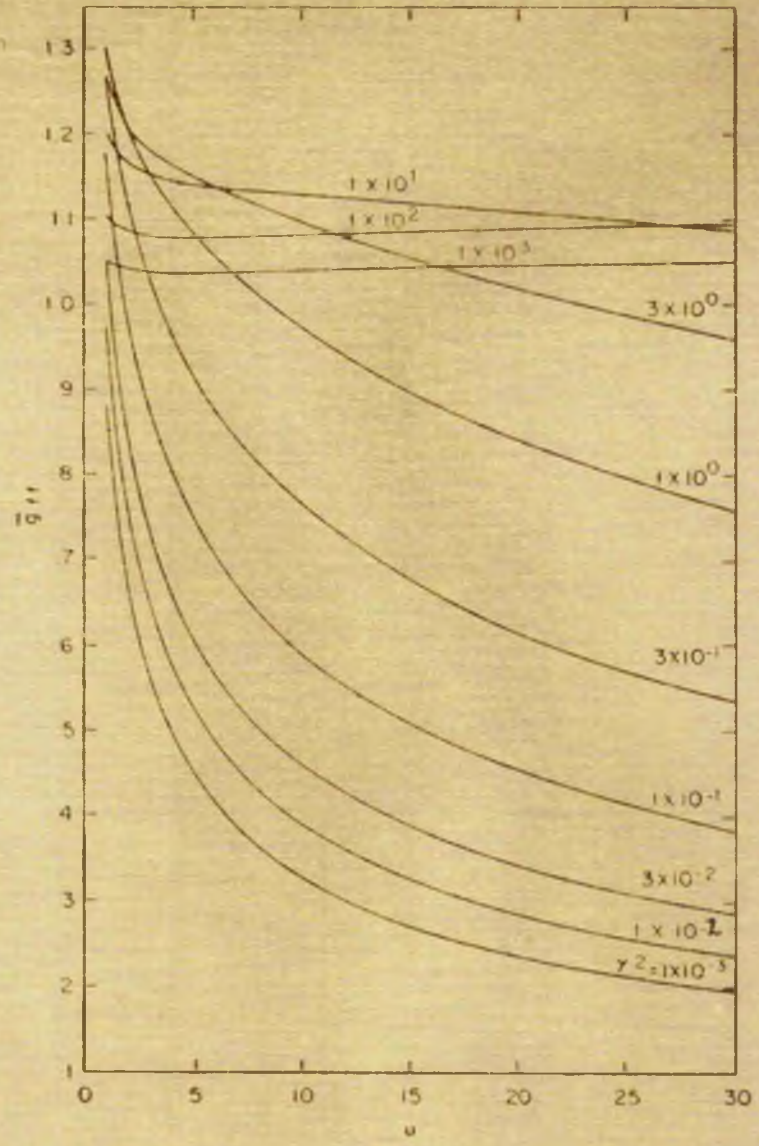


Fig 3. H. Temperature averaged free-free Gaunt factors as functions of u for various values of $\gamma^2 = Z^2 \frac{Ry}{kT}$.

The classical cross section

$$\sigma^{k}_{Aff}(\nu) = \frac{4\pi}{3\sqrt{3}} \frac{e^6}{hcm^2} \frac{Z^2}{\nu^3} \int \frac{f(V_s)}{V_s} dV_s \qquad (3.56)$$

varies inversely as the square root of the temperature since

$$\int \frac{f(V_s)}{V_s} dV_s = \left(\frac{2m}{\pi kT}\right)^{1/2} \qquad (3.57)$$

The Gaunt factor

$$\bar{g}_{ff}(\nu) = \sqrt{\frac{\pi kT}{2m}} \int \frac{f(V_s)}{V_s} g_{ff}(\nu)\, dV_s$$

has been evaluated and tabulated by Karsas and Latter as a function of the two temperature and frequency dependent variables

$$u = \frac{h\nu}{kT} \qquad , \qquad \gamma^2 = \frac{Z^2 R_y}{kT} \qquad (3.58)$$

The graphs 3H taken from the paper by Karsas and Latter (Ref 7) shows the temperature averaged free-free Gaunt factors as functions of u for various values of γ^2.

SCATTERING

The cross section for pure absorption by free electrons are small.

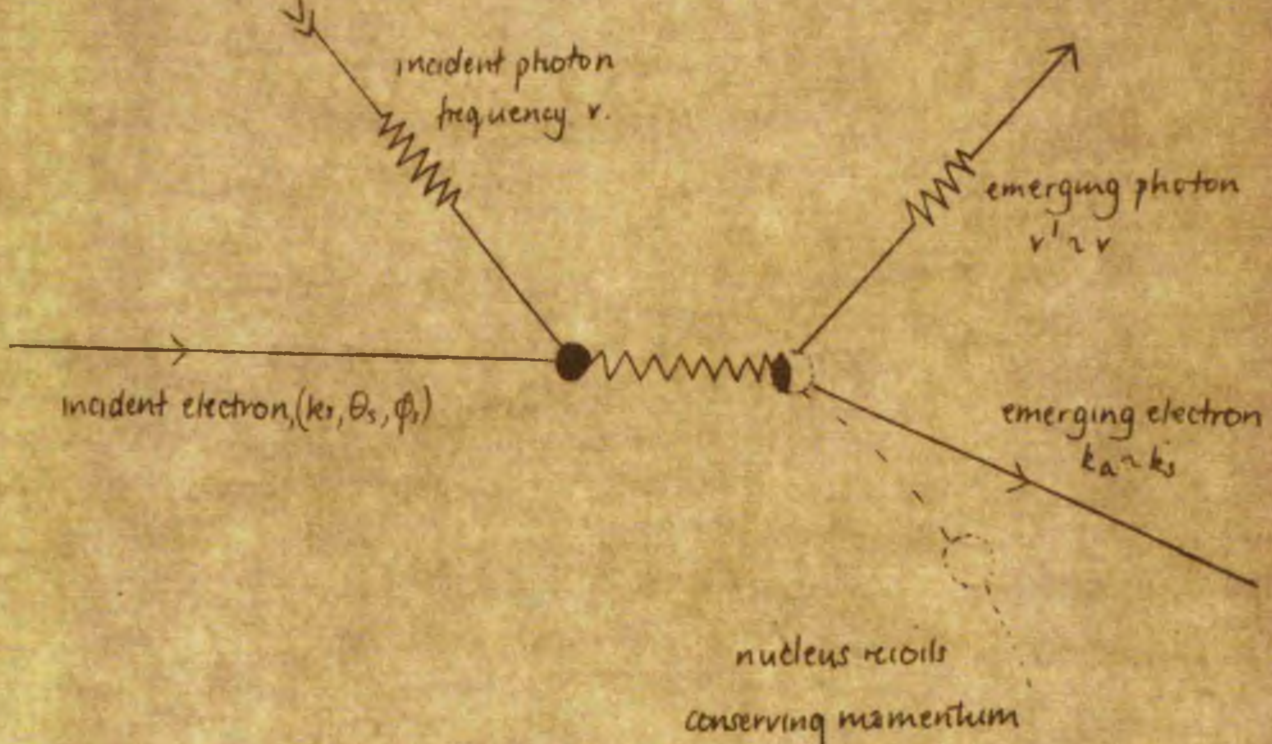


Fig. 3.I. Scattering Process

In fact it is only the scattered parts of the free wave functions which lead to absorption at all and first order Born approximation based only on their asymptotic plane wave behaviour gives a zero cross section. This implies that the second order process of scattering may be an equally important absorption process for free electrons.

In a scattering process the interaction between an incident photon and an electron perturbs the pair in such a way that the photon is absorbed with almost simultaneous re-emission in a new direction. (see Fig. 31) For photon energies much less than mc^2, the nonrelativistic case, the frequency of the scattered photon is almost the same as that of the incident photon and we have coherent scattering.

The total cross section for scattering of photons of frequency ν by an electron at rest is given by the relativistic formula of Klein Nishina (Heitler P221)

$$\sigma_s(\nu) = \sigma_0 \left[\tfrac{3}{4} \left\{ \frac{1+\gamma}{\gamma^3} \left[\frac{2\gamma(1+\gamma)}{1+2\gamma} \log(1+2\gamma) \right] + \frac{1}{2\gamma} \log(1+2\gamma) - \frac{1+3\gamma}{(1+2\gamma)^2} \right\} \right] \qquad (3.59)$$

where

$r_0^2 , r_0 = \frac{e^2}{mc^2}$

$$\sigma_0 = \frac{8\pi a_0^2}{3} , \qquad \gamma = \frac{h\nu}{\cancel{2\pi} mc^2} \qquad (3.60)$$

σ_0 is the classical Thomson cross section. Both the Planck and Rosseland means lay little weight on the absorption coefficient at photon frequencies with energies $h\nu$ much greater than 10kT. At temperatures of the order of 100eV, γ is of the order of 10^{-4} at most and hence the scattering cross-section per free electron is very nearly constant at the non relativistic and classical value σ_0 throughout the range of interest.

THE CONTINOUS ELEMENT SPECTRA

We now have cross sections for various absorption processes for individual atomic particles and wish to combine these for the total ensemble to form a spectrum for the mixture from which the opacity can be calculated.

In each gram of the element of nuclear charge Z there are A_0/M_z atoms where A_0 is Avogadro's number and M_Z is the atomic weight. Each atom has on the average n_{nl} electrons in the level nl with an average cross section σ_{nl} (which we assume to be zero at present below the lowest configuration component bound free edge, ignoring the line absorption). In addition there is a density of free electrons ρ_e adding and average of $\rho_e \sigma_{Aff}(\nu)$ to the cross section of each atom. Hence the cross section per gram of the element Z for pure absorption is

$$K_{Z,abs}(\nu) = \frac{A_0}{M_Z}\left(\sum_{nl} \bar{n}_{nl}\sigma_{nl}(\nu) + \rho_e \sigma_{Aff}(\nu)\right) \qquad (3.61)$$

By analogy with the derivation for the transition probability from the state s to the state a with a decrease in the number of photons in the radiation field, the transition probability from the state a to the state s with emission of a photon is the sum of two terms, a spontaneous part

$$P_{c\chi\nu,spont} = \frac{2}{3}\frac{e^2}{m^2\hbar}\frac{\nu}{c^3}\left|\langle\psi_{ia}|p|\psi_{is}\rangle\right|^2 q_0 \frac{\delta}{2\pi}(2\pi(\nu-\nu_{as})) \qquad (3.62)$$

and a term proportional to I(v)

$$P_{i\lambda\nu,\,stim} = \frac{1}{3}\frac{e^2}{m^2\hbar c\nu}\frac{I(\nu)}{h\nu}\left|\langle\psi_{is}|p|\psi_{ia}\rangle\right|^2\frac{q_i}{2\pi}\delta(2\pi(\nu-\nu_{as})) \quad (3.63)$$

It follows that, if the electrons obey Fermi-Dirac statistics the total stimulated emission at frequency v is just a factor

$$e^{-h\nu/kT} = e^{-u}$$

times the total pure absorption. Hence the total absorption is

$$k'_{Z,abs}(\nu) = k_{Z,abs}(\nu)\left(1-e^{-h\nu/kT}\right) \quad (3.64)$$

In addition we have an average of $\bar{Z}'$ free electrons per atom scattering radiation with cross section σ_s so that the total net absorption is

$$k_Z'(\nu) = \frac{A_0}{M_Z}\Big[\Big(\sum_{nl}\bar{n}_{nl}\sigma_{nl}(\nu) + \rho_e\sigma_{AH}(\nu)\Big)\Big(1-e^{-h\nu/kT}\Big)+\bar{Z}'\sigma_s\Big)\Big] \quad (3.65)$$

The dominant term in this expression is usually the bound free contribution which varies as $1/\nu^3$. For convenience it is better to change to the parameter $u = h\nu/kT$ and tabulate a function which remains all the absorption characteristics but remains within reasonable bounds. Such a function is $D_Z(u) = \dfrac{k_Z'(u)u^3}{C(1-e^{-u})}\left(\dfrac{kT}{R_y}\right)^3$ (3.66) where C is the numerical constant

$$C = \frac{A_0\, 64\, \pi^4 m e^{10}}{3\sqrt{3}\, c h^3 Ry^3} = 4.76704 \cdot 10^6 \qquad (3.67)$$

This function will now define the continuous spectrum of the element of nuclear charge Z, that is the element spectrum excluding the contribution from the line absorption. The absorption coefficient per gram of the mixture follows from combining the individual element spectra together according to their concentrations by weight.

$$D_M(u) = \sum \beta_Z D_Z(u) \qquad (3.68)$$

$$K_m'(u) = \frac{C(1-e^{-u})Ry^3}{u^3\ (kT)^3} D_M(u) \qquad (3.69)$$

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CHAPTER IV

LINE ABSORPTION

In deriving the transition probability leading to the absorption cross section for frequency v for an electron in any specified initial state, the variety of the possible simultaneous perturbations due to the potential field of the electrons surroundings was ignored. It was assumed that the electrons in each given ionic configuration remained indefinitely in undistorted states of fixed energy, for absorption to to take place. In the case of bound free absorption, consideration of the various perturber states implies that each infinitely sharp configuration edge should be replaced by a continous profile, but the effect on the opacity is small when superimposed on the configuration splitting of edges. However, the various perturber interactions become extremely important in the case of bound-bound transitions, as they lead to absorption over several narrow bands of frequency instead of infinitely narrow lines.

As in the case of the bound-free absorption edges, the effect of the various core configurations is to split each line into a number of components. These correspond to the dependence of the energy difference of the two levels concerned on the occupation numbers and the Slater integrals. The effect of perturbers outside the core is to produce a continuous range of energy perturbations and hence broaden each line component into a continuous profile. The magnitude of the interactions with the other core electrons is usually greater than of those with particles outside the core, so that in general the splitting with configuration tends to be greater than the broadening, and the components do not overlap.

The cross-sections for bound-bound transitions are large, and as already mentioned the broadening may be very great in the conditions of the stellar interior. At the lower temperatures the splitting of lines and the greater tendency of electrons to cluster in the lower bound levels as well as the emphasis on lower frequencies, all tend to make line absorption relatively more important.

The broadening mechanisms and the resulting profiles are complicated and this chapter is devoted to discussion of the problem in some detail, starting off with the theory of absorption according to time dependent perturbation theory. Fortunately at the temperatures under consideration here the opacity is not too sensitive to the exact profiles of the individual line components.

THE ABSORPTION OF RADIATION BY AN ELECTRON EMBEDDED IN A GENERAL EVOLVING CHARGE SYSTEM

We shall now return to the derivation of the cross-section for the absorption of radiation, treating the problem by time dependent perturbation theory, for an electron in a general charge system.

The hamiltonian for a charge system interacting with the radiation field is

$$H = \sum_i \left\{ e_i\varphi_i + \left(\underline{p}_i - \frac{e\underline{A}}{c}\right)^2 \Big/ 2m_i \right\} + \sum_\lambda H_\lambda \qquad (41)$$

where the index i refers to the ith charged particle of momentum p_i and mass m_i, in the electromagnetic field $\varphi_i, \underline{A}$ and the $\{H_\lambda\}$ are the hamiltonians of the radiation field at frequency v_λ. At time t=0 the possible eigen states $\Phi_k(t)$ of the time dependent Schrodinger equation for the hamiltonian H_s

$$H_s = \sum_i \left\{ e_i\varphi_i + \left(p_i - \frac{e}{c}A\right)^2/2m_i \right\} \qquad (4.2)$$

are approximately the products of the single particle eigen functions $\{\beta_{ik}(t)\}$ of the hamiltonians

$$h_i = e_i\bar{\varphi}_i(t) + p_i^2/2m_i$$

where $\bar{\varphi}_i(t)$ is the average potential of the ith particle due to the other particles at that time.

$$\Phi_k(t) = \prod_i \beta_{ik}(t) \qquad (4.3)$$

At any time t the states $\psi(t)$ of the particles may be expressed in terms of such functions.

The radiation states may be described by

$$\{R_k\} = \prod_\lambda |n_{\lambda k}\rangle e^{-2\pi i v_\lambda n_{\lambda k} t} \qquad (4.4)$$

where $n_{\lambda k} h\nu_\lambda$ is the energy of the radiation oscillator for frequency in the state k, and the exponential factor gives the time development of the states. The combined system of radiation and particles may be represented by wave functions of the form $\psi_j(t)\, R_k(t)$ and the interaction term

$$\sum_i \frac{p_i \cdot e\underline{A}}{mc}$$

in the hamiltonian H treated as a small perturbation. According to perturbation theory if a state is described by $\psi_s(0)\, R_f(0)$ at time t=0, the probability that it is in the state $\psi_a(T) R_g(T)$ at time T is

$$P(T) = \left| \frac{1}{\hbar} \int_0^T \langle \psi_a(t') R_g(t') \,|\, h_{\psi,R} \,|\, \psi_s(t') R_f(t') dt' \rangle dt' \right|^2 \tag{4.5}$$

where $h_{\psi,R}$ is the interaction hamiltonian.

When photons of frequency v are absorbed then the number of photons in the final states must be less than in the initial state. Expanding the vector potential as the sum of the contributions of the individual radiation oscillators

$$\underline{A} = \sum_\lambda q_\lambda \sqrt{4\pi c^2}\; \underline{e}_\lambda\, e^{i(\underline{k}_\lambda \cdot \underline{r})} \tag{4.6}$$

where $\underline{e}_\lambda$ is the polarisation vector and $\underline{k}$ the propagation vector for the oscillator λ, it is found that the probability of such transitions is zero unless

$$n_{\lambda f} = n_{\lambda g} - 1$$

In this case averaging over the polarisation and the direction of propagation of the radiation relative to the orientation of the system, the probability that a photon of frequency v has been absorbed due to this interaction, leaving the electron in a state a at time T is

$$P_{i,\nu,s} = \frac{1}{3}\,\frac{e^2}{m^2\hbar c\nu}\,\frac{I(\nu)}{h\nu}\left|\frac{1}{2\pi}\int_0^T \langle \psi_{ia}(t')|\,p_i\,e^{-2\pi i\nu t'}\,|\psi_{is}(t')\rangle\,dt'\right|^2 \qquad (47)$$

where the replacement of ψ_a and ψ_s by ψ_{ia} and ψ_{is} indicates that the wave functions may be regarded as functions of the coordinates of the ith particle on which the action of p_i has to be averaged over all other coordinates.

To find the average cross section for absorption for an electron in a given bound state with quantum numbers n and l initially, we have to average over the various possible wave functions and their development in time. The average cross section on summing over the available final states and dividing by the total incident flux in the time T, then becomes

$$\sigma_{i,\nu,s} = \frac{1}{3}\,\frac{e^2}{m^2\hbar c\nu}\,\mathrm{Ave}\,\frac{1}{T}\left\{\sum_a\left|\frac{1}{2\pi}\int_0^T \langle \psi_{ia}(t')|\,p_i\,e^{-2\pi i\nu t'}\,|\psi_{is}(t')\rangle\,dt'\right|^2\right\} \qquad (48)$$

THE CORRELATION FUNCTION

Supposing we write the part of the (~~wave function~~) cross section depending on the wave functions as $\overline{|C^2|}$, a sum of double integrals.

$$\overline{|C^2|} = \text{Ave}\left\{\frac{1}{4\pi^2 T}\sum_a \int_{t'=0}^{T}\int_{t''=0}^{T} \langle \psi_{1a}(t'')|\, p_1 e^{-2\pi i\nu t''}\,|\psi_{1\beta}(t'')\rangle \langle \psi_{1\beta}(t')|\, p_1 e^{+2\pi i\nu t'}\,|\psi_{1a}(t')\rangle\, dt'dt''\right\}$$

$$= \text{Ave}\left\{\frac{1}{4\pi^2 T}\sum_a \int_{t'=0}^{T}\int_{t''=0}^{T} f_a(t',t'')\,dt'dt''\right\} \qquad (4.9)$$

When the integrals in (4.9) are absolutely convergent then we may write each double integral

$$\int_0^T\int_0^T f_a(t',t'')\,dt'dt'' = \int_{t'=0}^{T}\int_{t''=t'}^{T} f_a(t',t'')\,dt'dt'' + \int_{t'=0}^{T}\int_{t''=0}^{t'} f_a(t',t'')\,dt'dt''$$

$$= \int_{t'=0}^{T}\int_{t''=t'}^{T+t'} f_a(t',t'')\,dt'dt'' + \int_{t''=0}^{T}\int_{t'=t''}^{T+t''} f_a(t',t'')\,dt'dt'' + \varepsilon(T) \qquad (4.10)$$

where $\varepsilon(T)$ tends to zero as T tends to infinity. Splitting up the integrals in this way and putting

$$\tau = |t'-t''|$$

the second part of each integral is the complex conjugate of the first and hence in the limit $T\to\infty$

$$\overline{|C^2|} = \lim_{T\to\infty} \text{Ave} \frac{\mathcal{H}_{el}}{2\pi^2 T} \sum_a \int_{t'=0}^{T}\int_{\tau=0}^{T} \left\langle \psi_{ia}(t'+\tau) \middle| p_i e^{-2\pi i\nu(t'+\tau)} \middle| \psi_{is}(t'+\tau) \right\rangle$$

$$\left\langle \psi_{is}(t') \middle| p_i e^{+2\pi i\nu t'} \middle| \psi_{ia}(t') \right\rangle dt'\, d\tau$$

$$= \frac{\mathcal{H}_{el}}{2\pi^2} \int_{\tau=0}^{\infty} C_i(\tau)\, d\tau .\, e^{-2\pi i\nu\tau} \qquad (4.11)$$

where $C_i(\tau)$ is the correlation function for the particle i.

$$C_i(\tau) = \text{Ave} \frac{1}{T} \sum_a \int_0^T \left\langle \psi_{ia}(t'+\tau) \middle| p_i \middle| \psi_{is}(t'+\tau) \right\rangle \left\langle \psi_{is}(t') \middle| p_i \middle| \psi_{ia}(t') \right\rangle dt' \qquad (4.12)$$

We shall now introduce the evolution operator $U(t_2,t_1)$ defined by

$$\psi_{ij}(t_2) = U(t_2,t_1)\, \psi_{ij}(t_1) \qquad (4.13)$$

with the property that

$$U(t'+\tau, 0) = U(t'+\tau, t')\, U(t', 0) \qquad (4.14)$$

We then have

$$C_1(\tau) = \lim_{T\to\infty} \text{Ave} \frac{1}{T} \sum_a \int_0^T \langle \psi_{1a}(t') | U(t'+\tau,t') p_1 U(t'+\tau,t') | \psi_{1s}(t') \rangle$$

$$\langle \psi_{1s}(t') | p_1 | \psi_{1a}(t') \rangle dt' \qquad (4.15)$$

THE CROSS SECTION IN THE ABSENCE OF PERTURBATIONS

In the ideal case when the electron is isolated and quite undisturbed until the interaction with the absorbed radiation takes place, then the hamiltonian and the energy of the electron remains constant. If $\psi_{1j}(0)$ is the solution of

$$h_1 \psi_{1j}(0) = E_j^0 \psi_{1j}(0) \qquad (4.16)$$

then the time dependent wave function $\psi_{1j}(t)$ which is the solution of

$$h_1 \psi_{1j}(t) = i\hbar \frac{\partial \psi_{1j}(t)}{\partial t} \qquad (4.17)$$

is just

$$\psi_{1j}(t) = e^{-iE_j^0 t/\hbar} \psi_{1j}(0) \qquad (4.18)$$

so that the operator $U(t_2,t_1)$ takes the simple form

$$U(t_2,t_1) = e^{-ih_1(t_2-t_1)/\hbar} \qquad (4.19)$$

In this case the correlation function is just

$$C_1(\tau) = \sum_a e^{-2\pi i \nu_{as}\tau} \left|\langle \psi_{1a}(0) | p_1 | \psi_{1s}(0)\rangle\right|^2 \qquad (4.20)$$

where $h\nu_{as} = h\nu_{as}^0 = E_a^0 - E_s^0$,

and

$$|\overline{C^2}| = \frac{1}{2\pi} \sum_a \delta(2\pi(\nu - \nu_{as})) \left|\langle \psi_{1a}(0) | p_1 | \psi_{1s}(0)\rangle\right|^2$$

The resulting transition probability (4.7) on restricting the final states a to some particular final state is

$$P_{1\nu s} = \frac{1}{3} \frac{e^2}{m^2 \hbar c \nu} \frac{I(\nu)}{h\nu} \left|\langle \psi_{1a}(0) | p_1 | \psi_{1s}(0)\rangle\right|^2 \frac{1}{2\pi} \delta(2\pi(\nu - \nu_{as})) \qquad (4.21)$$

which is the formula (3.1). The Dirac δ-function implies that absorption can only take place when $v=v_{as}$. However v_{as} itself will vary when we take account of the deviations from the stationary potential field and hamiltonian h_1 for which ψ_{1a} and ψ_{1s} are eigenfunctions.. Also if the motion of the nuclei is included the Doppler effect becomes evident. When all these considerations are taken into account absorption takes place over a range of frequencies and the δ function is replaced by a broadened line profile $b'(v)$. In general we may write

$$\sigma_{ivs} = \frac{1}{3} \sum_{a} \frac{e^2}{m^2 \hbar c v} \left| \langle \psi_{ia}(0) | p_i | \psi_{is}(0) \rangle \right|^2 \times b'(v) \quad (4.22)$$

where

$$\int b'(v) dv = 1 \qquad (4.23)$$

THE EVOLUTION OPERATOR

In the general time dependent case, suppose that at any time t the solutions of the time-independent Schrodinger equation for the instantaneous hamiltonian $h_i(t)$ for the ith electron, are the set $\{\beta_j(t)\}$ with energies $E_j(t)$.

