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METHODS OF OPACITY CALCULATIONS



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PHYSICS

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METHODS OF OPACITY CALCULATIONS

by

Harris Mayer



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## II.

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ABSTRACT

Methods for calculating the opacity of materials at high temperatures are discussed in this report. Minor improvements are outlined for the treatment of continuous absorption processes, and a small error usually made in treating the scattering process is corrected. In contrast to all previous calculations of opacity, the effect of line absorption is carefully examined, for it may well be the dominant process under certain conditions of temperature and density. Detailed methods for calculating the line absorption contribution are, therefore, developed. To illustrate the principles involved, the opacity of pure iron at a temperature of 1000 volts and normal density is worked out in detail. For this case, the opacity is  $20.2 \text{ cm}^2/\text{gram}$ , corresponding to a mean free path for radiation of  $6.31 \times 10^{-3} \text{ cm}$ . The ratio of the opacity including line effects to the opacity without lines is 3.2 .

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GLOSSARY OF NOTATION

A Reciprocal length, defined by (6.21).

A Helmholtz free energy, (A1.4).

$a_0$  Bohr radius =  $.5291 \times 10^{-8}$  cm.

$a_{ni}$  defined by (5.72), (6.46).

$a_Z'$  radius of ionic sphere, (4.24)

$B = \frac{Mc^2}{2kT u_0^2}$  in (5.33)

$B = \frac{2h\nu^3}{c^2} \frac{e^{-u}}{1-e^{-u}}$  as defined by (3.8)

$b_{ba}(\nu)$  dispersion factor for line absorptions (2.6)

$b'(u)$  dispersion factor for line absorption (5.11a)

c velocity of light

$\rho(\mathcal{E}_f)$  density of states of the free electron per unit energy interval (2.29)

$\rho_{iZ}$  degeneracy of the ith ionic level

$\rho_f$  density of initial state per df (2.26)

$D = \frac{u^3 \mu c}{A}$  reduced absorption coefficient (6.20)

$E_a$  energy of quantum state a of an ion (2.4)

$E_J$  energy of quantum state J of entire system (4.11)

e positive electronic charge

$f_{ba}, f_i$  electron number defined by (2.3)

$F(\nu, w)$  function defined by (2.34)

$\mathcal{G}_{b \rightarrow f}(\nu)$  Gaunt factor for bound-free transitions (2.22)

$\mathcal{G}_{ff}(\nu)$  Gaunt factor for free-free transitions

$\bar{\mathcal{G}}_{ff}$  Average Gaunt factor defined by (6.27)

$\mathcal{E}_{nk}(u)$  Frequency factor (5.82)

$\mathcal{E}'_{nk}(u)$  Frequency factor (5.71)



Glossary of Notation (continued)

$h$  Planck's constant

$$\hbar = \frac{h}{2\pi}$$

$I(\nu)$  Specific intensity of radiation see (2.2)

$I_n$  Ionization energy of an electron bound in the  $n$  shell, (2.21)

$K$  Mean opacity coefficient per unit mass  $\text{cm}^2/\text{gm}$ .

$k$  Boltzmann's constant

$\vec{k}$  Wave number vector in direction of propagation, (2.1)

$l_\nu$  Mean free path for radiation of frequency  $\nu$ , (3.15)

$M$  Mass of absorbing atoms, (2.16)

$M_Z$  Gram atomic weight, (6.1)

$M_K$  Number lines in  $K$ th class, (6.44)

$m$  Mass of electron, (2.3)

$N_0 = 6.023 \times 10^{23}$  Avogadro's Number

$N_b$  Number of atoms in initial state  $b$  (2.9)

$n_b$  Number of bound electrons

$n_f$  Number of free electrons

$n = n_b + n_f$  Total number of electrons in system (4.8)

$N$  Total number of atoms in system (4.6)

$N_Z$  Number of nuclei of atomic number  $Z$  in system (2.29)

$n_0$  Initial state of the scattering particle (2.32)

$\hat{n}$  Unit vector (3.17)

$\bar{N}_\nu$  Average number of quanta in each radiation oscillator (2.1)

$n(\epsilon_f) d(\epsilon_f)$  Number of states of free electron in energy interval  $d(\epsilon_f)$

$n(\vec{v}) d\vec{v}$  Number of electron with velocity vector between  $v$  and  $v + dv$  (3.3)

$$P = \frac{1}{1+r} \quad (5.5)$$

$P$  Pressure, (6.17)

Glossary of Notation (continued)