$$h_i(t)\beta_j(t) = E_j(t)\beta_j(t) \qquad (4.24)$$

The evolution operator U, may be determined relative to these states as basis, as a function of time. We may write

$$\begin{aligned} \psi_{ia}(t) &= \sum_{j} d_{iaj}(t)\, e^{-\frac{i}{\hbar}E_j^0 t} \beta_j(t) \\ \psi_{is}(t) &= \sum_{k} d_{isk}(t)\, e^{-\frac{i}{\hbar}E_k^0 t} \beta_k(t) \end{aligned} \qquad (4.25)$$

where E

where E_j^0 and E_k^0 are the energies of the states in the unperturbed case, so that the exponential factors give the development which the states would have in the approximation (4.18). The coefficients $d_{ixy}(t)\exp-\left(\frac{i}{\hbar}E_y^0 t\right)$ for all values of x and y provide the x,y elements for a matrix representation of U(t,o)

$$\left[U(t,0)\right]_{x,y} = d_{ixy}\, e^{-\frac{i}{\hbar}E_y^0 t}$$

and from (4.14)

$$U(t_1,t_2) = U(t_1,0)\left(U(t_2,0)\right)^{-1}$$

Now suppose that we divide up the time into several small intervals Δt_r such that $t_{r-1} < t < t_r$

and consider what happens if, during the interval Δt_r, the electron suffers a small change in the hamiltonian $h_{iP}(t)$ due to the surrounding field. In general the wave functions $\{\beta_j\}$ remain very much the same shape so that

$$\beta_j(t_r) \sim \beta_j(t_{r-1})$$

but the coefficients $\{d_{iaj}\}$ and $\{d_{isk}\}$ will differ both in phase and modulus. The changes in moduli implying that the electron i changes state, are referred to as the inelastic effects of the perturbation, the changes in phase as the elastic effects. The added effect of perturbations in the time interval t' to $t'+\tau$ may be written

$$U(t'+\tau,t') = U_{n+m-1} \quad \cdots \quad U_{n+1}U_n \qquad (4.26)$$

where

$$t_{n-1} < t' < t_n$$

$$t_{n+m-1} < t'+\tau < t_{n+m}$$

and

$$U_r = U(t_r, t_{r-1})$$

Time dependent perturbation theory determines the matrix for each individual U_r. In general the diagonal elements of U_r are the only ones of zero order and the off-diagonal elements are proportional to the strength of the perturbation. The diagonal elements can be written

$$(U_r)_{jj} = e^{-(\delta_{rj} + i\varphi_{rj}) - iE_j^0 \frac{\Delta t_r}{\hbar}} \qquad (4.27)$$

where

$$\varphi_{rj} = \int_{t_{r-1}}^{t_r} \frac{E_j(t) - E_j^0}{\hbar} dt$$

is the phase change produced in the state j by the perturbation, and the decay parameter, may be written in terms of the off-diagonal elements of U_r.

$$\delta_{rj} = \frac{1}{2} \sum_{k \neq j} \left| (U_r)_{jk} \right|^2 \qquad (4.28)$$

These off-diagonal elements are due to the probability that the interaction h_{iP} would send an electron in the state β_j at time t_{r-1}, into another state, β_k, by the time t_r.

$$(U_r)_{jk} = \frac{1}{\hbar} \int_{t_{r-1}}^{t_r} \langle \beta_j(t) | h_{ip} | \beta_k(t) \rangle e^{-i[E_j^0 - E_k^0]t/\hbar} dt \qquad (4.29)$$

In general $(U_r)_{jk}$ is small for each state k although the collective effect giving δ_{rj} may be considerable.

We may write each U_r

$$U_r = U_r^D + U_r^0 \tag{4.30}$$

where U_r^D is the diagonal part of U_r, and U_r^0 is the off-diagonal part which is proportional to the strength of the perturbation. The leading term in $U(t'+\tau,t')$ in (4.26) clearly comes from the product of the diagonal parts, which are commutative.

$$U(t'+\tau,t') = \prod_{r=n}^{n+m-1} U_r^D + \sum_{s=1}^{m} V_s(t'+\tau,t')$$

$$= U^D(t'+\tau,t') + \sum_{s=1}^{m} V_s(t'+\tau,t') \tag{4.31}$$

where

$$\begin{aligned} V_1(t'+\tau,t') = U^D_{n+m-1} \cdots\cdots & \quad U^D_{n+1} U^0_n + \cdots \\ \cdots + U^D_{n+m-1} \cdots & \quad U^D_{q+1} U^0_q U^D_{q-1} \cdots U^D_n + \cdots \\ & + U^0_{n+m-1} U^D_{n+m-2} \cdots\cdots U^D_n \end{aligned}$$

and $V_s(t'+\tau,t')$ gives the sum of all the products of m matrices in which s of the m are off diagonal and m-s are diagonal.

We have

$$C_i(\tau) = C_i^D(\tau) + \varepsilon$$

where $C_i^D(\tau)$ is the part of $C_i(\tau)$ due to the $\{U^D(t'+\tau,t')\}$ and ε represents the sum of the terms due to the matrices $V_s(t'+\tau,t')$.

Supposing we call the decay parameter and perturbational phase change in the time interval t_1 to t_2 for the state j , $\delta_j(t_2,t_1)$ and $\varphi_j(t_2,t_1)$

(that is, $d_{jj}(t_2) \sim e^{-(\delta_j(t_2,t_1)+i\varphi_j(t_2,t_1))}\, d_{jj}(t_1)$.)

then by (4.26)

$$\delta_j(t'+\tau,t') = \sum_{r=n}^{n+m-1} \delta_{jr}$$

and

$$\varphi_j(t'+\tau,t') = \sum_{r=n}^{n+m-1} \varphi_{jr} \tag{4.33}$$

where δ_{jr} and φ_{jr} are the decay parameter and phase change for the state j in the time interval Δt_r.

Since the $\{\psi_{ia}(t)\}$ and the available $\{\beta_j(t)\}$ form bases for the possible transition states we may use the closure property

$$\sum_j \langle\psi_{ij}|\cdot\quad\cdot|\psi_{ij}\rangle = \sum_j\sum_k \langle\psi_{ij}|\beta_k\rangle\langle\beta_k|\qquad|\beta_k\rangle\langle\beta_k|\psi_{ij}\rangle$$

$$= \sum_k\sum_j \langle\psi_{ij}|\beta_k\rangle\langle\beta_k|\psi_{ij}\rangle\langle\beta_k|\cdot\quad\cdot|\beta_k\rangle$$

$$= \sum_k \langle\beta_k|\cdot\quad\cdot|\beta_k\rangle$$

The summation over the states $\{\psi_{ia}(t)\}$ is thus equivalent to summation over the states $\{\beta_a(t)\}$ according to the probability that they are available

$$C_i^D(\tau) = \lim_{T\to\infty} \text{Ave} \sum_a\sum_k \frac{1}{T}\int_{t'=0}^{T} |d_{isk}(t')|^2 |\langle\beta_a(t')|\rho_i|\beta_k(t')\rangle|^2 \left(1-\frac{1}{\exp(\alpha+\beta E_a^0)+1}\right)$$
$$\times\exp-\left(\delta_a(t'+\tau,t')+\delta_k(t'+\tau,t')\right)$$
$$\times\exp-i\left(\varphi_a(t'+\tau,t')-\varphi_k(t'+\tau,t')\right) \tag{4.34}$$

The total radiation of frequency ν absorbed by the ensemble is the sum of that absorbed by each electron. If the material is in a steady state the distribution of electrons at time t' will be the same as at time $t=0$, that is, the total number of electrons instantaneously described by the state β_k at any time t' remains constant. Hence on summing over the contributions from all the electrons instantaneously in state β_k at time t' and dividing by the number of electrons in the state, and assuming that the various types of interaction occur randomly in time, the average absorption cross-section per electron in the state β_k for transitions to all states a is then

$$\sigma_{\nu k} = \mathcal{R}e\,\frac{1}{2\pi^2}\int_0^\infty e^{-2\pi i\nu\tau}\,C(\tau)\,d\tau \times \frac{1}{3}\frac{e^2}{m^2\hbar c\nu}\,,$$

$$\begin{aligned} C(\tau) = \mathrm{Ave}\sum_a \left|\langle\beta_a(0)|p|\beta_k(0)\rangle\right|^2 \exp -\left(\delta_a(\tau,0)+\delta_k(\tau,0)\right) \\ \times\left(1-\frac{1}{\exp(\alpha+\beta E_a^0)+1}\right)\times \exp\left\{+i\left(\varphi_a(\tau,0)-\varphi_k(\tau,0)\right)\right\}\exp 2\pi i\nu_{ak}^0\tau \\ = \left(1-\frac{1}{\exp(\alpha+\beta E_a^0)+1}\right)\sum_a \left|\langle\beta_a(0)|p|\beta_k(0)\rangle\right|^2 \sum_{\delta,\varphi} P(\delta,\varphi)\,e^{-\delta+i\varphi}\,e^{2\pi i\nu_{ak}^0\tau} \end{aligned} \qquad (4.35)$$

where $P(\delta,\varphi)$ is the probability of obtaining the value δ for the decay parameter

$$\delta = \delta_a(\tau,0) + \delta_k(\tau,0) \qquad (4.36)$$

and the differential phase change

$$\varphi = \varphi_k(\tau,0) - \varphi_a(\tau,0) \qquad (4.37)$$

and the averaging is over all possible values of δ and φ.

Suppose that at time t_{r-1} the states $\{\rho_j\}$ describe the electron in the field due to the nucleus and the other bound electrons in the ion, that is at that precise instant in time none of the surrounding charged particles are particularly close. Then in the time interval Δt_r the electron state is perturbed by the interaction with the radiation and by the surrounding particles. The interaction with the radiation does not alter the phase of the states $(\varphi_k = 0)$ but does, of course, cause transitions to other states, and hence gives a decay factor $\delta_{k,r}$ giving rise to "natural broadening". On the other hand the interactions with the other charged particles give rise to both elastic and inelastic effects which will depend on the charge, the position at time t_{r-1} and the velocity of each particle.

Let the mean rate at which inelastic transitions take place from the states $\{\rho_j\}$ due to the interaction with the radiation be $\gamma_{nat,j}$. Usually $\gamma_{nat,j}$ is small in spite of the intensity of radiation and contributes very little to the total broadening. The interaction is constant in time and the decay parameter δ_{rj} for the interval Δt_r giving the probability $e^{-2\delta_{rj}}$, that an inelastic transition does not take place from the state ρ_j in this interval takes the value

$$\delta_{rj,nat} = \frac{1}{2} \gamma_{nat,j} \Delta t_r \qquad (4.38)$$

Similarly the quantity determining the decay due to inelastic collisions is $\delta_{inel,j}$

$$\delta_{rj,inel} = \frac{1}{2} \gamma_{inel,j} \Delta t_r \qquad (4.39)$$

where $\gamma_{inel,j}$ is the average reaction rate with colliding particles for an electron in the state β_j .

In the case of elastic interactions with other particles the probability of a given type of particle perturbing an electron in a state β_j at any time, and the manner in which simultaneous interactions with several such particles may be considered, depend on the duration of the interactions relative to the lifetime of the state. If the perturbing particles remain almost stationary over the time interval in which the absorption takes place, then they may be treated by the Holtsmark theory. If, on the other hand, each particle is only close to the ion for a very short time, the phase is changed almost instantaneously, and the total phase change produced by non-overlapping dollisions will simply be the sum of the individual phase shifts. This is the basis of the "impact theory".

THE HOLTSMARK THEORY

The Holtsmark theory finds the probability that the perturbing particles produce an electric field F on the ion at time t=0. If the field $\underline{F} = \alpha \underline{F}_0$ for some constant $\underline{F}_0$, produces a change in energy $E_j(\alpha)$ for the state β_j , then, if $\underline{F}$ remains almost constant, inelastic transitions due to the field are unlikely, and the phase change according to the adiabatic theory in the time τ , is

$$\phi(\alpha) = \frac{E_j(\alpha)\tau}{\hbar} \qquad (440)$$

The simplest version of the theory takes the field F as that due to the nearest ion. In this case the probability that the nearest particle is of charge Z, and at a distance between R and R+dR from the perturbed ion is

$$dP(R) = 4\pi n R^2 \exp\left(-\tfrac{4}{3}\pi n R^3\right) P(Z_1)\, dR \qquad (4.41)$$

where n is the number density of slowly moving particles and $P(Z_1)$ is the fraction of these of charge Z_1. The homogeneous part of the field which this particle would exert on the ion is

$$\underline{F} = \frac{-Z_1 e \underline{R}}{R^3} \qquad (4.42)$$

and hence we can convert the expression (4.41) into a probability distribution in α where F_0 is conveniently chosen as

$$F_0 = \left(\frac{4\pi n}{3}\right)^{2/3} e \qquad (4.43)$$

$$dP(\alpha) = \sum_{Z_1} P(Z_1) \frac{3}{2\alpha} \left(\frac{Z_1}{\alpha}\right)^{3/2} e^{-\left(Z_1/\alpha\right)^{3/2}} d\alpha \qquad (4.44)$$

Treating the elastic effects in this approximation on their own

$$C(\tau) = \sum_a \int_0^\infty e^{i[E_a(\alpha) - E_k(\alpha)]\tau/\hbar} \frac{dP(\alpha)}{d\alpha} \cdot \frac{d\alpha}{d\nu} e^{+2\pi i \overset{\circ}{\nu}_{ak}\tau}$$

$$\times |\langle \phi_k(0) | p | \phi_a(0) \rangle|^2 d\nu \qquad (4.45)$$

and the cross-sections for transitions from the discrete states k with quantum numbers n and l, to states a with quantum numbers n' and l', with absorption of radiation frequency v, may then be written in terms of the oscillator strength f

$$\sigma_{v,k,a} = \frac{\pi e^2}{mc} f_{kA} \left(1 - \frac{1}{\exp(\alpha+\beta E_a^{\circ})+1}\right) b'_{ka}(v) \qquad (4.46)$$

where the line profile is

$$b'_{ka}(v) = \frac{dP(\alpha)}{d\alpha} . \frac{d\alpha}{dv} \qquad (4.47)$$

and $d\alpha/dv$ depends on the functional dependence on α of $E_k(\alpha)$ and $E_a(\alpha)$. If this is linear

$$\begin{aligned} E_a(\alpha) - E_k(\alpha) &= hc_1 \alpha \\ &= h\Delta v \\ &= h(v - v_{ak}^{\circ}) \end{aligned} \qquad (4.48)$$

then

$$\frac{d\alpha}{dv} = \frac{h}{c_1} \quad \text{and}$$

$$b'_{ka}(v) = \frac{3}{2}\frac{h}{c_1} \sum_{Z_1} P(Z_1) \left(\frac{Z_1 C_1}{\Delta v}\right)^{3/2} e^{-\left(\frac{Z_1 C_1}{\Delta v}\right)^{3/2}} \qquad (4.49)$$

If $E_a(\alpha) - E_k(\alpha)$ is quadratic in α or nearly so

$$\begin{aligned} E_a(\alpha) - E_k(\alpha) &= hc_2 \alpha^2 \\ &= h\Delta v \end{aligned} \qquad (4.50)$$

then

$$\frac{d\alpha}{dv} = \frac{1}{2}\sqrt{c_2/\Delta v}$$

and

$$b'_{ka}(\nu) = \sum_{Z_1} P(Z_1)\, \frac{3}{4}\sqrt{\frac{c_2}{\Delta\nu}} \left(\frac{Z_1 c_2}{\Delta\nu}\right)^{3/4} e^{-\left(\frac{Z_1 c_2}{\Delta\nu}\right)^{3/4}} \qquad (4.51)$$

$E_a(\alpha), E_k(\alpha), f_{ka}$ and $\overset{0}{\nu}_{ak}$ may all depend on the ionic configuration and $\sigma_{\nu,k,a}$ has also to be averaged over these according to their probability.

This approximation may be improved by taking into consideration the effect of the potential V(R) on the probability of a neighbouring particle at distance R through the Boltzmann factor (see for example Mayer P42, Ref. 12). The binary approximation has also been extended to the case of several ions of the same charge perturbing the central ion simultaneously, on the assumption that the interactions between the perturbing ions are negligible. The total field $\underline{F}$ exerted is then the vector sum of the individual perturber fields and the probability distribution for $\underline{F}$ may be calculated using Markoff chains (e.g. Chandrasekhar. Ref 5). The asymptotic behaviour of the line profile is the same as in the nearest neighbour approximation. The Holtsmark broadening is difficult to combine with other broadening effects and it is to be hoped that there are few lines in which broadening by slowly moving particles, generally the heavy ions, is of the same magnitude as other broadening mechanisms, such as the impact broadening.

THE IMPACT APPROXIMATION

We shall now review the impact approximation in which it is assumed that the phase shifts due to the distinct perturbations are scalarly additive and are either completed within the time τ if the time of closest approach is in this interval, or may be disregarded.

The phase change $\varphi_{J,r,\rho,V,Z_1,l}(\tau)$ produced in the one-electron eigenstate by one perturber of charge Z_1 in the time interval τ, depends on the time interval Δt_r in which it makes its closest approach ρ, the velocity $\underline{V}$, and in general on some other impact parameters l whose probability distribution W(1) is assumed known. The total phase change produced by all the perturbers is then

$$\varphi_J(\tau) = \sum_{r,x} \varphi_{Jrx}(\tau) \tag{4.52}$$

where $\varphi_{Jrx}(\tau)$ is the phase change produced by the $N(r,x)$ perturbers with the same collection of parameters (ρ, V, Z_1) (which will be designated by x), and which make their closest approach in the same time interval Δt_r.

$$\varphi_{Jrx}(\tau) = \sum_{i}^{N(r,x)} \varphi_{Jrxl_i}(\tau) \tag{4.53}$$

We shall first compute the probability distribution of the differential phase change between the states a and k

$$\varphi_{rx}(\tau) = \varphi_{krx}(\tau) - \varphi_{arx}(\tau)$$

due to the interactions with perturbers (r,x).

Suppose that v_x is the mean frequency with which perturbers with parameters x interact elastically with an electron in the state ρ_k, times the probability that the interaction with the state p_a would also be elastic. Then the probability that there are N(r,x) interactions of the type (r,x) contributing to the differential phase change $\varphi_{rx}(\tau)$ is

$$W\left(N(r,x)\right) = \frac{1}{\left(N(r,x)\right)!} \left(v_x \Delta t_r\right)^{N(r,x)} e^{-\Delta t_r v_x} \qquad (4.55)$$

We then have

$$P\left(\varphi_{rx}(\tau)\right) = \sum_{N(r,x)=0}^{\infty} \int_{l_1} \cdots \int_{l_{N(r,x)}} W(N(r,x)) \prod_{i=1}^{N(r,x)} W(l_i)\,dl_i \;\delta\left(\varphi_{rx} - \sum_{i=1}^{N(r,x)} \left(\varphi_{krxl_i} - \varphi_{arxl_i}\right)\right) \qquad (4.56)$$

Using the Dirichlet representation for the δ-function

$$\delta(z' - z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy\, e^{iy(z'-z)} \qquad (4.57)$$

this becomes

$$P\left(\varphi_{rx}(\tau)\right) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy\, e^{iy\varphi_{rx}(\tau) + v_x \Delta t_r \left[\alpha_{rx}(y) - 1\right]} \qquad (4.58)$$

provided

$$\alpha_{rx}(y) = \int W(l)\, e^{-iy\left(\varphi_{krxl} - \varphi_{arxl}\right)} dl \qquad (4.59)$$

We can now find the probability function P(δ, φ) in (4.35). The value of the decay parameter due to collisions and excitation or deexcitation by the radiation field is

$$\delta = \sum_{t_r<\tau} \delta_{ra} + \delta_{rk} = \sum_{t_r<\tau} \frac{\gamma}{2} \Delta t_r$$

where

$$\gamma = \left(\gamma_{nat,a} + \gamma_{nat,k} + \gamma_{inel,a} + \gamma_{inel,k}\right) \quad (4.60)$$

The probability of a phase difference φ between the states a and k due to the perturbation in time τ is

$$P(\varphi) = \iiint \prod_{r,x} \left(P(\varphi_{rx}(\tau))\, d\varphi_{rx}(\tau) \right) \delta\left(\varphi - \sum_{r,x} \varphi_{rx}(\tau)\right) \quad (4.61)$$

and hence

$$P(\delta,\varphi) = \iint \cdot \int \delta\left(\delta - \frac{\gamma}{2} \sum_{t_r<\tau} \Delta t_r\right) \delta\left(\varphi - \sum_{r,x} \varphi_{rx}(\tau)\right) \times \prod_{r,x} P\left(\varphi_{rx}(\tau) d\varphi_{rx}(\tau)\right) \quad (4.62)$$

Substituting for P($\varphi_{rx}(\tau)$) and using the Dirichlet representation for the δ-function we obtain

$$P(\delta,\varphi) = \delta\left(\delta - \frac{\gamma}{2} \sum_{t_r<\tau} \Delta t_r\right) \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{is\varphi} e^{\sum_{r,x} v_x \Delta t_r [\alpha_{rx}(s) - 1]} \quad (4.63)$$

Substituting this in (4.35) for the correlation function $C(\tau)$

$$C(\tau) = \sum_a C_{ak}(\tau) \times \left(1 - \frac{1}{\exp(\alpha+\beta E_a^0)+1}\right) |\langle \beta_a(0) | p | \beta_k(0) \rangle|^2$$

where

$$C_{ak}(\tau) = e^{-\sum_r \left(\gamma/2 + \sum_x v_x [\alpha_{rx}(1) - 1] \Delta t_r \right)} \tag{4.64}$$

Now applying the impact approximation, if r is such that t_r is less than τ then we assume that the phase change produced by the perturber, $\varphi_{jrxl}(\tau)$ is the total phase change produced by the perturber, $\varphi_{jrxl}(\infty)$ and this is independent of r.

$$\varphi_{jrxl}(\infty) = \varphi_{jxl}$$

In this case $\alpha_{rx}(1)$ is just

$$\alpha_{rx}(1) = \int dl\, W(l)\, e^{-i(\varphi_{kxl} - \varphi_{axl})} = \alpha_x(1) \tag{4.65}$$

If $t_r > \tau$ then $\varphi_{rx}(\tau) = 0$ (4.66)

and $\alpha_{rx}(1) = 1$

Hence $C_{ak}(\tau)$ becomes

$$C_{ak}(\tau) = e^{-[\gamma/2 + \sum_x v_x (\alpha_x(1) - 1)]\tau}$$

$$= e^{-(w_1 + i w_2)\tau}$$

on expanding the exponent as the sum of its real and imaginary parts.

Using (4.35) the cross-section for the absorption of radiation of frequency v for the electrons making transitions from one of the discrete states β_k with quantum numbers n,l, to the states β_a with quantum numbers n'l' in a given surrounding configuration I is

$$\sigma_{\nu,k,a} = \frac{\pi e^2}{mc} f_{KA} \, b'_{ka}(\nu) \tag{4.68}$$

f_{KA} is the oscillator strength and

$$b'_{ka}(\nu) = \frac{1}{2\pi^2} \frac{\omega_1}{\omega_1^2 + [2\pi(\nu-\nu^0_{ak}) - \omega_2]^2} \tag{4.69}$$

Hence to find the line profile in the impact approximation we need to know the phase shifts φ_{xl} and the mean frequencies v_x in addition to the transition rates $\gamma_{nat,j}$ and $\gamma_{inel,j}$ for the various pairs of states a and k.

v_x is just the mean frequency with which impacts of the type x occur, times the probability that such an impact does not terminate the states a and k,

$$\nu_x = 2\pi\rho \, V \, n(V,Z_1) \, e^{-\delta_{ax}} e^{-\delta_{kx}} \tag{4.70}$$

where $n(v,Z_1)$ is the density of particles of velocity V and charge Z_1. It is usually sufficiently accurate to take $e^{-\delta_{ax}}$ and $e^{-\delta_{kx}}$ as unity in this expression since those sets of parameters x which are likely to cause inelastic transitions cause rapidly fluctuating values $\alpha_x(1)$ which diminishes their contribution to w_1 and w_2.

Before calculating the phase shifts and transition rates there is an additional broadening factor which will be discussed, the effect of nuclear motion.

THE DOPPLER EFFECT

In the previous discussion the wave functions $\{\phi_k\}$ and all the particle coordinates have been relative to the nucleus of the radiating ion. If the velocities of radiating systems of mass M have a thermal distribution, but other broadening effects are negligible then Doppler broadening results in a Gaussian line shape.

$$\sigma_{v,k,a} = \frac{\pi e^2}{mc} f_{KA} \, b'_{ka}(v)$$

$$b'_{ka}(v) = \left(\frac{Mc^2}{2\pi kT v_{ak}^{0\,2}}\right)^{\frac{1}{2}} \exp - \left\{\left(\frac{Mc^2}{2kT} \frac{(v-v_{ak}^0)^2}{v_{ak}^{0\,2}}\right)\right\} \qquad (4.71)$$

with (half) half width

$$v_D = \left(\frac{2kT \log 2}{Mc^2}\right)^{\frac{1}{2}} v_{ak}^0 \qquad (4.72)$$

The movement of the frame of refence may be combined with other broadening processes which are statistically independent by folding the line shapes together. When the dispersion profile of the impact broadening

$$\frac{1}{\pi} \quad \frac{(\omega_1/2\pi)^2}{(\omega_1/2\pi)^2 + (v - v_{ak}^0 - \omega_2/2\pi)^2} \qquad (4.73)$$

of half width $\omega_1/2\pi$ and shifted by $\omega_2/2\pi$ from the unperturbed central frequency v_{ak}^0, is extended to include the Doppler motion the resulting profiles are the Voigt profiles V(a*,x)

$$b'_{ka}(\nu) = \frac{1}{\Delta}\,\frac{1}{\sqrt{\pi}}\,V\left(\frac{\omega_1/2\pi}{\Delta},\ \frac{\nu-\nu^0_{ak}-\omega_2/2\pi}{\Delta}\right) \qquad (4.74)$$

where

$$\Delta = \sqrt{\frac{2kT\,\nu^{0\,2}_{ak}}{Mc^2}} \quad \text{and} \quad V(a^*,x) = \frac{a^*}{\pi}\int \frac{e^{-y^2}}{(x-y)^2+a^{*2}}\,dy \qquad (4.75)$$

This profile will be sufficient when the Holsmark broadening due to slowly moving ions may be ignored, and the impact approximation is valid for almost all particles. We shall now calculate the natural broadening and inelastic impact broadening parameters $\gamma_{nat,j}$ and $\Gamma_{inel,j}$ and then proceed to find phase changes according to the Lindholm classical path approximation.

NATURAL BROADENING

To determine the natural broadening we have to find the mean rate at which the radiation of all frequencies incident on an electron in a state β_j, causes transitions to all other states β_j. This follows from (4.22) and (4.23).

If b_+ indicates a state β_{b^+} of energy E_{b^+} greater than E_j, the energy of the state β_j, then the probability of a transition from the state j to the available state b_+ per unit time is

$$W_{s\to b^+} = \iint \sigma_{\nu,s,b^+}\, b'(\nu)\, \frac{I(\nu,\Omega)}{h\nu}\, d\nu\, d\Omega$$

$$= \iint \frac{I(\nu,\Omega)}{h\nu}\cdot\frac{1}{3}\frac{e^2}{m^2\hbar c\nu}\, |\langle \beta_{b^+}|\,p\,|\beta_j\rangle|^2\, b'(\nu)\, d\nu\, d\Omega. \qquad (4.76)$$

$I(\nu,\Omega)$ is the intensity of radiation incident at the angle Ω and is given by

$$I(\nu,\Omega) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT}-1} \qquad (4.77)$$

Using the wave functions for an electron in the time averaged potential field of the ion for the $\{f_k\}$ and taking into account the availability of the final state, the probability per unit time of excitation to a h higher bound state is

$$W_{exc} = \sum_{B^+} \frac{8\pi^2 e^2}{mc^3} \nu_{jb^+}^2 \frac{f_{jB^+}}{e^{h\nu_{jb^+}/kT}-1}\left(1-\frac{1}{\exp(\alpha+\beta E_{b^+})+1}\right) \qquad (4.78)$$

where B^+ is the group of degenerate state b_+, f_{jB+} is the oscillator strength and ν_{jb+} is the natural frequency for the levels j and B^+.

The rate of excitation to the continuum is by analogy

$$W_{exc}^{cont} = \int_E \frac{8\pi^2 e^2}{mc^3} \nu_E^2 \frac{df}{dE}\left(\frac{1}{e^{h\nu/kT}-1}\right)\left(1-\frac{1}{\exp(\alpha+\beta E)+1}\right) dE \qquad (4.79)$$

Similarly the probability per unit time of losses from the state j due to stimulated emission is

$$W_{stim} = \sum_{B^-} \frac{8\pi^2 e^2}{mc^3} \nu_{jb^-}^2 \frac{f_{jb^-}}{e^{h\nu/kT}-1}\left(1-\frac{1}{\exp(\alpha+\beta E_{b^-})+1}\right) \qquad (4.80)$$

where B^- indicates a group of states $\{b^-\}$ of energy E_{b^-} less than E_J, and we have

$$f_{JB^-} = \frac{g_{b^-}}{g_J} f_{B^-J} \tag{4.81}$$

Using the fact that the stimulated emission is $\frac{1}{e^{h\nu/kT}-1}$ times the spontaneous emission the total rate of lossfrom state j by emission is

$$W_{dexc} = \sum_{B^-} \frac{8\pi^2 \nu_{Jb^-}^2}{mc^3} f_{JB^-} \left(\frac{e^{h\nu_{Jb^-}/kT}}{e^{h\nu_{Jb^-}/kT}-1} \right) \left(1 - \frac{1}{\exp(\alpha+\beta E_{b^-})+1} \right) \tag{4.82}$$

$\gamma_{nat,J}$ the mean transition rate from the level β_J due to the radiation is just the sum of the three contributions

$$W_{dexc}, \; W_{exc} \text{ and } W_{exc}^{ctm}$$

The reduced width $\Gamma_{nat,J} = \frac{\hbar}{2kT} \gamma_{nat,J}$ (4.83)

then becomes

$$\Gamma_{nat,J} = \frac{\alpha^3}{2} \frac{kT}{R_y} \left(\sum_{dexc} + \sum_{exc} + \int_{ctm} \right) \quad ; \quad \alpha = \frac{e^2}{\hbar c}$$

$$\sum_{dexc} = \sum_{B^-} \frac{u_{Jb^-}^2 f_{JB^-}}{1 - e^{-u_{Jb^-}}} \left(1 - \frac{1}{\exp(\alpha+\beta E_{b^-})+1} \right) ; \quad u_{Jb^-} = \frac{h\nu_{Jb^-}}{kT}$$

$$\sum_{exc} = \sum_{B^+} \frac{u_{Jb^+}^2 f_{JB^+}}{e^{u_{Jb^+}/kT} - 1} \left(1 - \frac{1}{\exp(\alpha+\beta E_{b^+})+1} \right) , \quad u_{Jb^+} = \frac{h\nu_{Jb^+}}{kT}$$

$$\int_{ctm} = \int \frac{u^2 \, df/du}{e^u - 1} \tag{4.84}$$

Usually the contribution from excitation to the continuum is small by comparison with the other terms. The integral may be simplified using the fact that the Gaunt factor is a slowly varying function of frequency which may be approximated by the value at the threshold frequency for the level j, $g_j(0)$.

Then

$$n^2 \frac{df}{du} = \frac{g_j(0)\, 16 Z^4 (Ry/kT)^2}{3\sqrt{3}\, \pi\, n^5\, u} \qquad (4.85)$$

and

$$\int_{ctm} = \frac{\alpha^3}{2} \frac{16 Z^4 g_j(0) (Ry/kT)}{3\sqrt{3}\, \pi\, n^5} \int_{u_j}^{\infty} \frac{1}{u(e^u - 1)} du \qquad (4.86)$$

$$= \frac{\alpha^3}{2} \frac{16 Z^4}{3\sqrt{3}\pi n^5} g_j(0) \frac{Ry}{kT} \times \sum_{r=1}^{\infty} E_1(r u_j) \quad ; \; u_j = \frac{-E_j}{kT}$$

if $E_1(x)$ is the exponential integral

$$E_1(x) = \int_x^{\infty} \frac{e^{-t}}{t} dt$$

Hence given the oscillator strengths and finding the necessary exponential integrals for the energy levels, we can calculate the average rate of transitions from any state j due to the radiation, that is the natural broadening paramters $\gamma_{nat,j}$

INELASTIC COLLISIONS

There are two possible ways in which a particle impinging on an ion can perturb a bound electron. Either the interaction between the particle and electron can lead to a transfer of energy from the perturber to the bound electron (or vice versa) in which case the interaction is inelastic, or the bound electron is only temporarily excited providing a phase shift but remaining in the same state after the impact. This section will consider the frequency with which inelastic collisions occur.

The collision of an electron with an ion represents a many body problem and as such is incapable of exact solution. The simplest and commonest approximation for the inelastic effects is the Born approximation which may be satisfactorily applied to excitation and ionisation of bound electrons when the energy transferred is small compared with the energy of the impinging particle. A complete account is given by T.R. Carson (Ref. 4) but a brief summary will be given here.

Supposing that a bound electron is in a state i of energy E_1 with wave function f_i, and we wish to know the frequency with which impinging electrons of charge Z_1 and velocity $V_i = \frac{\hbar k_i}{m} = \sqrt{\frac{2E}{m}}$, transfer energy to such electrons leaving them in a final state j of energy E_j. Since the energy must be conserved in such a case the final velocity of the particles will be

$$V_j = \frac{\hbar k_j}{m}, \tag{4.88}$$

$$\frac{\hbar^2(k_i^2 - k_j^2)}{2m} = E_j - E_i = \Delta E_{ij} \tag{4.89}$$

Describing the impinging particles by plane waves $e^{i\underline{K}.\underline{R}}$ in accordance with the Born approximation we may write the transition probability per unit time for the bound electron

$$A_{ij}(E) = N(E) \times V_i \times Q_{ij}(E) \times q(E_j) \qquad (4.90)$$

where $N(E)$ is the volume density of particles of energy E, $q(E_j)$ is the probability that the state $_j$ is available for the bound electron, and $Q_{ij}(E)$ is the result of scattering of the incident photons in all directions.

$$Q_{ij}(E) = \int I_{ij}(k_i, k_j, \Omega)\, d\Omega \qquad (4.91)$$

where $I_{ij}(k_i k_j, \Omega)$ is the differential scattering cross section for scattering angle Ω.

Applying the usual perturbation theory the Born approximation becomes

$$I_{ij}(k_i, k_j, \Omega) = \frac{m k_j^2}{\hbar^4 k_i} \left| \frac{1}{2\pi} \iint \exp^{-i \underline{k}_j \cdot \underline{R}} \rho_j^*(\underline{r}) \frac{Z_1 e^2}{|\underline{R} - \underline{r}|} \rho_i(\underline{r}) e^{i \underline{k}_i \cdot \underline{R}}\, d\underline{r}\, d\underline{R} \right|^2$$

$$(4.92)$$

where Z_1 is the charge of the perturbing particles.

On using Bethe's formula

$$\int \frac{\exp i \underline{K} \cdot \underline{R}}{|\underline{R} - \underline{r}|}\, d\underline{R} = \frac{4\pi}{K^2} \exp i \underline{K} \cdot \underline{r} \qquad (4.93)$$

and changing to the variable $\underline{K}$ instead of k_j,

the cross section becomes

$$Q_{ij}(E) = \int_{K = k_i - k_j}^{K = k_i + k_j} I_{ij}(k_i, K)\, dK$$

where

$$I_{ij}(k_i, K) = \frac{8\pi^2 m^2 Z_1^2 e^4}{\hbar^4 k_i^2 |K|^{-3}} \left| F_{ij}(K) \right|^2 \qquad (4.94)$$

in which

$$F_{ij}(K) = \int \exp i(\underline{K}.\underline{r})\, \phi_j^*(r)\, \phi_i(r)\, dr$$

The Bethe approximation for electron impact retains only the first non vanishing term in $F_{ij}(K)$ when exp $i(\underline{K}.\underline{r})$ is expanded in powers of $\underline{K}.\underline{r}$. This is valid when $\underline{K}.\underline{r}$ remains small over the dimensions of the atom. Approximating the wave functions ϕ_k by these for the time averaged potential again, the selection rules are then the same as for the radiative transitions and analogously may be designated as "allowed? or "forbidden" according to whether the linear or quadratic terms in K are the leading terms. Both allowed and forbidden transitions are considered in (Ref. 4) but since the forbidden transitions are very much less frequent than the allowed ones, they will contribute relatively little to the total probability of an inelastic collision for an electron in the state ϕ_i, and we need only consider the allowed transitions here.

Averaging over the initial states of energy E_i and summing over the final states of energy E_j we have

$$|F_{ij}(K)|^2 = \frac{K^2 \hbar^2}{2m\Delta E_{ij}} f_{I,J} \qquad (4.95)$$

when the final states belong to another bound level j.

$$I_{i,j}(k_i, K) = \frac{4me^4}{\hbar^2 k_i^2 K \Delta E_{ij}} f_{I,J} \qquad (4.96)$$

When the bound electron is excited to the continuum with energy between E_j and $E_j + dE_j$ then we may write the partial cross section as

$$\frac{dI_{I,J}(k_i, K)}{dE_j}\,\delta E_j = \left(\frac{4me^4}{\hbar^2 k_i^2 K \Delta E_{ij}}\;\frac{df_{I,J}}{dE_j}\right)\delta E_j \qquad (4.97)$$

Ej may range from 0 to $E - I_i$, where I_i is the ionization energy of the initial state, abd hence on integrating over E_j

$$I_i(k_i, K) = \int_0^{E-I_i} \frac{dI_{i,j}(k_i, K)}{dE_j}\, dE_j \qquad (4.98)$$

We may take account of the Bethe approximation by lowering the upper limit of the integration over K in (4.94)

$$Q_{ij}(E) = \int_{K_{min}}^{K_0} I_{ij}(k_i, K)\, dK \qquad (4.99)$$

Fortunately the dependence on K_o is not critical for the cross section is determined mainly by K_{min}. Calculations have shown that a good choice for K_o (see Bates. Ref. 2) is

$$\frac{\hbar^2 K_0^2}{2m} = E_0 = \frac{|\Delta E_{ij}|}{2} \qquad (4.100)$$

K_{min} may be expressed as an expansion in ΔE_{ij}. Although the Born approximation is not really valid at low impact energies, if second order terms are retained as well as first order,

$$K_{min} = {}^{m}/_{\hbar^2 k_i}\, \Delta E_{ij} \left(1 \pm \frac{|\Delta E_{ij}|}{4E}\right) \qquad (4.101)$$

where the upper sign refers to excitation and the lower to de-excitation, then the cross section has the right qualitative behaviour when E is no longer large compared with ΔE_{ij} , and the excitation cross section vanishes at the threshold $E=\Delta E_{ij}$, whereas the de-excitation cross-section remains finite when $E=0$.

$$Q_{ij}(E) = \frac{8\pi\hbar^2}{2m\,\Delta E_{ij}} f_{I,J}\left[\frac{R_y}{2E}\log\left\{\frac{4E_0}{(\Delta E_{ij})^2}\left(E-\frac{|\Delta E_{ij}|}{2}\right)\right\}\right] \qquad (4.102)$$

and for ionisation

$$Q_i(E) = \int\frac{dQ_{ij}}{dE_j}\,dE_j = \frac{8\pi\hbar^2}{2m}\int\frac{df_{I,J}}{dE_j}\,\frac{1}{|E_j-E_i|}\left[\frac{R_y}{2E}\log\left(\frac{4E_0}{(E_j-E_i)^2}\left[E-\frac{|E_j-E_i|}{2}\right]\right)\right]dE_j$$

$$(4.103)$$

The total frequency of electron impacts which excite the bound electron to a level j or ionise it, is given by integrating (4.90) over the energy of the impinging electron.

$$A_{ij}(E) = \int N(E)\,V_i\,Q_{ij}(E)\left(1-\frac{1}{\exp(\alpha+\beta E_j)+1}\right)dE$$

$$= \rho_e\,R_{ij}\left(1-\frac{1}{\exp(\alpha+\beta E_j)+1}\right) \qquad (4.104)$$

where ρ_e is the density of free elctrons and

$$R_{ij} = \overline{V_i\,Q_{ij}} = \int Q_{ij}(E)\sqrt{\frac{2E}{m}}\,f(E)\,dE \qquad (4.105)$$

where f(E)dE is the fraction of incident electrons with impact energies in the range E to E+dE and $Q_{ij}(E)$ is taken to be zero below the threshold for excitation. f(E) is very nearly

$$f(E)\,dE = \frac{2}{\sqrt{\pi}}\left(\frac{1}{kT}\right)^{3/2}\sqrt{E}\,e^{-E/kT}\,dE \qquad (4.106)$$

so that

$$R_{I,J} = \frac{2}{\sqrt{\pi}}\sqrt{\frac{2kT}{m}}\,8\pi\left(\frac{R_y}{kT}\right)\frac{\hbar^2}{2m}\,\frac{f_{I,J}}{x_{ij}}\,\frac{1}{2kT}\,I(x_{ij})\ ; \quad x_{ij} = \frac{\Delta E_{ij}}{kT} \qquad (4.107)$$

$$\alpha = E_0/\Delta E_{ij}$$

if

$$I(x) = \log 2\alpha\, e^{-x} + e^{-x/2}E_1(x/2) \quad \text{excitation}$$

$$= \log 2\alpha + e^{x/2}E_1(x/2) \quad \text{de-excitation}$$

For ionisation to the continuum

$$A_I = \rho_e R_I \qquad (4.108)$$

$$R_I = \frac{2}{\sqrt{\pi}}\sqrt{\frac{2kT}{M}}\,\frac{8\pi\hbar^2}{2m}\left(\frac{R_y}{kT}\right)\frac{1}{2kT}\int_{I_c/kT}^{\infty}\frac{I(x)}{x^4}\frac{df}{dx}\,dx$$

$$= \frac{128\hbar^3}{3\sqrt{3}\,\pi m^2 e^2}\left(\frac{R_y}{kT}\right)^{7/2}\frac{Z^4 g_1(0)}{n^5}\int_{I_c/kT}^{\infty}\frac{I(x)}{x^4}\,dx \qquad (4.109)$$

on using (4.85).

These formulae give us the mean rate at which electrons in state I undergo inelastic transitions as the result of collisions with free electrons knowing only the oscillator strengths and the density of free electrons. The cross sections for inelastic collisions with other ions will be of the same order of magnitude for the same velocity of impact. The reaction rates R_{ij} will thus be a factor $\sqrt{m/M}$ times the reaction rate for free electrons, where m and M are the reduced masses of electrons and of the perturbing ions respectively, and so the heavy particle collisions will only play a minor part in the inelastic broadening. The reduced width $\Gamma_{inel,i} = \frac{\hbar}{2kT}\gamma_{inel,i}$ is thus 4.110

$$\Gamma_{inel,i} = \frac{\hbar}{2kT}\left(\sum_J A_{ij} + A_i\right)$$

$$= (\rho_e a_0^3)\, 8\sqrt{\pi}\left(\frac{Ry}{kT}\right)^{2.5}\left(\sum_J \frac{f_{I,T}}{x_j}\bar{I}(x_j) + \frac{16Z^4}{3\sqrt{3}\pi n^5}\left(\frac{Ry}{kT}\right)^2\int_{I_i/kT}^{\infty}\frac{I(x)}{x^4}dx\right) \tag{4.111}$$

The exponential integrals are discussed in Appendix B.

ELASTIC PERTURBATIONS

In deriving the inelastic cross section we considered the probability that incident free electrons perturb the atom in such a way that a bound electron altered its orbit permanently. In the event that a collision between a charged particle and an ion containing an el electron described by the wave function ρ_J, does not produce an inelastic transition we wish to know the phase shift produced by the interaction. Usually the incident particles are of high angular momenta and may be treated by the Lindholm approximation in which they are assumed to move classically along straight line paths.

Suppose that a perturbing particle is described by a wave packet centred at position r(t) where r(t) takes on a minimum value ρ with spatial spread Δr, and with mean velocity V and uncertainty Δ V. If the particle is to be described classically then the wave packet must remain well localised during the time of interaction. This is true if $\Delta r/\rho$

and $\Delta V/V$ are small. Now $\Delta r \Delta V > \hbar/m$

and hence

$$\frac{\Delta r \Delta v}{\rho V} \sim \frac{1}{l} \qquad (4.112)$$

where the parameter l refers to the angular momentum with respect to the ion. Hence the angular momentum parameter must be large for the perturber to be treated classically.

For an electron with an average impact parameter ρ of $n^{-1/3}$ where n is the number of particles per cc, and a typical velocity of order $\sqrt{\frac{kT}{m}}$, l^3 is of the order

$$\Gamma = \frac{2(2\pi m k T)^{3/2}}{n h^3} \qquad (4.113)$$

In the case $T=10^{2.5}$, $P=10^{2.5}$, for the mixture in table 5.A we have a typical value for an electron of $l^3 \sim 600$

Small values of Γ imply that the gas is degenerate.

The additional assumption that the perturber trajectory is a straight line path and does not depend on the interaction with the ion, will be valid if the perturbers energy E_p is much greater than the interaction energy. If $E_p \sim kT$,

$$kT > \frac{Ze^2}{\rho}, \quad \text{ie } kT > Ze^2 n^{1/3} \qquad (4.114)$$

Suppose that a particle of charge Z_1 for which these assumptions are valid, moves along a straight line path with velocity V such that it makes its closest approach ρ to an ion with an electron in the state β_j at time t". The position of the particle at time t"+t is then

$$\underline{r}_p = \underline{\rho} + \underline{V}t \tag{4.115}$$

We wish to find the phase change $\varphi_{j,\rho,v,Z_1}(t_2,t_1)$ to the instantaneous eigenfunction $\beta_j(t)$ in the time interval (t_1, t_2)

$$\varphi_{j,\rho,V,Z_1}(t_2,t_1) = \int_{t_1}^{t_2} \frac{\Delta E_j}{\hbar}\,dt = \int_{\underline{\rho}+\underline{v}(t''-t_1)}^{\underline{\rho}+v(t''-t_2)} \Delta E_j \cdot \frac{d\underline{r}_p}{V} \tag{4.116}$$

where $\Delta E_j(t) = E_j(t) - E_j^{\circ}$,

E_j° being the unperturbed energy. If the impact is effectively completed in the time interval (t_1, t_2) then the limits of integration may be extended to plus and minus infinity.

At time t"+t, using first order perturbed wave functions with the $\beta_j(t_0)$ for some time t° before the perturbation, as the unperturbed wave functions, the energy of the interaction is to second order

$$\Delta E_j = \left\langle \beta_j(t^{\circ}) \left| \frac{Ze^2}{|\underline{\rho}+\underline{V}t-\underline{r}|} \right| \beta_j(t^{\circ}) \right\rangle + \sum_{k \neq j} \frac{\left| \left\langle \beta_j(t^{\circ}) \left| \frac{Ze^2}{|\underline{\rho}+\underline{V}t-\underline{r}|} \right| \beta_k(t^{\circ}) \right\rangle \right|^2}{E_k^{\circ} - E_j^{\circ}} \tag{4.117}$$

(N.B. The fact that the wave function β_j at time t"+t is not orthogonal to the $\beta_j(t^{\circ})$ represents only virtual transitions in this case. When $\underline{\rho}+\underline{V}t$ tends to infinity again the wave function returns to the state before the perturbation, $\beta_j(t^{\circ})$)

If θ_t is the angle between **r** and $\underline{\rho}+\underline{V}t$ then we may write

$$\frac{Z_1 e^2}{|\underline{\rho}+\underline{V}t-\underline{r}|} = \frac{Z_1 e^2}{\sqrt{\rho^2+V^2t^2}} \left(\sum_{s=0}^{\infty} \left(\frac{r}{\sqrt{\rho^2+V^2t^2}} \right)^s P_s(\cos\theta_t) \right) \tag{4.118}$$

assuming that the perturber has not penetrated inside the electron orbit. If the atom is randomly orientated with respect to the incident electron then

$$P_s(\cos\theta_t) = \frac{4\pi}{2l+1} \sum_{m=-l}^{m=+l} Y_l^{m*}(\theta_1,\varphi_1)\, Y_l^{m}(\theta,\varphi) \qquad (4.119)$$

where (θ,φ) are the bound electron angular coordinates, and (θ_1,φ_1) the angular coordinates of the perturber, are functions of time.

Taking the unperturbed wave functions as the time-averaged wave functions once more, the s=0 term on the right hand side of (4.118) produces the same phase change for every state and hence does not contribute to the line broadening. Now consider the first term in (4.117) as a sum of contributions from the various terms s. The odd terms all vanish since $r^n P_n(\cos\theta)$ is an operator of odd parity when n is odd, and in particular the s=1 term is zero. The s=2 term gives a total phase change

$$\Delta\phi_{2\; j,\rho,V,Z_1} = \frac{4\pi Z_1 e^2 3}{\sqrt{2\pi}\,\hbar\,(2s+1)\rho^2 V} \langle \beta_j | r^2 Y_2^0(\theta,\varphi) | \beta_j \rangle \qquad (4.120)$$

Specifying the state j by quantum numbers n,l,m,

$$\langle \beta_{nlm} | r^2 Y_2^0(\theta,\varphi) | \beta_{nlm} \rangle = \frac{n^2}{2Z^2}\sqrt{\frac{5}{4\pi}}\left[5n^2+1-3l(l+1)\right]\left[\frac{l(l+1)-3m^2}{(2l+3)(2l-1)}\right]$$

(4.121)

Although this matrix element does not vanish for any particular value of m, the average value over m is zero. Hence the contribution of these terms to $\alpha_x(1)$ on expanding expression (4.65) in powers of ϕ_v will be of order $\left(1/v^2\rho^4\right)$. Considering the second term in (4.117), the first contribution is from the s=1 term in the expansion (4.118), when the first term in (4.117) vanishes. We have for the state j=n,l,m,

$$\Delta\phi_{1,j,\rho,V,Z_1} = \frac{\pi}{2V\rho^3}\,\frac{Z_1^2e^4}{\hbar}\times\left\{\sum_{n'}\left(\frac{l+1}{3(2l+1)}\,\frac{|\langle R_{n'l+1}|r|R_{nl}\rangle|^2}{E^0_{n'l+1}-E^0_{nl}} + \frac{l}{3(2l+1)}\,\frac{|\langle R_{n'l-1}|r|R_{nl}\rangle|^2}{E^0_{n'l-1}-E^0_{nl}}\right)\right.$$

$$\left. + \int g(E)\frac{\left(\frac{(l+1)}{3(2l+1)}|\langle R_{E,l+1}|r|R_{nl}\rangle|^2+\frac{l}{3(2l+1)}|\langle R_{E,l-1}|r|R_{nl}\rangle|^2\right)dE}{E-E^0_{nl}}\right\}$$

$$= \frac{\alpha_r\,C_j}{V\rho^{r-1}} \qquad (4.122)$$

where

$$r=4.$$

$$\alpha_r = \frac{\sqrt{\pi}\,\Gamma\left(\frac{r-1}{2}\right)}{\Gamma(r/2)}$$

and

$$C_j = \frac{Z_1^2e^4\hbar}{2m}\left(\sum_{n'}\left(\frac{f_{nl,n'l+1}}{(E^0_{n',l+1}-E^0_{nl})^2}+\frac{f_{nl,n'l-1}}{(E^0_{n',l-1}-E^0_{nl})^2}\right)+\int\frac{\frac{df_{nl}}{dE}\,dE}{(E-E^0_{nl})^2}\right)$$

$$(4.123)$$

This phase shift is independent of the quantum number m, and depends only on the quantum numbers n and l for the perturbed state and the perturber parameters (ρ, V, $Z_1\bar{e}x$) Hence there is no averaging process over additional parameters for $\alpha_x(1)$ in (4.65). We have

$$\varphi_{Jxl} = \varphi_{Jx} = \Delta\phi_{1,J,\rho,V,Z_1} + O\left(\frac{1}{V^2\rho^4}\right) \qquad (4.124)$$

and for the line k,a

$$\alpha_x(1) = e^{-i(\varphi_{kx} - \varphi_{ax})} \qquad (4.125)$$

We can now calculate the real part of

$$w_{el} = w_{1,el} + i w_{2,el} = \sum_Z \iint v_x \left(\alpha_x(1) - 1\right) dV d\rho \qquad (4.126)$$

where the summation in (4.27) is now replaced by integration over V and p. $w_{2,el}$ is just the average shift due to all the particles outside the ion core, and is already allowed for in the energies of the wave functions for the average potential surrounding the ion. Using (4.70) for v_x we have

$$w_{1,el} = \sum_{Z_1} \iint d\rho \, dV \, 2\pi\rho \, V_n(V,Z_1)\left(1 - \cos\left(\frac{\alpha_r (C_a - C_k)}{V\rho^{r-1}}\right)\right)$$
$$\times \exp - (\delta_{ax} + \delta_{kx}) \qquad (4.127)$$

The δ_s , giving the probability of inelastic transitions, will only be appreciable for close impacts where the integrand is oscillating fast as a function of ρ, and hence we may neglect them altogether since they make little difference to $w_{1,el}$. Performing the integrations we obtain

$$\frac{\hbar}{kT}\, w_{1,el} = \sum_{Z_1} N_{Z_1}\, \frac{2\sqrt{\pi}}{3\sqrt{3}}\, 4\pi \left(\frac{2kT}{M_Z'}\right)^{1/6} \left(\frac{\pi}{2}\right)^{2/3} \left(\left|C_a - C_k\right|\right)^{2/3} \qquad (4.128)$$

where N_Z is the number density of particles of charge Z and reduced mass M'_Z, and the velocity distributions are assumed Maxwellian. The derivation of formula (4.128) by consideration of the general case

$$\varphi_k - \varphi_a = \frac{\alpha_r\,(C_k - C_a)}{V\rho^{r-1}} \qquad (4.129)$$

for any value of r is given in appendix C.

Since the coefficients are proportional to Z_1^2 and the mass dependence is only $\left(M_Z^1\right)^{-1/6}$, the contributions of ions and electrons are comparable.

THE LINE SPECTRUM

We now have expressions for all the necessary quantities required to calculate the line profile for absorption between the levels *k* and a in a given configuration I, and can add the line absorption into the spectrum.

The number of atoms of charge Z per gram of the element, in the configuration I is just the total number of atoms, A_0/M_Z times the probability of the configuration as given by (2.40)

$$N_{2,I} = A_0/M_2 \, P_I \qquad (4.130)$$

If the configuration I has n_{nl} electrons in the level l=nl, with average absorption cross sections $\sigma_{nl,n'l'}(\nu)$ at frequency ν for excitation into the level n'l', then the total line absorption minus the stimulated line emission per gram of the element is

$$K_2^{line}(\nu)\left(1-e^{-h\nu/kT}\right) = K_2^{'line} \qquad (4.131)$$

$$= \frac{A_0}{M_2}\sum_I \left\{ P_I \left[\sum_{nl} \bar{n}_{nl} \left(\sum_{n' \geq n} \sigma_{nl,n'l+1}(\nu) + \sum_{n'>n} \sigma_{nl,n'l-1}(\nu) \right) \right]_I \right\} (1-e^{-u})$$

The cross-section $\sigma_{nl,n'l'}(\nu)$ for l'=l±1 in the configuration I is

$$\sigma_{nl,n'l'}(\nu) = \frac{\pi e^2}{mc} f_{nl,n'l'} \, b'_{nl,n'l'}(\nu) \qquad (4.132)$$

The oscillator strength for the levels will depend on the inner parts of the wave functions. The potential gradient matrix element for pairs of states k and a will be approximately the same as the hydrogenic one for the corresponding states, and with an effective charge Z^*_{nl} appropriate to the screening of the inner orbit, k=nl, by the electrons inside it in the configuration in terms of the Slater screening constants

$$Z^*_{nl} = Z - \sum_{n''l'' < nl} n_{n''l''} \, \sigma_{nl,n''l''} \qquad (4.133)$$

This implies an oscillator strength

$$f_{nl,n'l'} = f^H_{nl,n'l'}\left(Z^*_{nl}, \nu_H\right)\left(\frac{\nu_H}{\nu}\right)^3 \qquad (4.134)$$

where

$$h\nu_H = Z^{*2}_{nl}\left(\frac{1}{n^2} - \frac{1}{n'^2}\right) R_y \qquad (4.135)$$

and the absorption strength again varies as $1/\nu^3$.

Treating all the surrounding particles in the impact approximation we have the line profile

$$b'_{nl,n'l'}(\nu) = \frac{1}{\Delta}\frac{1}{\sqrt{\pi}} V\left(\frac{\omega_1/2\pi}{\Delta}, \frac{\nu-\nu'_{ak}}{\Delta}\right) \qquad (4.136)$$

$$\Delta = \sqrt{\frac{2kT\,\nu_{ak}^{0\,2}}{Mc^2}} \quad ; \quad V(a^*,x) = \frac{a^*}{\pi}\int_{-\infty}^{+\infty}\frac{e^{-y^2}}{(x-y)^2+a^{*2}}\,dy$$

$$\frac{\hbar\omega_1}{kT} = \frac{1}{2}\left[\Gamma_{nat,nl} + \Gamma_{nat,n'l'} + \Gamma_{inel,nl} + \Gamma_{inel,n'l'}\right] + \frac{\hbar\omega_{1el}}{kT} \qquad (4.137)$$

and in terms of the average energy levels for the configuration I, (2.17),

$$h\nu'_{ak} = h\left(\nu^0_{ak} + \omega_2/2\pi\right) = \bar{E}_{n'l'} - \bar{E}_{nl} \qquad (4.138)$$

Changing to the variable $u=h\nu/kT$ by analogy with (3.66) the line spectrum for the element Z is

$$D_Z^{line}(u) = \frac{k_Z^{line}(u)\,u^3}{C}\left(\frac{kT}{Ry}\right)^3 \qquad (4.139)$$

This may be added on to the continuous spectrum for the element and the appropriate integrals evaluated over the resulting mixture spectrum to find the total Rosseland mean opacity.

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ELEMENT	Z	CONC. BY FRACTION NUMBER OF ATOMS	CONC. BY FRACTION OF TOTAL WEIGHT
HYDROGEN	1	.92477	.7440
HELIUM	2	.07387	.2360
CARBON	6	.00007	.0007
NITROGEN	7	.00026	.0029
OXYGEN	8	.00045	.0057
NEON	10	.00043	.0070
ALUMINIUM	13	.00007	.0015
SILICON	14	.00006	.0013
IRON	26	.00002	.0009

TABLE 5A-COMPOSITION OF MIXTURE

CHAPTER V

NUMERICAL PROCEDURES AND RESULTS

Programs have been devised in Fortran to calculate opacities along the lines indicated in the previous chapters, and these have already been used on the St Andrews University I.B.M. 1620 computer on a sample mixture at several pressures and temperatures. The program falls into four parts; the first finds the occupation numbers and energy levels, the second computes the continuous spectrum ignoring the splitting of edges with the ionic configurations, which is allowed for in the third section. Finally the last stage puts in the line contributions to the spectrum. The numerical procedures and approximations required in programming the calculations and sample results obtained at each stage will now be discussed.

The mixture of elements investigated and their relative concentrations are given in table 5A. This is a mixture already studied by Cox and has the relative concentration by weight of heavy elements $(Z>2)$, 0.02.

THE CALCULATION OF THE ENERGY LEVELS AND OCCUPATION NUMBERS

The theory in chapter II provides an iterative method of solution for the energy levels and occupation numbers. To produce a convergent sequence of iterations we have to make a reasonable guess at a set of trial solutions. At any specified temperature, sufficiently high pressures given a very high degree of ionization and it is sufficient to ignore all the bound electrons $n_{nl}=0$, and use Coulomb energy levels $E^{\sigma}_{nl}=-(Z^2/n^2)$Ry., for the trial values. The results of low pressure calculations can then be used as trial solutions at higher pressures.

For a perfect gas, neglecting the potential energy terms, we have from (2.37) for large α

$$\alpha \sim \log \frac{2V'}{\sum_z N_z \bar{Z}'} \left(\frac{2\pi kT}{h^2}\right)^{3/2} \qquad (5.1)$$

and from (2.39)

$$PV' \sim \sum_z N_z (1+\bar{Z}')kT \qquad (5.2)$$

so that $\exp(\alpha)$ varies as $T^{2.5}P^{-1}$.

Trial values of α were thus taken from such a formula

$$\alpha = \cdot 89 + 2\cdot 5 \log T - \log P \qquad (5.3)$$

where the temperature T is in electron volts and the pressure, P, in Megobars.

The Slater screening constants σ_{ij} for calculating the energy levels are given in appendix D, table A, as the symmetric array of numbers $\sigma_{ij}/n_i^2 = \sigma_{ji}/n_j^2$ where n_i is the principal quantum number of the level i screened by jth level electron. The calculations also require values of the $F_{1/2}(\alpha^*,\eta)$ and $F_{3/2}(\alpha^*,\eta)$ functions. Since $\eta = \beta\bar{U}$ is only a small correction term it is sufficient to express the incomplete Fermi-Dirac functions in terms of the complete integrals.

$$F_n(\alpha^*,\eta) = F_n(\alpha^*,0) - \frac{1}{n+1}\frac{(\eta)^{n+1}}{(1+\exp\alpha^*)} + O\left(\frac{\eta^{n+2}}{(n+2)(1+\exp\alpha^*)^2}\right) \qquad (5.4)$$

Z	Z	STATE	ENERGY RY	OCC NO
1	1	NO BOUND LEVELS		
2	2	1S	- 1.384	.01839
6	5.84	1S	- 30.147	.06613
		2S	- 3.239	.02127
		2P	- 3.224	.06381
7	6.79	1S	- 42.610	.11042
		2S	- 5.725	.02364
		2P	- 5.657	.07074
8	7.60	1S	- 56.960	.19543
		2S	- 8.467	.02658
		2P	- 8.378	.07945
		3S	- .428	.01767
		3P	- .321	.03187
		3D	- .146	.05040
10	9.03	1S	- 91.823	.65215
		2S	- 14.254	.03408
		2P	- 13.908	.10083
		3S	- 2.135	.02033
		3P	- 2.007	.06066
		3D	- 1.914	.1007
13	10.90	1S	-148.7	1.693
		2S	- 24.02	.0518
		2P	- 22.54	.1465
		3S	- 5.368	.0234
		3P	- 4.929	.0689
		3D	- 4.703	.1138
14	11.65	1S	-171.4	1.862
		2S	- 28.53	.06279
		2P	- 26.80	.1758
		3S	- 6.937	.0250
		3P	- 6.426	.0735
		3D	- 6.177	.1213
		4S	- .253	.0175
		4P	- .051	.0046
26	18.81	1S	-615.98	2.000
		2S	-121.46	1.269
		2P	-102.46	2.614
		3S	- 32.24	.0732
		3P	- 30.16	.2022
		3D	- 27.35	.3009
		4S	- 10.73	.02641
		4P	- 9.776	.08481
		4D	- 8.675	.1349
		4F	- 8.066	.18415
		5S	- 2.121	.0203
		5P	- 1.598	.0582
		5D	- .940	.0521
		5F	- .540	.0703
		5G	- .328	.0887

TABLE 5B-ENERGY LEVELS AND OCCUPATION NUMBERS LOG(T)=2.5 LOG(P)=2.5

For values of α greater than 4 the expansion of $F_n(\alpha^*,0)$ in terms of $\exp(-\alpha^*)$ converges rapidly

$$F_n(\alpha^*,0) = \sum_{s=1}^{\infty} (-1)^{s-1} \frac{\exp(-s\alpha^*)}{s^{n+1}} \int_0^{\infty} t^n e^{-t} dt \tag{5.5}$$

For values of α less than 4, the tables compiled by MacDougall and Stoner for $F_{1/2}(\alpha^*,0)$ and $F_{3/2}(\alpha^*,0)$ were used. These values are also tabulated in Appendix D in table B. A maximum of fifteen bound levels was allowed for each element.

The iterative method outlined at the end of chapter II converges rapidly providing the trial values are reasonably close. In any case convergence can always be obtained by taking intermediate steps in pressure.

A sample set of solutions for the average energy levels and occupation numbers for the mixture 5A at $T=10^{2.5}$ and $P=10^{2.5}$ Mbars is given in table 5B.

THE CONTINUOUS SPECTRUM WITHOUT CONFIGURATION SPLITTING OF THE EDGES

The second stage of calculating the opacity involves building up the absorption spectra of the elements for scattering, free-free electron transitions and a preliminary treatment for the bound free transitions without paying much attention to the behaviour of the absorption edges.

From equations (3.65) and (3.66) we have for the continuous element spectra

$$D_2(u) = \left(\frac{kT}{Ry}\right)^3 \cdot \frac{1}{\left(\frac{A_0\, 64\pi^4 m e^{10}}{3\sqrt{3}\, c h^3 Ry^3}\right)} \frac{A_0}{M_2}\left[\sum_{nl} \bar{n}_{nl}\, \sigma_{nl}(u)\, u^3 + \varphi_e\, \sigma_{AH}(u)\, u^3 + \bar{Z}'\sigma_s(1-e^{-u})^{-1}\right]$$

$$= \left(D_2(u)\right)_{bd\text{-}free} + \left(D_2(u)\right)_{free\text{-}free} + \left(D_2(u)\right)_{scatt.} \qquad (5.6)$$

The last term, the scattering contribution, never vanishes for any value of u and gives a lower limit for the opacity. It is therefore a convenient factor to consider first. Apart from the atomic weight of the element it depends only on the scattering cross section

$$\sigma_s = 6.65\ 205 \cdot 10^{-25}\, cm^2 \qquad (5.7)$$

and the average number of free electrons per atom of the element, $\bar{Z}'$. We have

$$\left(D_2(u)\right)_{scatt} = \cdot 840727 \cdot 10^{-7} \times \left(\frac{kT}{Ry}\right)^3 \frac{\bar{Z}'}{M_2}\left(1-e^{-u}\right)^{-1} \qquad (5.8)$$

The free-free absorption cross section depends on the temperature averaged Gaunt factor. The values tabulated by Karzas and Latter are given in appendix D table C. From equation (3.55) $\left(D_2(u)\right)_{free\text{-}free}$ becomes

$$\left(D_2(u)\right)_{free\text{-}free} = \frac{3.30045\,(\varphi_e \cdot 10^{-24})\,\bar{Z}'^2 \sqrt{Ry/kT}\,.\ \bar{g}_{ff}(u)}{M_2.} \qquad (5.9)$$

For the bound-free absorption equation (3.44) gives the average cross section above the highest component edge. However until the various ionic configurations have been considered the threshold of the highest configuration edge is unknown. As a preliminary approximation it is assumed that the absorption cross section takes the form (3.44) down to the frequency corresponding to the average energy level nl and the

ELEMENT	SCATTERING	+FREE-FREE ABSPN	+BD-FREE ABSPN	CONC	MIXTURE
HYDROGEN	.2857	.9582		.7440	.7129
HELIUM	.1984	.7507	.8680	.2360	.9288
CARBON	.1951	1.892	16.01	.0007	.9428
NITROGEN	.1944	2.166	38.01	.0029	1.084
OXYGEN	.1916	2.439	79.94	.0057	1.675
NEON	.1795	2.903	98.86	.0070	4.561
ALUMINIUM	.1621	3.509	38.28	.0015	5.720
SILICON	.1665	3.875	37.46	.0013	6.358
IRON	.1371	6.158	231.2	.0009	6.923

TABLE 5C-ROSSELAND MEAN OPACITY PER GRAM spectrum is adjusted below the highest edge in the next section of the program. The average value of Z_{eff}^{*4} for the configurations, $\bar{Z}_{eff}^{4}$ depends little on the various configurations of the outer orbit electrons since their screening constants are small, and it is only necessary to perform a relatively simple process for screening by electrons in the n=1 and n=2 shells. Thus the first approximation for is $\left(D_Z'(u)\right)_{\text{bd-free}}$

$$\left(D_Z'(u)\right)_{\text{bd-free}} = \sum_{\left\{M \mid u \geq -\frac{\bar{E}_M}{kT}\right\}} \left[\frac{\bar{n}_M \times Z^4}{M_Z \times n^5} g_M^H\left(\bar{Z}_{eff}, ukT + \bar{E}_M - K\right) \frac{\bar{Z}_{eff}^{*4}}{Z^4}\right] \tag{5.10}$$

The hydrogenic Gaunt factors are again those of Karzas and Latter and are listed in table D of appendix D.

On these lines the spectra of the elements in 5A have been computed at 1000 points between u=0 and u=20 for 12 different combinations of pressure and temperature. The resulting opacities per gram of the individual elements for the mixture at $T=10^{2.5}$, $P=10^{2.5}$, calculated after each stage of building up the spectra are given in table 5C, and show the relative importance of scattering, free-free absorption and bound free absorption in a typical case. The mixture spectrum was built up element by element and the opacity calculated each time, and these figures are also shown. It can be seen how elements with low concentrations can dominate the opacity of the mixture.

THE IONIC CONFIGURATIONS

To develop the spectrum further, the probability of the various contributing ionic configurations has to be computed. Because of the vast number of configurations it is desirable to omit all those which are so improbable that they are insignificant.

The probability of the configuration which has n_{iZ} electrons in the levels i in an atom of charge Z, is, according to (2.40)

$$P\{n_{iZ}\} = \prod_i \frac{g_{iZ}!}{n_{iZ}!\,(g_{iZ}-n_{iZ})!}\, p_i^{n_{iZ}}\, q_i^{(g_{iZ}-n_{iZ})} \qquad (5.11)$$

in which p_i and q_i for the level i are $p_i=\bar{n}_{iZ}/g_{iZ}$ and $q_i=1-p_i$. This is simply a product of the probabilities $P_{n_{iZ}}$ that there are n_{iZ} electrons in the level i.

In the case of the bound free absorption just one of the levels is involved in particular, and in the line absorption, two levels. For all possible occupation numbers of these particular levels we can consider which configurations of the other levels have a greater probability than say, ε^3, times the most probable configuration for these levels. This most probable configuration is the one in which we have the most probable number m_{iZ} in each level, where m_{iZ} is the biggest integer such that

$$m_{iZ} \leq g_{iZ}(p_i+1)$$

In the event of equality $m_{iZ}-1$ is equally probable. In some levels deviations from m_{iZ} will be unlikely. This will happen in deeply bound levels which are almost always full, $m_{iZ}=g_{iZ}$, or in very lightly bound levels which are almost always empty, $m_{iZ}=0$.

The probability that there are $m_{iz}+1$ electrons in a level i is

$$P_{m_{iz}+1} = P_{m_{iz}} \times \left(\frac{g_{iz}-m_{iz}}{m_{iz}+1} \right) \frac{p_i}{q_i} \tag{5.12}$$

and the probability that there are $m_{iz}-1$ electrons is

$$P_{m_{iz}-1} = P_{m_{iz}} \times \left(\frac{m_{iz}}{g_{iz}-m_{iz}+1} \right) \frac{q_i}{p_i} \tag{5.13}$$

Suppose that

$$P_{m_{iz}+1} < \varepsilon P_{m_{iz}} \tag{5.14}$$

then

$$P_{m_{iz}+2} < \varepsilon^2 P_{m_{iz}}$$

and similarly, if

$$P_{m_{iz}-1} < \varepsilon P_{m_{iz}}, \tag{5.15}$$

$$P_{m_{iz}-2} < \varepsilon^2 P_{m_{iz}}$$

If both (5.14) and (5.15) hold then

$$\frac{p_i}{q_i} < \frac{\varepsilon (m_{iz}+1)}{(g_{iz}-m_{iz})}$$

and

$$\frac{p_i}{q_i} > \frac{m_{iz}}{(g_{iz}-m_{iz}+1)\varepsilon}$$

This implies that

$$\varepsilon^2 > \frac{m_{1Z}}{m_{1Z}+1} \, \frac{(g_{1Z}-m_{1Z})}{(g_{1Z}-m_{1Z}+1)}$$

The right hand side of this inequality is zero if $m_{1Z}=0$ or $m_{1Z}=g_{1Z}$ but otherwise it is greater than $\frac{1}{4}$.

Hence if m_{1Z} is a clear maximum so that the two next most probable numbers are both less probable by a factor ε, then either $m_{1Z}=0$, and the next two most probable values are 1 or 2, or $m_{1Z}=g_{1Z}$ and the next most probable are $g_{1Z}-1$ and $g_{1Z}-2$. Furthermore the probability of the fourth most probable occupation numbers in these cases is less than and we may exclude configurations with such an occupation number. For such levels the number of possibilities to be considered for the occupation of the level is then three at most. Furthermore the probability of configurations in which two such levels have their third most probable occupation numbers may also be neglected.

In the calculations the levels not involved as initial or final states in the absorption process, were divided up according to whether their most probable occupation numbers were at least ten times as probable as the next two most probable numbers (i.e.$\varepsilon=1/10$), or not. In the former case only the three most probable possibilities were considered, and if the conditions did not hold, occupation numbers were considered both above and below m_{1Z} until n_{1Z} was such that $P_{n_{1Z}} < \varepsilon^3 P_{m_{1Z}}$. The numbers of configurations considered were then reduced to feasible proportions, and it is estimated that the total probabilities of the configurations excluded in this way was less than 1%.

SPLITTING OF BOUND-FREE ABSORPTION EDGES

When the various probabilities of the ionic configurations have been computed the bound free absorption edges can be corrected for configuration splitting. The average cross section in the region of the edges for a level nl is given by (3.45) and in calculating the edges were extended down to the threshold positions for the average energy levels $\bar{E}_{nl}$, using the cross sections obtained by expanding the range of validity of the cross-sections (3.44) to these frequencies. This means that

$$\left(D_2(u)\right)_{bd\text{-}free} = \left(D_2^{'}(u)\right)_{bd.free} + \sum_{nl}\sum_{I} P_I \left(\frac{Z^4}{M_2 n^5} n_{nl} \Delta_{nl,I}(u)\right) \qquad (5.17)$$

where

$$\Delta_{nl,I}(u) = g_{nl}^{H}(2,0) \times \left(\frac{(Z_{eff}^{*4})_I - \bar{Z}_{eff}^{4}}{Z^4}\right)_{nl,I} \qquad \text{if } u_{nl,I} < u < -\frac{\bar{E}_{nl}}{kT}$$

and

$$= 0 \qquad \text{when } u < u_{nl,I} \text{ or } u > -\frac{\bar{E}_{nl}}{kT} \quad)$$

or

$$\Delta_{nl,I}(u) = -\,g_{nl}^{H}(2,0)\left(\frac{\bar{Z}_{eff}^{4}}{Z^4}\right)_{nl,I} \qquad \text{if } -\frac{\bar{E}_{nl}}{kT} < u < u_{nl,I}$$

and

$$= 0 \qquad \text{when } u < -\frac{\bar{E}_{nl}}{kT} \text{ or } u > u_{nl,I}$$

$u_{nl,I}$ is the threshold for the level nl in the configuration I.

LOG P	5.5	4.5	3.5	2.5	1.5	0.5	-0.5	-1.5
LOG T								
3.0	3.196 3.198	1.082 1.085	.5153 .5159	.3797 .3803				
2.5			21.33 21.63	6.923 7.691	1.419 1.527	.4947 .5008		
2.0					61.88 71.10	10.64 14.66	1.753 1.976	.5555 .5715

TABLE 5D-ROSSELAND MEAN OPACITIES BEFORE AND AFTER SPLITTING OF EDGES

The difference in opacity of the mixture 5.A when the edges were split in this way is shown for 12 different pressure and temperature conditions in table 5D by comparing the Rosseland mean opacities before and after splitting was included. The effect is more evident at lower temperatures as we should expect.

THE LINE SPECTRUM

The contribution of the line spectrum follows from (4.131) and (4.134). It depends on the line splitting with configurations and on the profile of each component given by (4.136)

$$\left(D_z(u)\right)_{line} = \sum_{nl\to n'l'} \left(\sum_I \frac{3\sqrt{3}\pi}{16} \frac{\left(\frac{Ry}{kT}\right)}{M_z} P_I f^{H}_{nl,n'l'}\left(Z^*_{nl,I}, \nu_H\right) Z^{*\,6}_{nl,I} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right)^3\right.$$

$$\left. \times \frac{1}{\sqrt{\pi}} \sqrt{\frac{Mc^2 Ry}{2Ry\,kT}} \frac{1}{u_0} V(a^*, u)\right)$$

$$\frac{3\sqrt{3}\pi}{16} = 1.020260 \qquad \frac{Mc^2}{2Ry} = 3.922143 \cdot 10^7 M_z$$

The Lorentz half-width in (4.137) due to natural broadening and inelastic and elastic perturbations may be calculated from the average energy levels and oscillator strengths irrespective of the ionic configuration. As each configuration component and its probability is considered the central frequency for the line can be calculated and this gives the Doppler width and determines the line profile. The hydrogenic oscillator strengths are given in Appendix D, table E, for pairs of states with different principal quantum numbers n and n'. For the oscillator strengths between levels of the same n we have

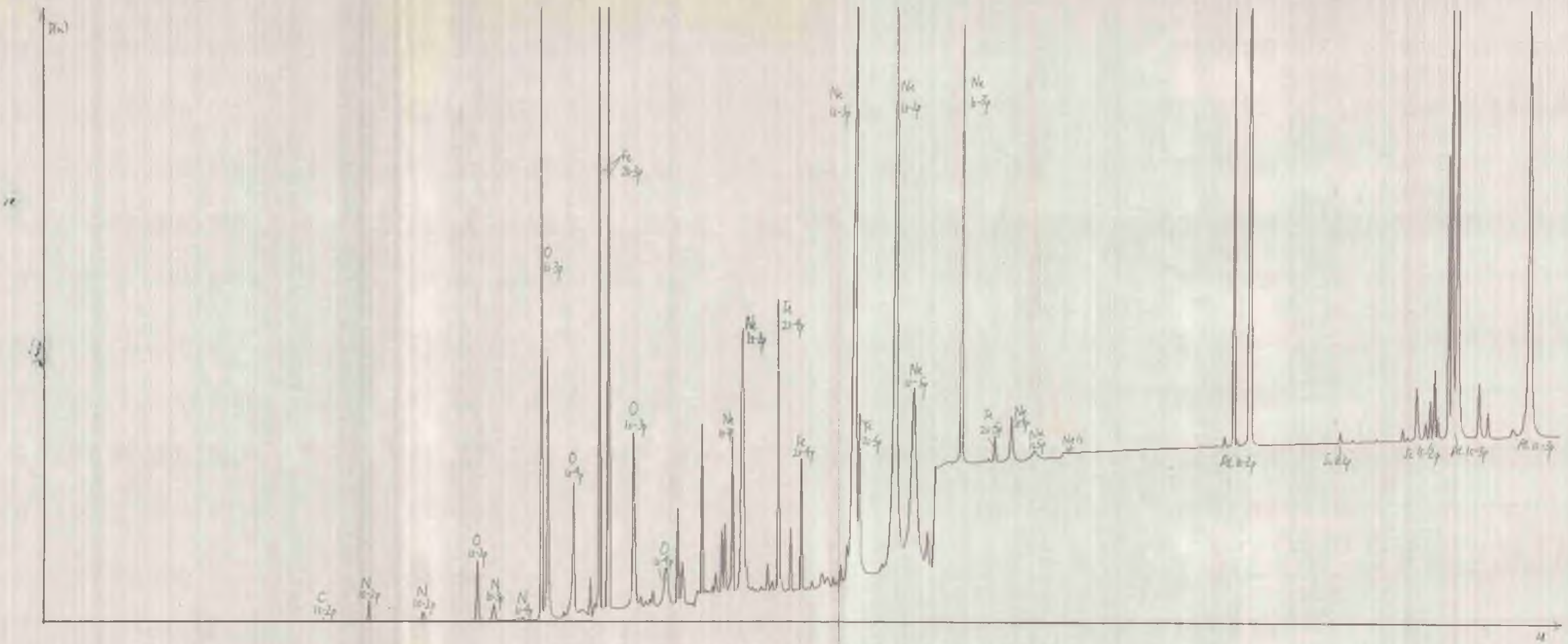

FIG 5E MIXTURE SPECTRUM T= 110eV P= 3.6 Mtorr

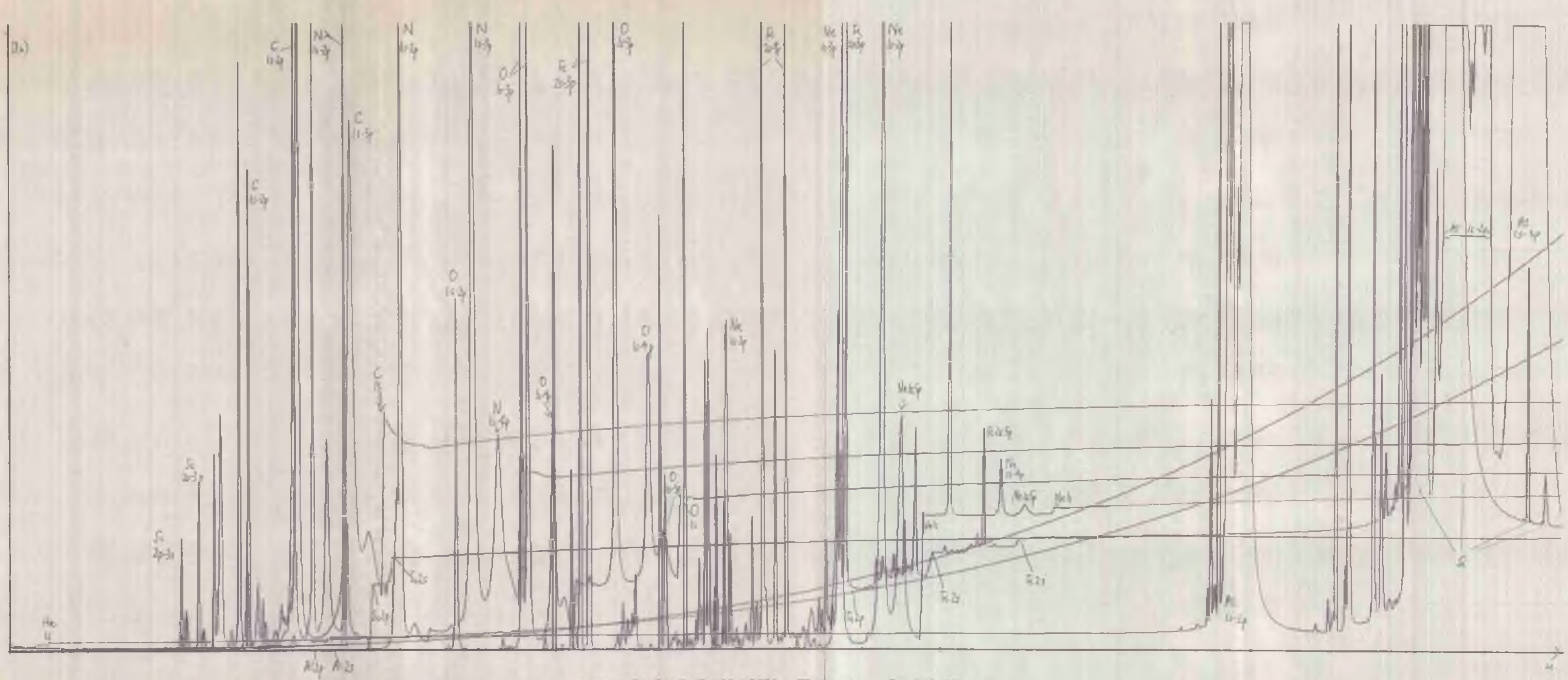

Fig 5F ELEMENT SPECTRA T= 10 eV P= 316 Mbars

$$f_{nl,\,nl+1} = \frac{l+1}{2l+1}\,\frac{3n^2}{4Z^2}\left(n^2-(l+1)^2\right)\left(\frac{E_{nl+1}-E_{nl}}{Ry}\right)$$

$$f_{nl,\,nl-1} = \frac{l}{2l+1}\,\frac{3n^2}{4Z^2}\left(n^2-l^2\right)\left(\frac{E_{nl}-E_{nl-1}}{Ry}\right) \qquad (5\ 20)$$

In the calculations the components of each line were added in to the spectrum separately, starting at the line centre and working outwards into the wings until the absorption strength was less than one per cent of the background spectrum. The necessary values of the Voigt function were extracted from the tables of Posener and are listed in Appendix D, table F. For values of a^* greater than 10 the profile is effectively Lorents. In the extreme wings of the line the asymptotic form

$$V(a^*,x) = e^{-x^2} + \frac{a^*}{\sqrt{\pi}\,x^2} + o\left(a^{*2}x^{-4}\right)$$

was used.

The natural broadening was always very small compared with the broadening due to inelastic collisions, and this was usually rather less than the elastic interaction broadening. The Doppler width was normally less than the Lorents width, that is $a^* > 1$. Increasing the ratio of the inelastic broadening considerably relative to the other broadening processes, and hence altering the ratio of the Lorents width to the Doppler width, did not reveal great sensitivity to the line profile. There was slightly more effect at lower temperatures.

The element spectra including lines are shown in the graphs 5.F

LOG T	LOG P	PLANCK.CTM	ROSS.CTM	COX.CTM	PLANCK.LIN	ROSS.LIN	COX.LIN
3.0	5.5	99.71	3.196	2.934	99.86	3.293	2.997
3.0	4.5	11.69	1.082	1.155	120.5	1.165	1.208
3.0	3.5	1.553	.5153	.5667	1.672	.5443	.5887
3.0	2.5	.4715	.3797	.3906	.5125	.3915	.3961
2.5	3.5	206.6	21.33	17.91	222.7	23.56	19.88
2.5	2.5	25.19	6.923	6.359	35.20	10.31	8.374
2.5	1.5	3.184	1.419	1.531	5.916	2.588	2.116
2.5	0.5	.6520	.4947	.5308	1.913	.6090	.5863
2.0	1.5	421.3	61.88	52.40	503.8	119.8	84.62
2.0	0.5	51.92	10.64	11.05	86.50	27.07	19.33
2.0	-0.5	6.125	1.753	2.027	19.55	3.176	2.926
2.0	-1.5	1.003	.5555	-	15.50	.6730	-

TABLE 5G-OPACITIES OF MIXTURE AND COMPARISON VALUES FROM THE COX OPACITIES for the case $T=100$eV and $P=.316$Mbars. The mixture spectrum is superimposed in fig 5.E with the element spectra combined according to their concentrations. The richness of lines in the regions $5 \leq u < 12$ demonstrates clearly how the line absorption can be important; in the case shown it increases the opacity by about 55%. The Planck and Rosseland mean opacities including the line absorption and splitting of absorption edges are given in the fourth and fifth columns of figures in table 5.G, for the twelve pressure and temperature conditions investigated.

COMPARISON OF RESULTS AND CONCLUSIONS

The most recent opacities published are those of Cox at Los Alamos. These were also based on Mayer's method for finding the occupation numbers, and used hydrogenic Gaunt factors and oscillator strengths. In the second and third columns of table 5.G the Rosseland mean for the continuous spectrum of the mixture without configuration splitting of the edges, is compared with the corresponding values obtained by interpolation in Cox's table of opacities for the same mixture. Cox calculated the bound energy levels by taking the Bohr hydrogen-like theory for the nuclear charge diminished by the average shielding by the bound electrons according to the screening constants, and adding the perturbation of the free electrons. The average number of perturbing electrons interacting with an electron in the same level i was taken as $(1 - 1/g_{12})$ times the average number in the level, and the energy levels were all adjusted for depression of the continuum. Hence the ionization energies calculated by Cox tend to be lower than the present ones. This increases the continuous opacity and accounts for the fact that the Cox values are larger at the lower pressures at each given temperature, where the free electron perturbations and the bound-free absorption are less significant.

However at higher densities the bound free absorption and the energy perturbations due to the free electrons, become more important. The effective charges used by Cox in determining the appropriate bound-free hydrogenic Gaunt factors were taken from the ionization energies of the bound states, which include both bound and free electron perturbations and depression of the continuum, and these are considerably less than the effective charges used in this thesis at higher densities. Since the bound free cross sections are proportional to the fourth power of the effective charge (apart from the slow variation in the hydrogenic Gaunt factor) the present values of the opacity increase above Cox's values as the density and pressure increase at constant temperature.

It is believed that at present no values of the opacity have been published which include splitting of edges, and as table 5.D indicates this can easily increase the opacity by 10% or so.

Several other calculations have considered the line absorption. The Rosseland mean opacities given by Cox on adding lines with a Lorentz profile, and a half-width due to Sternheimer representing the inelastic collision width, are given in column 6 of table 5G. In agreement with his results the figures in column 5 indicate the importance of the line absorption, which can double the opacity. In fact, the present line treatment using the Voigt profile and combining the different broadening mechanisms of which the elastic interactions are often more effective than the inelastic collisions, tends to show even a slightly larger increase in the opacity due to the line absorption than the Cox values.

It is now hoped to extend these calculations and compute the Rosseland mean opacities for different mixtures and many more pressures and temperatures within the range considered here in order to provide adequate tables for interpolation in the construction of stellar models.

BIBLIOGRAPHY, CHAPTER V

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	1965	Stars and Stellar Systems Vol. VIII, Stellar Structure (Chicago), P.195
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APPENDIX A. THE FERMI-DIRAC STATISTICS AND THE GRAND ENSEMBLE

Let μ_{iz} be the subspace in the vector space μ of possible electron states in an atom of charge Z, corresponding to the energy E_{iz}. In an ensemble of n electrons and N_Z atoms of type Z we may describe a systems distribution by the number of electrons, $N_Z n_i$ in each subspace μ_{iz}. The vector space describing the possible states of the ensemble is isomorphic to the subspace of antisymmetric vectors in the n-fold tensor product of μ spaces. The choice of the anti-symmetric states corresponds to the Pauli exclusion principle whereby no two electrons can occupy the same state simultaneously.

Supposing that the average number of states per atom of energy approximately equal to E_{iz} is g_{iZ} (i.e. g_{iZ} is the dimension of μ_{iz}) then if we wish to put $N_Z n_{iZ}$ electrons into the $N_Z g_{iZ}$ available distinct states, supposing that the electrons are distinct, we have

$$N_z g_{iz}(N_z g_{iz}-1)(N_z g_{iz}-2)\cdots = \frac{(N_z g_{iz})!}{(N_z(g_{iz}-n_{iz}))!}$$

vectors corresponding to the same distribution in the iZ state. Allowing for the indistinguishability of the electrons we have

$$G = \prod_i \frac{(N_z g_{iz})!}{(N_z(g_{iz}-n_{iz}))!\,(N_z n_{iz})!}$$

vectors corresponding to the distribution $\{n_{iZ}\}$.

It follows that the a priori probability of the distribution characterised by $\{n_{iZ}\}$ is proportional to

$$P = \prod_{Z} \prod_{i} \frac{(N_Z(g_{iZ}))!}{(N_Z(g_{iZ}-n_{iZ}))!\,(N_Z n_{iZ})!} \qquad A(1)$$

Hence we have, assuming that N_{ZgiZ}, $N_Z(g_{iZ}-n_{iZ})$, and $N_Z n_{iZ}$ are large

$$\log P = \sum_Z N_Z \sum_i \Big\{ (n_{iZ}-g_{iZ}) \log N_Z (g_{iZ}-n_{iZ}) - n_{iZ} \log N_Z n_{iZ} + g_{iZ} \log N_Z g_{iZ} \Big\} \qquad (A.2)$$

(This follows from Stirling's formulae

$$n! \sim \sqrt{2\pi n}\,(n/e)^n$$

$$\log n! \sim n \log n - n + \tfrac{1}{2} \log (2\pi n)$$

)

Supposing we allow a slight variation in the n_{iZ} and the g_{iZ}

$$-\delta \log P = \sum_Z N_Z \sum_i \Big\{ -\delta n_{iZ} \log N_Z (g_{iZ}-n_{iZ}) - \delta n_{iZ} + \delta n_{iZ} \log N_Z n_{iZ} + \delta n_{iZ} \Big\} + \sum_Z N_Z$$

Hence when the degeneracy is a variable function of the n_{iZ}

$$\delta g_{iZ} = \sum_j \frac{\partial g_{iZ}}{\partial n_{jZ}} \delta n_{jZ}$$

and so

$$-\delta \log P = \sum_Z N_Z \Big\{ \sum_i \delta n_{iZ} \left(\log N_Z n_{iZ} - \log N_Z (g_{iZ} - n_{iZ}) \right) + \sum_i \sum_j \frac{\partial g_{iZ}}{\partial n_{jZ}} \delta n_{jZ} \left[\log N_Z (g_{iZ} - n_{iZ}) - \log N_Z g_{iZ} \right]$$

$$= \sum_Z N_Z \Big\{ \sum_i \delta n_{iZ} \Big[\log n_{iZ} - \log (g_{iZ} - n_{iZ}) + \sum_j \frac{\partial g_{jZ}}{\partial n_{iZ}} \begin{bmatrix} \log (g_{jZ} - n_{jZ}) \\ - \log g_{jZ} \end{bmatrix}$$

(A.3)

We wish to consider variations in (A3) subject to the conditions that the total number of electrons remains constant and that the total energy of the system is constant. The first condition gives

$$\sum_i \delta n_{iZ} = 0$$

The total energy E of the electrons is the sum of their kinetic energies and of their interactions with the nuclei and each other. Let E_{jkZ} be the average interaction of the jZth and kZth state electrons, then the energy of the electrons in an ion with m_{iZ} in the levels i may be written as a quadratic expression in the m_{iZ}

$$E_{ion} = \sum_i m_{iZ} E^0_{iZ} + \frac{1}{2} \sum_i \sum_j m_{iZ} m_{jZ} E_{jiZ} - \sum_i \max(0, m_{iZ}-1) E_{iiZ} m_{iZ}$$

(A.4)

where E^0_{iZ} is the interaction with the nucleus plus the kinetic energy of an ith level electron.

This suggests that we write the average energy of the ion in the form

$$\bar{E}_{ion} = \sum n_{iz} \left(E_{iz}^{\circ} + \frac{1}{2} \sum_{j} n'_{ji} E_{jiz} \right) \qquad (A.5)$$

where n'_{jiz} is the average number of jth state electrons interacting with another in the ith.

By symmetry

$$n_{iz} n'_{jiz} = n_{jz} n'_{ijz} \qquad (A.6)$$

and if the variations in the $\{n_{iz}\}$ are independent then

$$n_{iz} \delta n'_{jiz} = \delta n_{jz} n'_{ijz} \qquad (A.7)$$

Hence the variation in the total energy is

$$\delta E = \sum N_z \left\{ \sum \delta n_{iz} \left(E_{iz}^{\circ} + \sum_{j} n'_{jiz} E_{ijz} \right) \right\}$$

(N.B. There is no distinction here between discrete and continuum levels. The indices j and i refer to any energy subspaces μ_{iz}, μ_{jz}).

The most probable distribution will be that for which P has a maximum, that is

$$-\delta \log P = 0$$

subject to the conditions

$$\delta n = \sum_{i} \delta n_i = 0$$

$$\delta E = 0$$

Using the method of Lagrange multipliers

$$-\delta \log P + \alpha \delta n + \beta \delta E = 0$$

and assuming that the δn_{iz} are linearly independent we now have

$$-\log n_{iz} + \log(g_{iz} - n_{iz}) - C_i = \alpha + \beta E_{iz}$$

where

$$E_{iz} = E_{iz}^{0} + \sum_{j} n'_{jiz} E_{jiz} \quad \text{(which leads to 2.21)} \qquad (A.9)$$

and

$$C_i = \sum_{j} \frac{\partial g_{jz}}{\partial n_{iz}} \left[\log(g_{jz} - n_{jz}) - \log g_{jz} \right] \qquad (A.10)$$

On considering the total energy

$$\beta = 1/kT$$

and α must be chosen such that the total number of electrons is correct. Hence

$$n_{iz} = \frac{g_{iz}}{\exp(\alpha + \beta E_{iz} + C_i) + 1} \qquad (A.11)$$

THE DEGENERACY FUNCTION

In calculating the probability of an electron occupying a given state i it is normally assumed that the number of ways of arranging the $N_Z n_{iZ}$ electrons in the level is given by an expression of the form

$$\frac{(N_z g_{iz})!}{(N_z(g_{iz} - n_{iz}))!\,(N_z n_{iz})!} \qquad (A.12)$$

The degeneracy function will be defined such that this expression always does give the a priori probability of the distribution corresponding to the occupation numbers $\{n_{12}\}$ being the number of permitted arrangements of the electrons in the levels. Supposing we consider small changes in the occupation numbers and the corresponding effect on the degeneracy by selecting one more state for occupation and suppose first of all, that we select a state in the ith level itself for which we have a choice of $N_Z m_{iZ}$ states. Then the number of possible configurations of the

$$N_2 (n_{12} + \delta n_{12}) = N_2 \left(n_{12} + 1/N_Z\right)$$

electrons is

$$\frac{(N_Z g_{12})!}{(N_2(g_{12}-n_{12}))!\,(N_2(n_{12}))!} \times \frac{N_2 m_{12}}{(N_2(n_{12}+\delta n_{12}))} = \frac{[N_2(g_{12}+\delta g_{12})]!}{(N_2(g_{12}+\delta g_{12}-n_{12}-\delta n_{12}))!\,(N_2(n_{12}+\delta n_{12}))!} \qquad (A.13)$$

Using Stirlings formula for the factorials of large numbers we have

$$\begin{aligned} &N_Z g_{12} \log N_Z g_{12} - N_Z g_{12} - N_2 (g_{12}-n_{12}) \log N_2 (g_{12}-n_{12}) + N_2 (g_{12}-n_{12}) \\ &\qquad + \log N_Z m_{12} \qquad\qquad (A\,14) \\ &= N_Z (g_{12}+\delta g_{12}) \log N_2 (g_{12}+\delta g_{12}) - N_2 (g_{12}+\delta g_{12}) \\ &- N_2 (g_{12}+\delta g_{12}-n_{12}-\delta n_{12}) \log N_2 (g_{12}+\delta g_{12}-n_{12}-\delta n_{12}) + N_2 (g_{12}+\delta g_{12}-n_{12}-\delta n_{12}) \end{aligned}$$

Retaining terms in δn_{12} and δg_{12} to first order only we obtain

$$\frac{\delta g_{12}}{\delta n_{12}} = \frac{\log\left(\frac{g_{12}-n_{12}}{m_{12}}\right)}{\log\left(\frac{g_{12}-n_{12}}{g_{12}}\right)} \quad \text{where} \qquad (A.15)$$

m_{iz} is the average number of states available in the level i. When $m_{12} = g_{12} - n_{12}$, that is, any state which is not occupied is available, then $\delta g_{12}/\delta n_{12}$ is zero and g_{iz} is a constant as in the usual statistics. If $g_{iz,max}$ is the maximum degeneracy of level i can have and the n_{iz} are such that a fraction u are not full with an average number q_i, and a fraction (1-u) are full with an average number p_i of electrons then

$$m_{12} = f_{12}\, u\, (g_{12max} - q_i)$$
$$n_{12} = f_{12}(1-u)p_i + f_{12} u q_i \qquad (A\ 16)$$

Eliminating u

$$m_{12} = \frac{(g_{12max} - q_i)(p_i f_{12} - n_{12})}{(p_i - q_i)}$$

If we insert this expression for m_{iz} in (A15) and change to new variables

$$G_{12} = g_{12}/f_{12}$$

$$N_{12} = n_{12}/f_{12}$$

then f_{iz} depends only on the occupation numbers n_{jz}, and hence

$$\frac{\partial G_{12}}{\partial N_{12}} = \log\left(\frac{(G_{12}-N_{12})(p-q)}{(g_{12max}-q)(p-N_{12})} \Big/ \log\left(\frac{G_{12}-N_{12}}{G_{15}}\right)\right) \qquad (A\ 18)$$

When the n_{iz} becomes so large that the ith levels are largely filled up then in general few of the remaining atoms will still be able to take more than one electron in the level so that

$$q \sim p-1$$

In this case (A18) may be integrated to give G_{12} as a function of N_{12}. When $N_{12}=1$, then $N_2 G_{12}$ is equal to the number of ways of choosing one state from all the available states so that

$$N_2 G_{12} = N_2\, g_{12max}$$

A solution giving this boundary condition is

$$F(g_{12max}) - F(g_{12max}+1-p_1) - F(p_1-N_{12}) + (N_{12}+1-p_1)\log(g_{12max}+1-p_1)$$

$$= F(G_{12}) - F(G_{12}-N_{12}) \qquad (A.19)$$

where $F(y) = y\log y$

If we partly ignore the dependence of g_{12} on the average occupation numbers of the other levels by taking f_{12} to be constant, hence neglecting the small changes in f_{12} and p_1 for small changes in the n_{j2}, so that

$$\frac{\partial g_{12}}{\partial n_{j2}} = 0 \qquad i \neq j$$

then

$$g_{12} = f_{12}\, G_{12} \quad \text{with } G_{12} \text{ given by (A.19)} \qquad (A.20)$$

$$\& \quad C_1 = \frac{\partial G_{12}}{\partial N_{12}} \log\left(\frac{G_{12}-N_{12}}{G_{12}}\right) = \log\left(\frac{(G_{12}-N_{12})}{(g_{12max}+1-p_1)(p_1-n_{12})}\right)$$

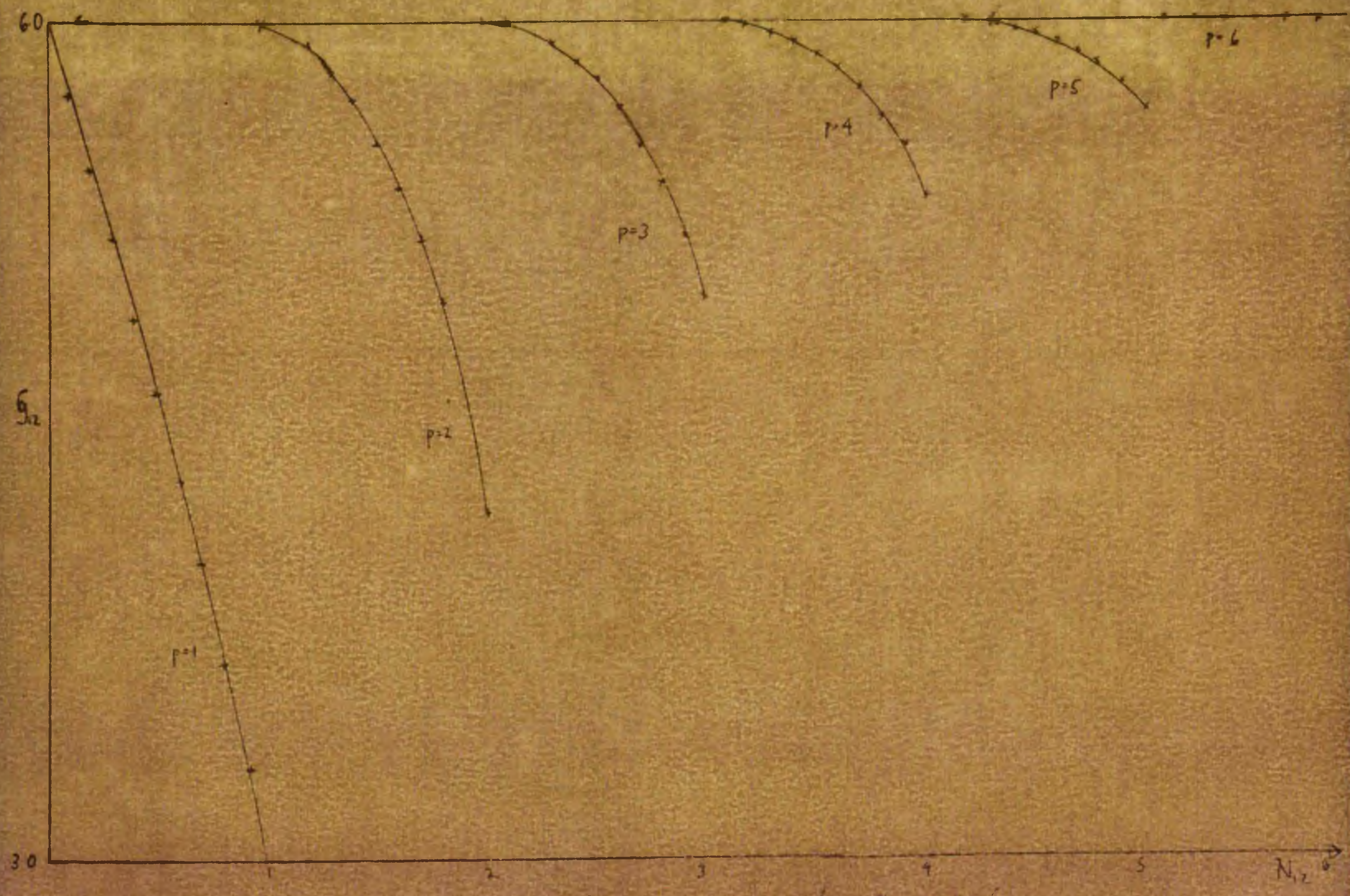

Fig. A.A. Effective degeneracy function for values of p=1 to 6 for $g_{12,max} = 6$.

As n_{iZ} tends to p_i this expression for C_i becomes infinite unless simultaneously n_{iZ} tends to G_{iZ}, the degenerate case. When $p_i=g_{iZ,max}$ then $G_{iZ}=g_{iZ,\ max}$ and C_i is zero corresponding to the usual statistics.

Hence the tightly bound electron levels are unaffected by these considerations and since the unoccupied continuum states are also all always available $p=g_{iZ},$ max for these too. However for levels in the transition regions which can not take the full $g_{iZ,max}$ electrons and remain stable, then C_i and G_{iZ} will vary. The graphs (A.A) show the effective degeneracy G_{iZ} as a function of N_{iZ} in the case $g_{iZ,max}=6$ for the integral values of p_i from one to six. In each graph G_{iZ} drops steeply as the occupation number tends to the maximum value p_i.

APPENDIX B. THE EXPONENTIAL INTEGRALS

The exponential integrals $E_n(x)$ for $x \geqslant 0$ are defined by

$$E_n(x) = \int_x^\infty \frac{e^{-t}}{t^n}\,dt$$

They are required for n=1 in the evaluation of the inelastic collision rate and the natural broadening.

For values of x less than 1 the power series expansion in x for $E_1(x)$ is convergent

$$E_1(x) = -\gamma - \log x - \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{n.n!}$$

For values of $x \geqslant 1$ the function $x.e^x.E_1(x)$ may be approximated as the ratio of two polynomials in x. Accuracy to within 2.10^{-8} may be obtained using polynomials of degree four

$$x e^x E_1(x) = \frac{x^4 + a_1 x^3 + a_2 x^2 + a_3 x + a_4}{x^4 + b_1 x^3 + b_2 x^2 + b_3 x + b_4} + \varepsilon(x) \; ; \quad |\varepsilon(x)| < 2.10^{-8}.$$

The coefficients are taken from Abramowitz and Stegun, Ref 1 - P.231

$a_1 = 8.5733287401$ $b_1 = 9.5733223454$

$a_2 = 18.0590160730$ $b_2 = 25.6329561486$

$a_3 = 8.6347608925$ $b_3 = 21.0996530877$

$a_4 = .2677737343$ $b_4 = 3.9584969228$

The integrals required in equation (4.111)

$$\int_{x_c}^{\infty} \frac{I(x)}{x^4}\,dx = \frac{1}{8}\int_{T}^{\infty} \frac{e^{-t}E_1(t)\,dt}{t^4} \qquad \text{where} \quad T = \frac{x_c}{2}$$

may be expressed in terms of $E_1(T)$ and $E_1(2T)$ using the recurrence relation

$$E_{n+1}(x) = \frac{1}{n}\left[\frac{e^{-x}}{x^n} - E_n(x)\right]$$

and integration by parts. The result is

$$\frac{1}{8}\int_{T}^{\infty} \frac{e^{-t}E_1(t)}{t^4}\,dt = \frac{1}{8}\left\{ \frac{e^{-T}E_1(T)}{3T}\left[\frac{1}{T^2} - \frac{1}{2T} + \frac{1}{2}\right] - \frac{e^{-2T}}{9T}\left[\frac{1}{T^2} - \frac{7}{4T} + 5\right] \right.$$
$$\left. - \frac{1}{12}\left[E_1(T)\right]^2 + \frac{10}{9}E_1(2T) \right\}$$

Ref:- 1956. Abramowitz and Stegun. Handbook of Mathematical Functions. Dover. P.231

APPENDIX C. THE EVALUATION OF THE INTEGRALS FOR THE LINE HALF WIDTHS IN THE IMPACT APPROXIMATION

The total phase shifts produced by a perturber of charge Z_{11} with velocity V and impact parameter ρ, may be written in the form

$$\Delta\varphi_{J,\rho,V,Z_1} = \frac{\alpha_r C_J}{V\rho^{r-1}}$$

where

$$\alpha_r = \frac{\sqrt{\pi}\,\Gamma\left(\frac{r-1}{2}\right)}{\Gamma(r/2)}$$

and C_j is a constant.

This leads to a half width for the elastic impacts for the line k, a, given by

$$\frac{w_{i,el}}{2\pi} = \sum_{Z} \iint d\rho\, dV\, 2\pi\rho\, V n(V,Z_1)\left(1 - \cos\left(\frac{\alpha_r (C_a - C_k)}{V\rho^{r-1}}\right)\right)$$

$n(V,Z_1)$ is the number density of perturbers of charge Z_1 with velocity V relative to the nucleus of the perturbed ion Z, where the velocity distribution is assumed Maxwellian.

$$n(V,Z_1) = N_{Z_1} \times n_{Z_1}(v)$$

$$n_{Z_1}(v) = \frac{\pi}{2}\left(\frac{2M_{Z_1}'}{\pi kT}\right) V^2 e^{-M_{Z_1}'V^2/2kT} \quad , \quad M_{Z_1}' = \frac{M_{Z_1} M_2}{M_{Z_1} + M_2}$$

and N_{Z_1} = number of particles per cc. of charge Z_1.

To evaluate the integrals for each charge Z_1 put

$$I_1 = \int_0^\infty \int_0^\infty dV\, d\rho\, 2\pi\rho\, V n_{Z_1}(V)\left(1 - \cos\left(\frac{\alpha_r (C_a - C_k)}{V\rho^{r-1}}\right)\right)$$

and make the change of variable

$$t = \frac{\alpha_r (C_a - C_k)}{V\rho^{r-1}}$$

Then

$$\bar{I}_1 = \int_{V=0}^\infty \left(\frac{\alpha_r (C_a - C_k)}{V}\right)^{2/1-r} V n_{Z_1}(v)\, \frac{2\pi}{r-1} \int_{t=0}^\infty (1-\cos t)\, t^{-\alpha}\, dt$$

where $\alpha = 1 + 2/r-1$

$$\int_{t=0}^\infty (1-\cos t)\, t^{-\alpha}\, dt = \left[(1-\cos t)\frac{t^{1-\alpha}}{1-\alpha}\right]_0^\infty - \int_0^\infty \sin t \cdot \frac{t^{1-\alpha}}{1-\alpha}\, dt$$

$$= -\frac{1}{1-\alpha}\, \Gamma(2-\alpha) \sin\left((2-\alpha)\pi/2\right) \quad \text{if } 1 < 2-\alpha < 3$$

since $\int_0^\infty \sin t \cdot t^{z-1}\, dt = \Gamma(z) \sin\frac{\pi z}{2}$

Hence

$$\bar{I}_1 = \int_{V=0}^\infty \left(\frac{\alpha_r (C_a - C_k)}{V}\right)^{2/r-1} V n_{Z_1}(v)\, \frac{2\pi}{2} \cdot \Gamma\left(\frac{r-3}{r-1}\right) \cos\frac{\pi}{r-1}$$

Similarly the shift $\frac{\omega_{2,el}}{2\pi}$ is

$$\frac{\omega_{2,el}}{2\pi} = \sum_{Z_1} \iint dV\, d\rho\, 2\pi\rho\, V n(Z_1, V) \sin\left(\frac{\alpha_r (C_a - C_k)}{V\rho^{r-1}}\right)$$

$$= \sum_{Z_1} N_{Z_1} (\bar{I}_2)_{Z_1}$$

where

$$\left(\bar{I}_2\right)_{Z_1} = \int_{V=0}^{\infty} \left(\frac{\alpha_r (C_a - C_k)}{V}\right)^{2/r-1} V n_{Z_1}(V)\, 2\pi\, \Gamma\left(\tfrac{r-3}{r-1}\right) \sin\tfrac{\pi}{r-1}\, dV$$

Using

$$\int_{V=0}^{\infty} V^{\frac{r-3}{r-1}} n_{Z_1}(V)\, V\, dV = \frac{2}{\sqrt{\pi}} \left(\frac{2kT}{M_2'}\right)^{\frac{r-3}{2(r-1)}} \Gamma\left(\tfrac{2r-3}{r-1}\right)$$

$$\frac{w_1 u}{2\pi} = \sum_{Z_1} N_{Z_1} \frac{2}{\sqrt{\pi}} \left(\frac{2kT}{M_2'}\right)^{\frac{r-3}{2(r-1)}} \Gamma\left(\tfrac{r-3}{r-1}\right) \cos\tfrac{\pi}{r-1} (\alpha_r)^{2/3} (C_a - C_k)^{2/3} \Gamma\left(\tfrac{2r-3}{2r-1}\right)$$

$$= \sum_{Z_1} N_{Z_1} \frac{2\sqrt{\pi}\cdot 4\pi}{3\sqrt{3}} \left(\frac{2kT}{M_2'}\right)^{1/6} \left(\frac{\pi}{2}\right)^{2/3} (C_a - C_k)^{2/3} \quad \text{if } r=4$$

since $\Gamma(\frac{1}{3})\Gamma(5/3) = 2/3\, \Gamma(1/3)\Gamma(2/3) = \frac{2\pi}{3\sin\pi/3} = \frac{4\pi}{3\sqrt{3}}.$

This is the formula (4.128).

APPENDIX D. TABLES

Table A - Slater Screening Constants

Table B - Fermi-Dirac Functions

Table C - Free-free Gaunt Factors

Table D - Bound-free Gaunt Factors

Table E - Hydrogenic Oscillator Strengths

Table F - Voigt Function

	1	2	3	4	5	6
1	.625005	.209881	.242803	.099442	.108831	.111028
2	.209881	.150395	.162114	.084119	.090017	.103583
3	.242803	.162114	.181645	.086761	.093949	.106336
4	.099442	.084119	.086761	.066411	.068798	.073139
5	.108831	.090017	.093949	.068798	.071873	.076936
6	.111028	.103583	.106336	.073139	.076936	.086051
7	.057638	.051356	.052406	.044911	.045701	.047171
8	.061521	.053998	.055522	.046516	.047498	.049130
9	.062455	.059079	.060264	.049875	.050874	.053301
10	.062504	.062127	.062296	.055961	.057114	.059403
11	.037520	.034346	.034871	.031193	.031572	.032278
12	.039495	.035728	.036481	.032098	.032565	.033339
13	.039976	.038209	.038816	.033895	.034358	.035457
14	.040004	.039735	.039853	.036524	.037053	.038195
15	.040005	.039993	.039999	.039302	.039471	.039751

TABLE A SLATER SCREENING CONSTANTS $\sigma_{nl,n'l'}/a^2$

	7	8	9	10	11	12	13	14	15
1	.057638	.061521	.062455	.062504	.037520	.039495	.039976	.040004	.040005
2	.051356	.053998	.059079	.062127	.034346	.035728	.038209	.039735	.039993
3	.052406	.055522	.060264	.062296	.034871	.036481	.038816	.039853	.039999
4	.044911	.046516	.049875	.055961	.031193	.032098	.033895	.036524	.039302
5	.045701	.047498	.050874	.057114	.031572	.032565	.034358	.037053	.039471
6	.047171	.049130	.053301	.059403	.032278	.033339	.035457	.038195	.039751
7	.037277	.038043	.039474	.041476	.027816	.028411	.029618	.031606	.034560
8	.038043	.038940	.040515	.042678	.028132	.028772	.030001	.032013	.035099
9	.039474	.040515	.042678	.045322	.028729	.029413	.030820	.032857	.036201
10	.041476	.042678	.045322	.050231	.029587	.030318	.031855	.034374	.037887
11	.027816	.028132	.028729	.029587	.023831	.024148	.024749	.025602	.026679
12	.028411	.028772	.029413	.030318	.024148	.024501	.025145	.026045	.027173
13	.029618	.030001	.030820	.031855	.024749	.025145	.025936	.026964	.028221
14	.031606	.032013	.032857	.034374	.025602	.026045	.026964	.028418	.029989
15	.034560	.035099	.036201	.037887	.026679	.027173	.028221	.029989	.032957

TABLE A. SLATER GREENIAN [illegible]

	$2/3XF_{3/2}$	$F_{1/2}$		$2/3XF_{3/2}$	$F_{1/2}$
0.0	.768 536	.678 094	2.0	.117 200	.114 588
0.1	.703 351	.626 152	2.1	.106 273	.104 116
0.2	.643 197	.577 470	2.2	.096 347	.094 566
0.3	.587 752	.531 931	2.3	.087 332	.085 864
0.4	.536 710	.489 414	2.4	.079 148	.077 938
0.5	.489 773	.449 793	2.5	.071 720	.070 724
0.6	.446 659	.412 937	2.6	.064 981	.064 161
0.7	.407 098	.378 714	2.7	.058 868	.058 194
0.8	.370 833	.346 989	2.8	.053 324	.052 770
0.9	.337 621	.317 630	2.9	.048 298	.047 842
1.0	.307 232	.290 501	3.0	.043 741	.043 366
1.1	.279 451	.265 471	3.1	.039 611	.039 303
1.2	.254 073	.242 410	3.2	.035 868	.035 615
1.3	.230 907	.221 193	3.3	.032 476	.032 269
1.4	.209 777	.201 696	3.4	.029 404	.029 233
1.5	.190 515	.183 802	3.5	.026 620	.026 480
1.6	.172 967	.167 397	3.6	.024 099	.023 984
1.7	.156 989	.152 373	3.7	.021 816	.021 721
1.8	.142 449	.138 627	3.8	.019 748	.019 670
1.9	.129 224	.126 063	3.9	.017 875	.017 812
			4.0	.016 179	.016 128

TABLE B FERMI-DIRAC FUNCTIONS

$\log_{10} \gamma^2$ u	-3.00	-2.75	-2.50	-2.25	-2.00	-1.75	-1.50
.0001	5.52	5.51	5.51	5.50	5.49	5.48	5.46
.0003	4.91	4.91	4.91	4.90	4.89	4.88	4.86
.0010	4.25	4.25	4.25	4.24	4.24	4.22	4.20
.0030	3.65	3.65	3.65	3.65	3.64	3.63	3.62
.0100	3.01	3.01	3.01	3.01	3.01	3.00	2.99
.0300	2.43	2.44	2.44	2.45	2.45	2.46	2.45
.1000	1.83	1.84	1.85	1.87	1.88	1.90	1.91
.3000	1.33	1.35	1.36	1.38	1.41	1.44	1.47
.5000	1.13	1.14	1.16	1.18	1.21	1.25	1.28
1.0000	.88	.89	.91	.93	.96	1.00	1.05
1.5000	.75	.76	.78	.80	.84	.88	.92
2.0000	.66	.68	.69	.72	.75	.79	.84
3.0000	.56	.57	.59	.62	.64	.68	.73
4.0000	.49	.50	.52	.54	.57	.61	.65
5.0000	.45	.46	.47	.49	.52	.56	.60
6.0000	.41	.42	.43	.45	.48	.52	.56
7.0000	.38	.39	.40	.43	.45	.49	.53
8.0000	.36	.37	.38	.40	.43	.46	.50
9.0000	.34	.35	.36	.38	.40	.44	.47
10.0000	.32	.33	.34	.36	.39	.42	.45
11.0000	.31	.32	.33	.35	.37	.40	.44
12.0000	.30	.31	.32	.33	.35	.38	.42
13.0000	.29	.30	.30	.32	.34	.37	.41
14.0000	.28	.28	.29	.31	.33	.36	.39
15.0000	.27	.27	.28	.30	.32	.35	.38
16.0000	.26	.27	.28	.29	.31	.34	.37
17.0000	.25	.26	.27	.28	.30	.33	.36
18.0000	.24	.25	.26	.28	.29	.32	.35
19.0000	.24	.24	.25	.27	.29	.31	.34
20.0000	.23	.24	.25	.26	.28	.31	.34

TABLE C Temperature averaged free free Gaunt factors $u = \frac{h\nu}{kT}$, $\gamma^2 = \frac{Z^2 R_y}{kT}$

	-1.00	-.50	0.00	.50	1.00	2.00	3.00
.0001	5.37	5.23	5.00	4.74	4.43	3.82	3.21
.0003	4.77	4.64	4.41	4.15	3.85	3.27	2.72
.0010	4.13	3.99	3.78	3.53	3.24	2.70	2.20
.0030	3.55	3.42	3.22	2.99	2.72	2.23	1.81
.0100	2.94	2.83	2.65	2.44	2.21	1.80	1.49
.0300	2.42	2.34	2.19	2.02	1.82	1.51	1.28
.1000	1.92	1.88	1.78	1.65	1.50	1.28	1.15
.3000	1.53	1.55	1.50	1.41	1.31	1.16	1.08
.5000	1.37	1.42	1.40	1.34	1.25	1.13	1.06
1.0000	1.17	1.26	1.29	1.26	1.19	1.10	1.04
1.5000	1.05	1.17	1.24	1.22	1.17	1.09	1.04
2.0000	.98	1.11	1.20	1.20	1.16	1.08	1.04
3.0000	.87	1.02	1.15	1.17	1.15	1.08	1.04
4.0000	.80	.96	1.11	1.16	1.14	1.07	1.03
5.0000	.74	.91	1.08	1.14	1.14	1.07	1.03
6.0000	.70	.87	1.05	1.13	1.13	1.07	1.03
7.0000	.66	.84	1.03	1.12	1.13	1.07	1.03
8.0000	.63	.81	1.00	1.11	1.13	1.08	1.03
9.0000	.61	.78	.98	1.10	1.13	1.08	1.04
10.0000	.58	.76	.97	1.09	1.12	1.08	1.04
11.0000	.56	.74	.95	1.08	1.12	1.08	1.04
12.0000	.55	.72	.93	1.07	1.12	1.08	1.04
13.0000	.53	.70	.92	1.06	1.12	1.08	1.04
14.0000	.52	.69	.91	1.06	1.12	1.08	1.04
15.0000	.50	.67	.89	1.05	1.11	1.08	1.04
16.0000	.49	.66	.88	1.04	1.11	1.08	1.04
17.0000	.48	.64	.87	1.03	1.11	1.08	1.04
18.0000	.47	.63	.86	1.03	1.11	1.08	1.04
19.0000	.46	.62	.85	1.02	1.11	1.08	1.04
20.0000	.45	.61	.84	1.01	1.10	1.08	1.04

TABLE C Temperature averaged free-free Gaunt factors (cont

BOUND-FREE GAUNT FACTORS

$n = 1, n = 2$

Electron Energy, E/Z^2R_y	Photon Energy, $h\nu/Z^2R_y$	Level, $1s$	Photon Energy, $h\nu/Z^2R_y$	Level $2s$	Level $2p$	$\bar{g}$
	$n = 1$		$n = 2$			
1000 (13)*	1000 (13)	6928 (−5)	1000 (13)	2771 (−4)	6928 (−17)	6928 (−5)
1111 (12)	1111 (12)	2078 (−4)	1111 (12)	8314	1871 (−15)	2078 (−4)
1000 (11)	1000 (11)	6928	1000 (11)	2771 (−3)	6928 (−14)	6928
1111 (10)	1111 (10)	2078 (−3)	1111 (10)	8313	1870 (−12)	2078 (−3)
1000 (9)	1000 (9)	6926	1000 (9)	2770 (−2)	6926 (−11)	6926
1111 (8)	1111 (8)	2076 (−2)	1111 (8)	8306	1869 (−9)	2076 (−2)
1000 (7)	1000 (7)	6906	1000 (7)	2763 (−1)	6906 (−8)	6906
1111 (6)	1111 (6)	2059 (−1)	1111 (6)	8236	1853 (−6)	2059 (−1)
4000 (5)	4000 (5)	3410	4000 (5)	1364 (0)	8525	3410
2041	2041	4745	2041	1898	2325 (−5)	4745
1000	1000	6715	1000	2686	6714	6715
4444 (4)	4445 (4)	9917	4445 (4)	3966	2231 (−4)	9918
2500	2501	1302 (0)	2500	5207	5206	1302 (0)
1111	1112	1894	1111	7572	1703 (−3)	1894
4000 (3)	4010 (3)	2971	4002 (3)	1187 (1)	7411	2972
2041	2051	3918	2043	1565	1912 (−2)	3923
1000	1010	5129	1002	2042	5087	5142
4444 (2)	4544 (2)	6687	4469 (2)	2645	1477 (−1)	6724
2500	2600	7800	2525	3059	3019	7875
1600	1700	8585	1625	3331	5100	8711
1111	1211	9129	1136	3497	7642	9316
6250 (1)	7250 (1)	9729	6500 (1)	3612	1373 (0)	1006 (1)
4000	5000	9939	4250	3553	2055	1043
2778	3778	9948	3028	3408	2752	1058
2041	3041	9856	2291	3225	3425	1063
1562	2562	9721	1812	3031	4045	1062
1235	2235	9571	1485	2842	4607	1056
1000	2000	9423	1250	2664	5106	1049
6944 (0)	1694	9157	9444 (0)	2334	5925	1035
4444	1444	8850	6944	2000	6784	1009
2500	1250	8531	5000	1626	7587	9755 (0)
1111	1111	8246	3611	1279	8192	9342
4000 (−1)	1040	8076	2900	1067	8459	9011
2041	1020	8026	2704	1003	8518	8896
1000	1010	7999	2600	9686 (0)	8549	8830
4444 (−2)	1004	7985	2541	9498	8558	8793
2500	1002	7980	2525	9431	8562	8779
1111	1001	7976	2511	9384	8565	8770
1000 (−3)	1000	7973	2501	9349	8567	8763
1111 (−4)	1000	7973	2500	9346	8567	8761
1000 (−5)	1000	7973	2500	9346	8567	8761
1111 (−6)	1000	7973	2500	9346	8567	8761
1000 (−7)	1000	7973	2500	9346	8567	8761
1111 (−8)	1000	7973	2500	9346	8567	8761
1000 (−9)	1000	7973	2500	9346	8567	8761
1111 (−10)	1000	7973	2500	9346	8567	8761
1000 (−11)	1000	7973	2500	9346	8567	8761
1111 (−12)	1000	7973	2500	9346	8567	8761
1000 (−13)	1000	7973	2500	9346	8567	8761
1111 (−14)	1000	7973	2500	9346	8567	8761
1000 (−15)	1000	7973	2500	9346	8567	8761

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

Table D P1

n = 3

Electron Energy, E/Z^2R_y	Photon Energy, $h\nu/Z^2R_y$	Level			Σ
		3s	3p	3d	
1000 (15)*	1000 (15)	6235 (−4)	1848 (−16)	1369 (−29)	6928 (−5)
1111 (12)	1111 (12)	1071 (−3)	4988 (−15)	5326 (−27)	2078 (−4)
1000 (11)	1000 (11)	6235	1847 (−13)	1368 (−24)	6928
1111 (10)	1111 (10)	1070 (−2)	4988 (−12)	5325 (−22)	2078 (−3)
1000 (9)	1000 (9)	6233	1847 (−10)	1368 (−19)	6926
1111 (8)	1111 (8)	1069 (−1)	4984 (−9)	5322 (−17)	2076 (−2)
1000 (7)	1000 (7)	6216	1842 (−7)	1364 (−14)	6906
1111 (6)	1111 (6)	1055 (0)	4942 (−6)	5294 (−12)	2059 (−1)
4000 (5)	4000 (5)	5069	2273 (−5)	4210 (−11)	5410
2041	2041	4270	6199	2250 (−10)	4745
1000	1000	6043	1790 (−4)	1326 (−9)	6715
4444 (4)	4443 (4)	8924	5949	9915	9918
2500	2500	1171 (1)	1388 (−3)	4113 (−8)	1302 (0)
1111	1111	1704	4541	3027 (−7)	1894
4000 (3)	4001 (3)	2670	1976 (−2)	3658 (−6)	2973
2041	2042	3516	5097	1849 (−5)	3924
1000	1001	4589	1355 (−1)	1003 (−4)	5144
4444 (2)	4456 (2)	5939	3930	6542	6731
2500	2511	6858	8022	2372 (−3)	7889
1600	1611	7455	1552 (0)	6239	8735
1111	1122	7804	2021	1540 (−2)	9552
6250 (1)	6361 (1)	8009	3608	4236	1015 (1)
4000	4111	7818	5557	9765	1055
2778	2889	7420	7101	1849 (−1)	1072
2041	2152	6954	8732	5064	1081
1562	1673	6458	1019 (1)	4611	1083
1235	1346	5976	1144	6460	1081
1000	1111	5524	1249	8563	1078
6944 (0)	8056 (0)	4756	1402	1332 (0)	1068
4444	5556	3834	1523	2107	1051
2500	3611	2875	1559	3332	1024
1111	2222	1976	1454	5059	9854 (0)
4000 (−1)	1511	1416	1277	6551	9458
2041	1315	1246	1199	7042	9293
1000	1211	1155	1150	7555	9189
4444 (−2)	1156	1102	1122	7495	9128
2500	1136	1085	1111	7552	9105
1111	1122	1072	1104	7593	9089
1000 (−3)	1112	1062	1098	7623	9076
1111 (−4)	1111	1062	1098	7626	9075
1000 (−5)	1111	1062	1098	7626	9075
1111 (−6)	1111	1062	1098	7626	9075
1000 (−7)	1111	1062	1098	7626	9075
1111 (−8)	1111	1062	1098	7626	9075
1000 (−9)	1111	1062	1098	7626	9075
1111 (−10)	1111	1062	1098	7626	9075
1000 (−11)	1111	1062	1098	7626	9075
1111 (−12)	1111	1062	1098	7626	9075
1000 (−13)	1111	1062	1098	7626	9075
1111 (−14)	1111	1062	1098	7626	9075
1000 (−15)	1111	1062	1098	7626	9075

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

Table D P2

n = 4

Electron Energy, E/Z²R_y	Photon Energy, hν/Z²R_y	Level				4
		4s	4p	4d	4f	
1000 (13)*	1000 (13)	1109 (−3)	3464 (−16)	3464 (−29)		6928 (−5)
1111 (12)	1111 (12)	3326	9353 (−15)	8418 (−27)		2078 (−4)
1000 (11)	1000 (11)	1108 (−2)	3464 (−13)	3464 (−24)	1133 (−35)	6928
1111 (10)	1111 (10)	3325	9352 (−12)	8417 (−22)	2329 (−32)	2078 (−3)
1000 (9)	1000 (9)	1108 (−1)	3463 (−10)	3463 (−19)	1134 (−28)	6926
1111 (8)	1111 (8)	3322	9344 (−9)	8410 (−17)	2323 (−25)	2076 (−2)
1000 (7)	1000 (7)	1105 (0)	3453 (−7)	3453 (−14)	1131 (−21)	6906
1111 (6)	1111 (6)	3294	9265 (−6)	8339 (−12)	2302 (−18)	2059 (−1)
4000 (5)	4000 (5)	5436	4263 (−5)	1066 (−10)	8881 (−17)	3410
2041	2041	7591	1162 (−4)	3696	9303 (−16)	4745
1000	1000	1074 (1)	3337	3337 (−9)	1119 (−14)	6715
4444 (4)	4444 (4)	1586	1115 (−3)	2310 (−8)	1882 (−13)	9918
2500	2500	2083	2603	1041 (−7)	1388 (−12)	1302 (0)
1111	1111	3028	8515	7663	2299 (−11)	1894
4000 (3)	4001 (3)	4746	3704 (−2)	9260 (−6)	7715 (−10)	2973
2041	2042	6250	9555	4681 (−5)	7643 (−9)	3924
1000	1001	8156	2540 (−1)	2539 (−4)	8437 (−8)	5145
4444 (2)	4451 (2)	1055 (2)	7364	1633 (−3)	1239 (−6)	6733
2500	2506	1218	1502 (0)	5994	7973	7894
1600	1606	1322	2540	1575 (−2)	3270 (−5)	8745
1111	1117	1383	5778	3381	1009 (−4)	9365
6250 (1)	6312 (1)	1417	6750	1066 (−1)	5629	1015 (1)
4000	4062	1379	9962	2448	2010 (−3)	1036
2778	2840	1306	1316 (1)	4617	5422	1077
2041	2103	1217	1611	7613	1207 (−2)	1087
1562	1625	1123	1871	1140 (0)	2340	1091
1235	1297	1036	2090	1587	4083	1091
1000	1062	9326 (1)	2267	2090	6366	1089
6944 (0)	7569 (0)	8069	2312	3204	1413 (−1)	1082
4444	5069	6397	2667	4945	3238	1069
2500	3125	4614	2617	7469	7987	1047
1111	1736	2929	2240	1033 (1)	1992 (0)	1014
4000 (−1)	1025	1863	1734	1169	3808	9736 (0)
2041	9291 (−1)	1559	1521	1173	4721	9542
1000	7250	1358	1388	1159	5333	9408
4444 (−2)	6694	1259	1311	1146	5708	9323
2500	6500	1225	1283	1140	5848	9291
1111	6361	1200	1263	1133	5950	9267
1000 (−3)	6260	1181	1248	1131	6026	9249
1111 (−4)	6251	1180	1246	1131	6033	9248
1000 (−5)	6250	1179	1246	1131	6034	9247
1111 (−6)	6250	1179	1246	1131	6034	9247
1000 (−7)	6250	1179	1246	1131	6034	9247
1111 (−8)	6250	1179	1246	1131	6034	9247
1000 (−9)	6250	1179	1246	1131	6034	9247
1111 (−10)	6250	1179	1246	1131	6034	9247
1000 (−11)	6250	1179	1246	1131	6034	9247
1111 (−12)	6250	1179	1246	1131	6034	9247
1000 (−13)	6250	1179	1246	1131	6034	9247
1111 (−14)	6250	1179	1246	1131	6034	9247
1000 (−15)	6250	1179	1246	1131	6034	9247

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

Table D P3

n = 5

Electron Energy, E/Z^2Ry	Photon Energy, $h\nu/Z^2Ry$	Level					Σ
		5s	5p	5d	5f	5g	
1000 (13)*	1000 (13)	1732 (−3)	5543 (−16)	6208 (−29)			6928 (−5)
1111 (12)	1111 (12)	5196	1496 (−14)	1508 (−26)			2078 (−4)
1000 (11)	1000 (11)	1732 (−2)	5542 (−13)	6207 (−24)	3027 (−35)		6928
1111 (10)	1111 (10)	5196	1496 (−11)	1508 (−21)	6619 (−32)		2078 (−3)
1000 (9)	1000 (9)	1732 (−1)	5541 (−10)	6206 (−19)	3026 (−28)		6926
1111 (8)	1111 (8)	5191	1495 (−8)	1507 (−16)	6614 (−25)	1020 (−33)	2076 (−2)
1000 (7)	1000 (7)	1727 (0)	5525 (−7)	6188 (−14)	3017 (−21)	5175 (−29)	6906
1111 (6)	1111 (6)	5147	1482 (−5)	1494 (−11)	6558 (−18)	1012 (−24)	2059 (−1)
4000 (5)	4000 (5)	8525	6820	1910 (−10)	2328 (−16)	9977 (−25)	5410
2041	2041	1186 (1)	1060 (−4)	1021 (−9)	2459 (−15)	2048 (−21)	4745
1000	1000	1679	5371	6016	2933 (−14)	3029 (−20)	6715
4444 (4)	4444 (4)	2479	1785 (−3)	4497 (−8)	4934 (−13)	1903 (−18)	9918
2500	2500	3254	4165	1866 (−7)	3639 (−12)	2495 (−17)	1302 (0)
1111	1111	4732	1362 (−2)	1373 (−6)	6026 (−11)	9297 (−16)	1894
4000 (3)	4000 (3)	7415	5927	1659 (−5)	2022 (−9)	8666 (−14)	2973
2041	2041	9765	1529 (−1)	8387	2003 (−8)	1682 (−12)	3924
1000	1000	1274 (2)	4064	4549 (−4)	2217 (−7)	3798 (−11)	5146
4444 (2)	4448 (2)	1648	1178 (0)	2964 (−3)	3247 (−6)	1251 (−9)	6754
2500	2504	1902	2402	1073 (−2)	2088 (−5)	1450 (−8)	7897
1600	1604	2064	4045	2820	8561	9149	8747
1111	1115	2158	6037	6050	2640 (−4)	4059 (−7)	9371
6250 (1)	6290 (1)	2208	1074 (1)	1904 (−1)	1471 (−3)	4009 (−6)	1016 (1)
4000	4040	2146	1588	4568	5245	2225 (−5)	1058
2778	2818	2029	2094	8221	1412 (−2)	8588	1080
2041	2081	1888	2559	1352 (0)	3136	2584 (−4)	1090
1562	1602	1742	2964	2019	6061	6484	1095
1235	1275	1600	3302	2804	1054 (−1)	1418 (−3)	1095
1000	1040	1467	3573	3681	1690	2785	1094
6944 (0)	7344	1255	3935	3603	3610	8425	1089
4444	4844	9689 (1)	4127	8539	8212	2906 (−2)	1078
2500	2900	6845	3960	1258 (1)	1961 (0)	1139 (−1)	1060
1111	1511	4145	3220	1650	4616	5234	1030
4000 (−1)	8000 (−1)	2422	2275	1690	7969	1706 (0)	9925 (0)
2041	6041	1887	1878	1590	9242	2618	9719
1000	5000	1588	1631	1492	9890	3383	9563
4444 (−2)	4444	1424	1488	1421	1018 (1)	3918	9458
2500	4250	1366	1435	1392	1027	4132	9416
1111	4111	1324	1397	1370	1033	4295	9383
1000 (−3)	4010	1293	1369	1354	1036	4418	9361
1111 (−4)	4001	1290	1366	1353	1037	4429	9358
1000 (−5)	4000	1290	1366	1352	1037	4431	9358
1111 (−6)	4000	1290	1366	1352	1037	4431	9358
1000 (−7)	4000	1290	1366	1352	1037	4431	9358
1111 (−8)	4000	1290	1366	1352	1037	4431	9358
1000 (−9)	4000	1290	1366	1352	1037	4431	9358
1111 (−10)	4000	1290	1366	1352	1037	4431	9358
1000 (−11)	4000	1290	1366	1352	1037	4431	9358
1111 (−12)	4000	1290	1366	1352	1037	4431	9358
1000 (−13)	4000	1290	1366	1352	1037	4431	9358
1111 (−14)	4000	1290	1366	1352	1037	4431	9358
1000 (−15)	4000	1290	1366	1352	1037	4431	9358

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

Table D.P4

TABLE E

Bound-bound Oscillator Strengths

$l = 0$

n \ n′l′	2,1	3,1	4,1	5,1	6,1	7,1	8,1	9,1
1	4162 (0)*	7910 (−1)	2899 (−1)	1594 (−1)	7799 (−2)	4184 (−2)	3183 (−2)	2216 (−2)
2	0000	4349 (0)	1028 (0)	4199	.2165 (−1)	.1274 (−1)	8180	5503
3	−.4077 (−1)	0000	.4847	1210 (0)	3139	.2737	1633 (−1)	1086 (−1)
4	−9133 (−2)	−9673 (−1)	0000	.5442	1501 (0)	5963	3227	1980
5	−.3640	−.2220	−1587	0000	.6078	.1549 (0)	6737	3675
6	−1854	−.9097 (−2)	−.3701 (−1)	−.2256	0000	6736	.1713 (0)	7482
7	−1084	−.4736	−1520	−.3240 (−1)	−2902	0000	7406	1881 (0)
8	−6923 (−3)	−.2824	−8047 (−2)	−2180	−6833 (−1)	−.5577	0000	8096
9	−.4711	−.1856	−4850	−1133	−2849	−8446 (−1)	−4259	0000
10	−3357	−.1268	−3106	−7008 (−2)	−.1316	−.3528	−1007	−4946
11	−.2480	−9161 (−3)	−.2222	−.4633	−.9251 (−3)	−.1881	−4212 (−1)	−.1171
12	−1807	−6852	−.1619	−.5252	−6128	−.1149	−2249	−4900 (−1)
13	−1469	−.3268	−.1321	−2504	−4819	−.7647 (−2)	−.1376	−3819
14	−.1167	−.4143	−9439 (−3)	−1808	−.3180	−.3403	−.9178 (−2)	−1694
15	−9453 (−4)	−3321	−7481	−1408	−2421	−3891	−6908	−1078
16	−.7793	−2704	−6042	−.1120	−1895	−3048	−4815	−7999 (−2)

n \ n′l′	10,1	11,1	12,1	13,1	14,1	15,1	16,1	
1	1607 (−2)	1200 (−2)	9214 (−3)	7227 (−3)	.5774 (−3)	4686 (−3)	3836 (−3)	
2	3988	.2932	2248 (−2)	1735 (−2)	1394 (−2)	1127 (−2)	9244	
3	.7594	.5484	.4117	.3173	2502	2009	1650 (−2)	
4	1516 (−1)	9264	6797	5152	4007	3184	.2574	
5	2273	.1324 (−1)	.1081 (−1)	7986	6095	4769	3811	
6	4098	2348	1717	1224 (−1)	9088	6967	5478	
7	8211	4508	2810	1900	.1359 (−1)	1015 (−1)	.7791	
8	.2047 (0)	8951	4807	3065	2076	.1408	.1112 (−1)	
9	8770	.2215 (0)	9645	5508	3513	2248	1614	
10	0000	.9459	2580 (0)	1096 (0)	5689	.3557	2415	
11	−5636	0000	1015 (1)	2546	1106 (0)	6074	3798	
12	−.1535	−.6329	.0000	1084 (1)	2712	1177 (0)	6456	
13	−5590 (−1)	−1300	−7025 (0)	0000	1154 (1)	2878	1247 (0)	
14	−2990	−6282	−.1665	−7719 (0)	.0000	1224 (1)	3045	
15	−1852	−3561 (−1)	−6975 (−1)	−1830	−8416 (0)	0000	1293 (1)	
16	−1225	−.2061	−.3732	−7669 (−1)	−1996	−9114 (0)	0000	

$l = 1$

n \ n′l′	1,0	2,0	3,0	3,2	4,0	4,2	5,0	5,2
2	−1387 (0)	.0000	.1359 (−1)	.6958 (0)	3045 (−2)	.1218 (0)	1213 (−2)	.4457 (−1)
3	−.2637 (−1)	−1450 (0)	0000	0000	3225 (−1)	6183	7428	1592 (0)
4	−9664 (−2)	−5421 (−1)	−1616 (0)	−1032 (−1)	0000	.0000	3291 (−1)	4095
5	−4646	−.1388	−4054 (−1)	−5683 (−2)	−1814 (0)	−.4637 (−1)	0000	0000
6	−2690	−.7210 (−2)	−.1715	−1403	−4894 (−1)	−.9729 (−2)	−2026 (0)	−7959 (−1)
7	−.1605	−.4247	−.9123 (−2)	−7019 (−3)	−1988	−.3790	−5165 (−1)	−1722
8	−1061	−2727	−.5516	−4079	−1076	−1923	−2246	−6804 (−2)
9	−7587 (−3)	−.1061	−3621	−2607	−6599 (−2)	−1135	−.1225	−3491
10	−5551	−.3539	−.2918	−1779	−4589	−7318	−.7578 (−2)	−.2071
11	−4002	−.9040 (−3)	−1828	−1274	−5088	−.5041	−.5080	−1547
12	−3071	−7494	−1572	−.9463 (−4)	−.2266	−3641	−.3602	−9542 (−3)
13	−2409	−5845	−1058	−7258	−.1717	−2726	−2662	−.6787
14	−1925	−4646	−8542 (−3)	−5688	−1536	−2100	−2031	−.5110
15	−.1562	−3756	−6698	−4528	−1081	−1695	−1590	−3956
16	−1285	−3081	−5465	−3678	−8582 (−3)	−1550	−.1270	−.3134

n \ n′l′	6,0	6,2	7,0	7,2	8,0	8,2	9,0	9,2
2	6180 (−3)	.2165 (−1)	3615 (−3)	.1253 (−1)	2508 (−3)	.7736 (−2)	.1570 (−3)	3220 (−2)
3	3032 (−2)	.3614	.1579 (−2)	.2901	9412	.1721 (−1)	6119	1115 (−1)
4	.1234 (−1)	.1483 (0)	.3094	.6235	.2682 (−2)	3350	.1617 (−2)	2081
5	7434	.6247	1749 (−1)	1570 (0)	.7267	6735	.3851	.3636
6	0000	0000	9672	6314	2278 (−1)	1650 (0)	9498	.7212
7	−2245 (0)	−1171	0000	.0000	.1192 (0)	4845	2815 (−1)	1750 (0)
8	−.5718 (−1)	−2564 (−1)	−2489 (0)	−1564	0000	0000	.1430 (0)	7210
9	−2404	−1023	−6271 (−1)	−5488 (−1)	−2695	−.1975	0000	0000
10	−1566	−5283 (−2)	−.2737	−.1593	−6825 (−1)	−4615 (−1)	−2025	−2394
11	−8495 (−2)	−.3152	−1502	−7250 (−2)	−2977	−.1782	−7870 (−1)	−3896 (−1)
12	−5725	−2080	−.9568 (−2)	−.4551	−1636	−9287 (−2)	−.5215	−.2186
13	−4079	−1488	−6554	−.3042	−.1022	−5580	−.1767	−.1542
14	−.3029	−1087	−4950	−1986	−6921 (−2)	−3671	−.1104	−6870 (−2)
15	−2522	−7918 (−3)	−.3976	−.1434	−4861	−.2572	−7482 (−2)	−.4333
16	−.1826	−.6154	−.2597	−.1102	−.3707	−1888	−.3379	−.3186

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

TABLE E—continued

$l = 1$

n \ v'F	10,0	10,2	11,0	11,2	12,0	12,2	13,0
2	.1119 (−3)*	.3695 (−2)	.8860 (−4)	.2714 (−3)	.6280 (−4)	.2094 (−2)	.4050 (−6)
3	.4227	.7606	.3054 (−3)	.5545	.2286 (−5)	.4140	.1736 (−5)
4	.1062 (−1)	.1533 (−1)	.7405	.9529	.3590	.6015	.4070
5	.2356	.2240	.1566 (−2)	.1501 (−1)	.1086 (−2)	.1061 (−1)	.7947
6	.3052	.3940	.3077	.2440	.2043	.1643	.1400 (−2)
7	.1176 (−1)	.7635	.6270	.4203	.3029	.2680	.2549
8	.3557	.1046 (0)	.1004 (−1)	.8091	.7027	.4457	.4506
9	.1640 (0)	.7600	.9902	.1944 (0)	.1635 (−1)	.8529	.8729
10	.0000	.0000	.1879 (0)	.8000	.4438	.2044 (0)	.1063 (−1)
11	−.3155	−.2825	.0000	.0000	.2110 (0)	.8427	.3800
12	−.7952 (−1)	−.6996 (−1)	−.3583	−.3259	.0000	.0000	.2941 (0)
13	−.3452	−.2601	−.8406 (−1)	−.7416 (−1)	−.3634	−.3699	.0000
14	−.1096	−.1562	−.3607	−.3023	−.9040 (−1)	−.8430 (−1)	−.3046
15	−.1186	−.8215 (−2)	−.2025	−.1306	−.3922	−.3432	−.9593 (−1)
16	−.8051 (−2)	−.3425	−.1266	−.9580 (−2)	−.2132	−.1019	−.4157

n \ v'F	13,2	14,0	14,2	15,0	15,2	16,0	16,2
2	.1596 (−2)	.3092 (−4)	.1263 (−2)	.5144 (−4)	.1020 (−2)	.2370 (−4)	.8347 (−3)
3	.3180	.1381 (−3)	.2409	.1107 (−3)	.2081	.5015	.1629 (−2)
4	.5148	.3155	.3995	.2497	.3166	.2014 (−3)	.2535
5	.7818	.6026	.5952	.4009	.4630	.3735	.3718
6	.1109 (−1)	.1060 (−2)	.8670	.8070	.6640	.4018	.5215
7	.1171	.1802	.1266 (−1)	.1330 (−2)	.9482	.1016 (−2)	.7235
8	.2708	.3059	.1890	.2167	.1356 (−1)	.1604	.1013 (−1)
9	.4706	.3546	.2949	.3571	.2004	.2338	.1446
10	.8960	.9865	.4952	.6108	.3107	.4006	.2115
11	.2146 (0)	.2894 (−1)	.9409	.1120 (−1)	.5196	.6070	.3208
12	.8855	.5550	.2250 (0)	.2525	.9832	.1264 (−1)	.5460
13	.0000	.2573 (0)	.9290	.6102	.2854 (0)	.2556	.1090 (0)
14	−.4144	.0000	.0000	.2805 (0)	.9750	.6604	.3408
15	−.9494 (−1)	−.4078	−.4392	.0000	.0000	.3040 (0)	.1017 (1)
16	−.3086	−.1015	−.1033	−.4511	−.5042	.0000	.0000

$l = 2$

n \ v'F	2,1	3,1	4,1	4,3	5,1	5,3	6,1
3	−.4175 (0)	.0000	.1099 (−1)	.1018 (1)	.2210 (−2)	.1566 (0)	.8420 (−3)
4	−.7508 (−1)	−.3710 (0)	.0000	.0800	.2782 (−1)	.8902	.3857 (−2)
5	−.2662	−.8354 (−1)	−.3636 (0)	−.1242 (−1)	.0000	.0000	.4800 (−1)
6	−.1290	−.3568	−.8908 (−1)	−.2216 (−2)	−.5748 (0)	−.5239 (−1)	.0000
7	−.7598 (−2)	−.1741	−.3753	−.7982 (−3)	−.8419 (−1)	−.6205 (−2)	−.9908 (0)
8	−.4654	−.1033	−.1998	−.3802	−.4053	−.2282	−.9940 (−1)
9	−.3132	−.6692 (−2)	−.1212	−.2158	−.2194	−.1118	−.4527
10	−.2216	−.4611	−.8000 (−2)	−.1560	−.1969	−.6425 (−3)	−.2564
11	−.1628	−.3326	−.3397	−.9199 (−4)	−.9085 (−2)	−.4086	−.1466
12	−.1253	−.2484	−.4009	−.6355	−.6564	−.2706	−.9858 (−2)
13	−.9176 (−3)	−.1908	−.3089	−.4855	−.4691	−.1990	−.7014
14	−.7589	−.1499	−.2596	−.3709	−.3571	−.1489	−.5282
15	−.6119	−.1201	−.1899	−.2905	−.2790	−.1143	−.3884
16	−.5088	−.9774 (−3)	−.1533	−.2522	−.2226	−.8998 (−4)	−.3129

n \ v'F	6,3	7,1	7,3	8,1	8,3	9,1	9,3
3	.3589 (−1)	.4212 (−3)	.2539 (−1)	.2408 (−3)	.1442 (−1)	.1566 (−3)	.9094 (−2)
4	.1862 (0)	.2374 (−2)	.7224	.1135 (−2)	.3639	.6797	.2149 (−1)
5	.8445	.1053 (−1)	.1908 (0)	.4082	.8082	.2094 (−2)	.4241
6	.0000	.7024	.8329	.1539 (−1)	.2090 (0)	.6197	.8623
7	−.5788 (−1)	.0000	.0000	.9985	.8393	.2081 (−1)	.2109 (0)
8	−.1149	−.4106 (0)	−.8674 (−1)	.0000	.0000	.1104 (0)	.8558
9	−.4314 (−2)	−.1050	−.1771	−.4326 (0)	−.3181	.0000	.0000
10	−.2141	−.4592 (−1)	−.6754 (−2)	−.1167	−.2463 (−1)	−.4560	−.1515
11	−.1241	−.2522	−.3583	−.4859 (−1)	−.9909 (−2)	−.1186	−.5208 (−1)
12	−.7930 (−3)	−.1572	−.1975	−.2674	−.4796	−.5117 (−1)	−.1249
13	−.3451	−.1063	−.1272	−.1675	−.2815	−.2824	−.6589 (−2)
14	−.3928	−.7597 (−2)	−.8757 (−3)	−.1134	−.1019	−.1770	−.3756
15	−.2940	−.1639	−.6855	−.8136 (−2)	−.1257	−.1208	−.2429
16	−.2267	−.4552	−.4738	−.6081	−.9122 (−3)	−.8646 (−3)	−.1679

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below.

TABLE E—continued

$l = 2$

$n'l'$ / n	10,1	10,3	11,1	11,3	12,1	12,3	13,1		
3	1067 (−3)*	.6881 (−2)	.7643 (−4)	4911 (−2)	.5678 (−4)	3179 (−2)	.4343 (−4)		
4	4391	.1306 (−1)	.3025 (−3)	9337	.2104 (−3)	6881	.1633 (−3)		
5	.1242 (−2)	.2552	.8084	.1677 (−1)	.3605	1171 (−1)	4072		
6	.3170	.4619	1091 (−2)	2824	1256 (−2)	.1878	8613		
7	.8358	.9049	4534	4909	2599	5031	1703 (−2)		
8	.2649 (−1)	.2171 (0)	1070 (−1)	.9451	3372	5157	5548		
9	1456 (0)	.8708	3236	.2242 (0)	.1312 (−1)	9798	6833		
10	0000	0000	1694 (0)	9861	3838	.2318 (0)	1560 (−1)		
11	−.4809	−.1062	0000	0000	1933 (0)	9364	4490		
12	−.1227	−.9994 (−1)	−.9056	−.2221	0000	0000	2220 (0)		
13	−.3581 (−1)	−.1566	−.1288	−.4812 (−1)	−.3313	−.2308	0000		
14	−.2971	−.7906 (−2)	−.5646 (−1)	−.1090	−.1330	−.5693 (−1)	−.5574		
15	−.1864	−.4723	−.5118	−.9716 (−2)	−.3912 (−1)	−.2241	−.1412		
16	−.1269	−.3071	−.1957	−.3763	−.3264	−.1151	−.6179 (−1)		

$n'l'$ / n	13,3	14,1	14,3	15,1	15,3	16,1	16,3		
3	2418 (−2)	.5401 (−4)	1886 (−2)	2717 (−4)	1301 (−2)	2207 (−4)	1216 (−2)		
4	.3148	1260 (−3)	3964	.9932	.5123	7982	2509		
5	.8354	3066	.6466	2374 (−3)	3023	1881 (−3)	3989		
6	1325 (−1)	6285	.9762	4751	7436	3693	5813		
7	2033	1192 (−2)	1443 (−1)	8724	1071 (−1)	6613	.8205 (−1)		
8	3208	.2203	.2163	1344 (−2)	.1343	.1133 (−2)	1131		
9	3984	.4127	.3562	2721	.2278	1911	1633		
10	1016 (0)	.8170	.5601	4929	.3508	.3233	2383		
11	2997	.1814 (−1)	1092 (0)	9514	3812	3748	3647		
12	9689	.5070	2479	2071 (−1)	.1089 (0)	1088 (−1)	6021		
13	.0000	2486 (0)	1003 (1)	3697	2364	2331	1126 (0)		
14	−.2983	0000	0000	2733 (0)	1038 (1)	6329	2648		
15	−.6319 (−1)	−.3838	−.3344 (0)	0000	0000	3025 (0)	1073 (1)		
16	−.2594	−.1478	−.7400 (−1)	−.6104	−.3729 (0)	0000	0000		

$l = 3$

$n'l'$ / n	3,2	4,2	5,2	5,4	6,2	6,4	7,2	7,4	8,2
4	−.7268 (0)	0000	.8871 (−2)	.1546 (1)	.1985 (−2)	1824 (0)	.5644 (−3)	.3838 (−1)	2716 (−3)
5	−.1119	−.6339 (0)	0000	0000	.2528 (−1)	.1183 (1)	.4432 (−2)	2287 (0)	1630 (−2)
6	−.5849 (−1)	−.1390	−.6031 (0)	−.9485 (−2)	0000	0000	.4133 (−1)	1110 (1)	.8205
7	−.1828	−.3160 (−1)	−.1406	−.1509	−.3950 (0)	−.2346 (−1)	0000	0000	.6195 (−1)
8	−.1030	−.2614	−.5775 (−1)	−.9007 (−3)	−.1455	−.4417 (−2)	−.3995 (0)	−.4611 (−1)	.0000
9	−.6453 (−2)	−.1535	−.3029	−.2297	−.6159 (−1)	−.1329	−.1502	−.8436 (−4)	−.6113 (0)
10	−.4543	−.9899 (−2)	−.1823	−.1263	−.3299	−.7184 (−3)	−.6464 (−1)	−.3014	−.1330
11	−.3080	−.6812	−.1198	−.7772 (−4)	−.2017	−.4010	−.3508	−.1441	−.6737 (−1)
12	−.2271	−.4013	−.8566 (−2)	−.3178	−.1342	−.2497	−.2115	−.8139 (−3)	−.3683
13	−.1727	−.3677	−.6110	−.3647	−.9463 (−2)	−.1676	−.1432	−.5109	−.2290
14	−.1547	−.2831	−.4619	−.2679	−.6875	−.1188	−.1032	−.3451	−.1547
15	−.1072	−.2231	−.3588	−.2033	−.5311	−.8776 (−4)	−.7691 (−2)	−.2459	−.1121
16	−.8683 (−3)	−.1792	−.2849	−.1587	−.4133	−.6696	−.5860	−.1824	−.8219 (−2)

$n'l'$ / n	8,4	9,2	9,4	10,2	10,4	11,2	11,4	12,2	12,4
4	2633 (−1)	.1342 (−3)	1437 (−1)	.9713 (−4)	.8979 (−2)	.6571 (−4)	.3981 (−2)	4661 (−4)	4215 (−2)
5	.8450	.7983	.4148	.4389 (−3)	.2386 (−1)	.2919 (−3)	1319 (−1)	.1990 (−3)	.1896 (−1)
6	2433 (0)	.3081 (−2)	.9733	1529 (−2)	.4890	.8867	.2956	.5678	.1922
7	1073 (1)	1363 (−1)	.2338 (0)	.4824	1048 (0)	.2417 (−2)	.3318	1411 (−2)	.3552
8	.0000	.8438	1063 (1)	.1760 (−1)	2601	.6788	1099 (0)	.3425	.5888
9	−.7021 (−1)	0000	0000	1082 (0)	.1063 (1)	.2292 (−1)	2658	.8920	1141 (0)
10	−.1359	−.6277 (0)	−.9693 (−1)	0000	0000	1330 (0)	1076 (1)	.7835 (−1)	.2717
11	−.4076 (−2)	−.1602	−.1903	−.6472	−.1257 (0)	0000	0000	1386 (0)	1093 (1)
12	−.2369	−.6999 (−1)	−.7046 (−2)	−.1636	−.2324 (−1)	−.6689	−.1361 (0)	0000	0000
13	−.1346	−.3846	−.3451	−.7258 (−1)	−.9466 (−2)	−.1712	−.3191 (−1)	−.6921	−.1878 (0)
14	−.8908 (−3)	−.2401	−.1988	−.4801	−.4673	−.7317 (−1)	−.1209	−.1771	−.3894 (−1)
15	−.5776	−.1627	−.1258	−.2503	−.2698	−.4132	−.6013 (−2)	−.7779 (−1)	−.1409
16	−.4132	−.1166	−.8374 (−3)	−.1702	−.1721	−.2605	−.3487	−.4301	−.7443 (−2)

$n'l'$ / n	13,2	13,4	14,2	14,4	15,2	15,4	16,2	16,4	
4	.5468 (−4)	.3895 (−2)	.2848 (−4)	.2589 (−2)	2073 (−4)	1830 (−2)	.1658 (−4)	1436 (−2)	
5	.1427 (−3)	.7428	1063 (−3)	5536	.8167	4252	6427	5547	
6	.5893	1332 (−1)	.2806	.9678	.2100 (−3)	7290	.1620 (−3)	9650	
7	.9083	.2197	6233	1541 (−1)	.4525	1130 (−1)	5599	.8561	
8	.2810 (−2)	.5602	1300 (−2)	2400	.8980	1697	.6316	.2253 (−1)	
9	4528	.6177	2849	5812	1751 (−2)	2558	.1199 (−2)	1070	
10	.1119 (−1)	.1177 (0)	5785	6421	3374	3988	2194	2690	
11	.5437	.2779	1333 (−1)	1211 (0)	.6940	6641	4116	4142	
12	.1849 (0)	.1115 (1)	4039	.2845	1601 (−1)	1244 (0)	.8223	.6847	
13	0000	.0000	2117 (0)	1148 (1)	.4456	2914	1033 (−1)	1277 (0)	
14	−.7165	−.2206 (0)	.0000	.0000	2588 (0)	1167 (1)	.3286	.2983	
15	−.1831	−.4628 (−1)	−.7417	−.2342 (0)	0000	.0000	2664 (0)	1196 (1)	
16	−.8044 (−1)	−.1782	−.1893	−.5388 (−1)	−.7677	−.2886 (0)	0000	0000	

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below.

TABLE ℰ—continued

$l = 4$

$n \backslash l'$	4,3	5,3	6,3	6,5	7,3	7,5	8,3	8,5
5	− 1047 (1)*	0000	7376 (− 2)	1676 (1)	1174 (− 2)	2018 (0)	3893 (− 3)	3992 (− 1)
6	− 1418 (0)	− 9220 (0)	0000	0000	1980 (− 1)	1492 (1)	3455 (− 2)	2657 (0)
7	− 4541 (− 1)	− 1779	− 8652 (0)	− 7693 (− 2)	0000	0000	3386 (− 1)	1392 (1)
8	− 2063	− 6372 (− 1)	− 1908	− 1101	− 8363 (0)	− 2099	0000	0000
9	− 1135	− 3226	− 7570 (− 1)	− 3398 (− 3)	− 1974	− 3356 (− 2)	− 8270 (0)	− 3854 (− 1)
10	− 6984 (− 2)	− 1856	− 3881	− 1482	− 8131 (− 1)	− 1086	− 2023	− 6558 (− 2)
11	− 4652	− 1181	− 2299	− 7847 (− 4)	− 4291	− 4087 (− 3)	− 8352 (− 1)	− 2318
12	− 3277	− 8033 (− 2)	− 1495	− 4705	− 2991	− 2641	− 4380	− 1021
13	− 2407	− .5777	− 1036	− 3067	− 1709	− 1604	− 2801	− 5599 (− 3)
14	− 1827	− 4306	− .7527 (− 2)	− .2126	− 1198	− 1056	− 1866	− 3417
15	− 1423	− 3307	− 5670	− 1543	− 8790 (− 2)	− 7378 (− 4)	− 1320	− 2281
16	− 1135	− 2603	− 4395	− 1161	− 6674	− 5587	− 9747 (− 2)	− 1605

$n \backslash l'$	9,3	9,5	10,3	10,5	11,3	11,5	12,3	12,5
5	1787 (− 3)	2592 (− 1)	9821 (− 4)	1373 (− 1)	6049 (− 4)	8270 (− 2)	4027 (− 4)	5415 (− 2)
6	1109 (− 2)	9504	5588 (− 3)	4400	3119 (− 3)	2466 (− 1)	1942 (− 3)	1559 (− 1)
7	6377	2909 (0)	2544 (− 2)	1110 (0)	1123 (− 2)	5530	6330	5209
8	3461 (− 1)	1557 (1)	1042 (− 1)	5031	3795	1215 (0)	1858 (− 2)	6261
9	0000	0000	7540	1308 (1)	1480 (− 1)	3107	5480	1283 (0)
10	− 8285 (0)	− .5957 (− 1)	0000	0000	9779	1296 (1)	1963 (− 1)	5166
11	− 2068	− 1061	− 8370 (0)	− 8281 (− 1)	0000	0000	1214 (0)	1291 (1)
12	− 8871 (− 1)	− 5689 (− 2)	− .2115	− 1534	− 8503 (0)	− 1083 (0)	0000	0000
13	− 4804	− 1727	− 9155 (− 1)	− 5451 (− 2)	− 2162	− 2063 (− 1)	− .8671	− 1556 (0)
14	− 2965	− .9587 (− 3)	− 4994	− 2588	− 6418 (− 1)	− 7461 (− 2)	2213	− 2643 (− 1)
15	− 1990	− 5933	− 3102	− 1430	− 5163	− 3502	− 9677 (− 1)	− 9682 (− 2)
16	− 1415	− 3964	− 2092	− .9037 (− 3)	− 3222	− 2023	− 5326	− 4692

$n \backslash l'$	13,3	13,5	14,3	14,5	15,3	15,5	16,3	16,5
5	2856 (− 4)	3767 (− 2)	2084 (− 4)	2742 (− 2)	1382 (− 4)	2067 (− 3)	1254 (− 4)	1605 (− 2)
6	1503 (− 3)	1035 (− 1)	9239	7345	6825	5431	5208	4147
7	.5974	2054	2684 (− 3)	1407 (− 1)	1912 (− 3)	.1013 (− 1)	1419 (− 3)	7582
8	1047 (− 2)	3719	6617	2422	4492	1682	3214	1225 (− 1)
9	2684	6764	1540 (− 2)	4084	9783	3693	6668	.1889
10	7563	1336 (0)	3636	7138	2098 (− 2)	4359	1539 (− 2)	2901
11	2482 (− 1)	.3220	9404	1377 (0)	4677	7455	2712	4579
12	1461 (0)	1302 (1)	3029 (− 1)	3275	1138 (− 1)	1413 (0)	5791	7687
13	0000	0000	1716 (0)	1313 (1)	3600	3331	1386 (− 1)	1446 (0)
14	− 8844	− 1642 (0)	0000	0000	1977 (0)	1555 (1)	4190	3390
15	− 2266	− 3261 (− 1)	− 9076	− 1940 (0)	0000	0000	2243 (0)	1354 (1)
16	− 9934 (− 1)	− 1208	− 2322	− 3913 (− 1)	− 9304	− 2248 (0)	0000	0000

$l = 5$

$n \backslash l'$	5,4	6,4	7,4	7,6	8,4	8,6	9,4	9,6
6	− 1372 (1)	0000	6294 (− 2)	2008 (1)	9010 (− 3)	2169 (0)	2783 (− 3)	3979 (− 1)
7	− .1631 (0)	− .1221 (1)	0000	0000	1718 (− 1)	1806 (1)	2729 (− 2)	2977 (0)
8	− 4902 (− 1)	− 2174 (0)	− 1139 (1)	− 6479 (− 2)	0000	0000	3155 (− 1)	1603 (1)
9	− 2121	− 7613 (− 1)	− 2380 (0)	− 8412 (− 3)	− 1094 (1)	− 1789 (− 1)	0000	0000
10	− 1125	− 3600	− 9079 (− 1)	− 2420	− 2480 (0)	− 2620 (− 2)	− 1070 (1)	− 3318 (− 1)
11	− 6767 (− 2)	− 2017	− 4525	− 1002	− 9944 (− 1)	− 8041 (− 3)	− 2542 (0)	− 3262 (− 2)
12	− 4450	− .1259	− 2626	− 5100 (− 4)	− 3122	− 3460	− 1051	− 1691
13	− 3082	− 8467 (− 2)	− 1680	− 2965	− 3043	− 1806	− 5554 (− 1)	− 7483 (− 3)
14	− .2243	− 6009	− .1151	− 1888	− 1982	− 1068	− 3341	− 3982
15	− 1691	− 4444	− 8291 (− 2)	− 1285	− 1376	− 6887 (− 4)	− 2203	− 2586
16	− .1311	− 3393	− 6204	− 9184 (− 3)	− .1002	− 4728	− 1546	− 1553

$n \backslash l'$	10,4	10,6	11,4	11,6	12,4	12,6	13,4	13,6
6	1212 (− 3)	2455 (− 1)	6421 (− 4)	1233 (− 1)	3848 (− 4)	7326 (− 2)	2509 (− 4)	4694 (− 2)
7	8809	9866	3999 (− 3)	4482	2161 (− 3)	.2437 (− 1)	1312 (− 3)	1487 (− 1)
8	3566 (− 2)	3328 (0)	1815 (− 2)	.1218 (0)	8352	3881	4381	3331
9	4898 (− 1)	1611 (1)	8679	3505	3010 (− 2)	1360 (0)	1415 (− 2)	6834
10	0000	0000	6775 (− 1)	.1967 (1)	1255 (− 1)	3605	4460	1434 (0)
11	− 1060 (1)	− 3138 (− 1)	.0000	0000	.8864	1541 (1)	1698 (− 1)	3675
12	− 2590 (0)	− 8662 (− 2)	− 1060 (1)	− .7251 (− 1)	0000	0000	1109 (0)	1529 (1)
13	− 1093	− 2878	− 2633 (0)	− 1271	− 1066 (1)	− 9553 (− 1)	0000	0000
14	− 3840 (− 1)	− 1502	− .1127	− 4356 (− 2)	− 2679 (0)	− .1732	− 1076 (1)	− 1203 (0)
15	− 3567	− 7031 (− 3)	− 6083 (− 1)	− 1995	− 1156	− 6052 (− 2)	− 2725 (0)	− 2240 (− 1)
16	− 2574	− 4239	− .3746	− 1090	− 6289 (− 1)	− 2815	− 1185	− 7936 (− 2)

*The number in parentheses indicates the power of ten multiplying the entry and succeeding entries below

```
A                0.00000     .10000     .30000     .50000     .75000


V(A,0)           1.00000     .89646     .73460     .61569     .50694
INT.VAL                .94599     .80902     .67079     .55699     .46443


WIDTH/2           .83255     .88716    1.00433    1.13160    1.30367
INT.VAL                .85952     .94444    1.06675    1.21599    1.39466



  X
 0.00            1.00000    1.00000    1.00000    1.00000    1.00000
  .10             .99309     .99299     .99277     .99256     .99229
  .20             .97265     .97226     .97145     .97063     .96963
  .30             .93952     .93870     .93702     .93534     .93330
  .40             .89503     .89373     .89110     .88847     .88531


  .70             .71203     .71003     .70606     .70222     .69775
 1.00             .50000     .50000     .50000     .50000     .50000
 1.50             .21022     .21874     .23416     .24731     .26063
 2.00             .06520     .07732     .10260     .12260     .14148
 2.20             .03492     .05028     .07599     .09594     .11450


 2.40             .01845     .03338     .05806     .07697     .09446
 2.60             .00923     .02308     .04583     .06320     .07927
 2.80             .00436     .01682     .03728     .05295     .06751
 3.00             .00195     .01295     .03109     .04510     .05822
 3.40             .00033     .00873     .02286     .03402     .04466


 4.00             .00002     .00576     .01576     .02389     .03181
 5.00            0.00000     .00348     .00970     .01491     .02009
 6.00            0.00000     .00235     .00661     .01022     .01386
 7.00            0.00000     .00170     .00480     .00745     .01014
 8.00            0.00000     .00129     .00365     .00568     .00774


 9.00            0.00000     .00101     .00287     .00447     .00610
10.00            0.00000     .00082     .00232     .00361     .00494
12.00            0.00000     .00056     .00160     .00250     .00342
15.00            0.00000     .00036     .00102     .00160     .00219
20.00            0.00000     .00020     .00057     .00090     .00123



          TABLE F. THE VOIGT FUNCTION V(A,X*WIDTH/2)/V(A,0)
```

```
A                1.00000    1.50000    2.00000    4.00000   10.00000


V(A,0)            .42758     .32159     .25540     .13700     .05614
INT.VAL                .36809     .28511     .17900     .07980    0.0000


WIDTH/2          1.48848    1.88866    2.31843    4.17840   10.07435
INT.VAL                1.68426    2.10068    3.23002    7.10531    0.0000


   X
  0.00           1.00000    1.00000    1.00000    1.00000    1.00000
   .10            .99204     .99161     .99126     .99057     .99016
   .20            .96868     .96704     .96577     .96322     .96154
   .30            .93138     .92808     .92555     .92060     .91743
   .40            .88237     .87738     .87363     .86647     .86207


   .70            .69375     .68736     .68288     .67524     .67114
  1.00            .50000     .50000     .50000     .50000     .50000
  1.50            .27087     .28448     .29226     .30297     .30769
  2.00            .15516     .17235     .18178     .19446     .20000
  2.20            .12782     .14446     .15358     .16586     .17123


  2.40            .10697     .12261     .13121     .14283     .14793
  2.60            .09079     .10525     .11324     .12408     .12887
  2.80            .07801     .09127     .09863     .10867     .11312
  3.00            .06775     .07985     .08661     .09588     .10000
  3.40            .05249     .06256     .06824     .07610     .07962


  4.00            .03774     .04547     .04988     .05604     .05882
  5.00            .02403     .02925     .03227     .03652     .03846
  6.00            .01665     .02037     .02254     .02562     .02703
  7.00            .01221     .01499     .01662     .01893     .02000
  8.00            .00934     .01149     .01275     .01455     .01538


  9.00            .00737     .00908     .01009     .01153     .01220
 10.00            .00597     .00736     .00818     .00936     .00990
 12.00            .00414     .00512     .00569     .00651     .00690
 15.00            .00265     .00328     .00365     .00418     .00442
 20.00            .00149     .00184     .00205     .00235     .00249


            TABLE F. THE VOIGT FUNCTION V(A,X*WIDTH/2)/V(A,0)
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