- $P_J$  Probability given by (4.13)
- $Q$  Electronic partition function of the system (AI.1)
- $q$  Availability of final state (2.29)
- $r = \frac{\mu_l}{\mu_c}$  = ratio of line absorption to continuous background (5.5)
- $\overline{r^2}$  Value of  $r^2$  averaged over the bound wave functions (4.27)
- $r_0 = \frac{e^2}{mc^2}$  Classical electrons radius (2.34)
- $Rhc$  Rydberg energy = 13.607 volts (2.25)
- $S(u)$  Stromgren function Tabulated in Table VI (6.30)
- $S$  Eq. (5.11a)
- $S$  Entropy (AI.11)
- $T$  Absolute temperature (2.16)
- $u = \frac{h\nu}{kT}$  as defined by (3.8a)
- $V$  Volume of system (2.9)
- $V_{ij}$  Sum of Coulomb and exchange electron interactions (4.12)
- $w$  Transition probability as defined by (2.1)
- $w = \cos \theta$  (2.34)
- $w_{ab}^s(\nu)$  Transition probability for spontaneous emission (2.10)
- $w_{ab}^i(\nu)$  Probability for induced emission (2.11)
- $Z'$  Effective nuclear charge (2.25)
- $Z^*$  Effective nuclear charge (6.7)
- $Z$  Effective nuclear charge (AI.15)
- $\alpha = e^2/hc = 1/137.03$  fine structure constant
- $\alpha'$  See (4.13)
- $\alpha''$  See (4.17)
- $\alpha^*$ :  $-kT\alpha^*$  is free energy of electrons (4.41a)
- $\vec{\alpha}_j$  Dirac velocity matrix for  $j$ th electron (2.1)

-x-

Glossary of Notation (continued)

$$\beta = \frac{1}{kT}$$

$$\Gamma = \frac{\gamma}{4\pi kT} \quad \text{Dimensionless half breadth, defined in (5.21)}$$

$$\frac{\gamma}{2\pi} \quad \text{Breadth of spectral line (2.15)}$$

$$\gamma = \frac{h\nu'}{mc^2} \quad (2.34)$$

$$\vec{\epsilon} \quad \text{Direction of polarization (2.1)}$$

$$\epsilon(r) \quad \text{Potential energy (4.49)}$$

$$\epsilon_f \quad \text{Energy of free electron}$$

$$\bar{\epsilon}_i \quad \text{Ionization energy of the } i\text{th} \text{ electron (4.22)}$$

$$\bar{\bar{\epsilon}}_i \quad \text{Average energy of electron in } i\text{th} \text{ state (AI.10)}$$

$$\Theta \quad \text{Scattering angle (2.32)}$$

$$\Lambda \quad \text{Rosseland mean-free path (3.18)}$$

$$\Lambda_c \quad \text{Mean free path ignoring lines (5.7)}$$

$$\Lambda_l \quad \text{Contribution of lines to Rosseland mean free path (5.8)}$$

$$\mu \quad \text{Absorption coefficient, as defined in (5.3)}$$

$$\mu_c \quad \text{Absorption due to continuous processes alone (5.4)}$$

$$\mu_l \quad \text{Absorption due to lines (2.9), (5.4)}$$

$$\mu_s \quad \text{Scattering coefficient, i.e. inverse mean free path for scattering. (2.33)}$$

$$\nu' \quad \text{Frequency}$$

$$\rho \quad \text{Density (3.25)}$$

$$\sigma_{i,j} \quad \text{Screening constants, defined by (4.23) Tabulated in Table II}$$

$$d\sigma \quad \text{Surface element (3.1)}$$

$$\phi_0 = \frac{8\pi}{3} \left\{ \frac{e^2}{mc^2} \right\}^2 = .6654 \times 10^{-24} \text{ cm. Thomson cross-section (6.24)}$$

$$\phi_{ta}(\nu') \quad \text{Absorption cross-section. Eq. (2.8)}$$

Glossary of Notation (continued)

- $\phi_f$  Electrostatic potential, defined by (4.26)
- $\phi$  Differential scattering cross-section (2.32)
- $\chi_k$  Electron wave function (4.2)
- $\Omega_j$  Density of states, defined by (4.14)

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I. INTRODUCTION

The opacity of materials at extremely high temperatures is important in the study of stellar interiors. As such, it has engaged the interest of astrophysicists for the last thirty years. The most recent study of this problem is by Morse<sup>(1)</sup>. Following the tradition in the field, Morse considers only three fundamental processes as contributing to the opacity - photo-electric absorption (bound-free transitions), collision absorption (free-free transitions) and Compton scattering. It was pointed out by Edward Teller that a fourth process, line absorption, might often prove to be the determining one in the opacity. At his suggestion, therefore, the problem was investigated anew.

Previous workers<sup>(2)</sup> had recognized that sufficient absorption strength was present in the line spectrum to increase the opacity by factors of 2 to 4. It was argued, however, that individual lines are extremely sharp, and although they are very strong compared to the continuous absorption processes, they would simply make a very small region of the spectrum opaque to radiation. Since the mean free path for radiation ( $\sim$ reciprocal of the opacity) is a weighted frequency average of the reciprocal absorption coefficient, the blackness of these small regions would not appreciably alter the mean free path. Teller pointed out two reasons for suspecting these conclusions: 1) Individual lines were apt to be very much broader under the extreme temperature and density conditions of stellar interiors than under normal terrestrial conditions 2) There would be an enormous number of lines arising from the complicated electrostatic interactions at these temperatures.

The reasoning behind these suspicions is qualitatively very simple. At high temperatures, an element will be found in many states of ionization. Furthermore each ion type will exist in a number of excited states. For example, calculations show that iron at temperatures of 1000 volts and densities 5 times normal, i.e. 39.3

(1) Astrophysical Journals 92 pp. 27-49, 1940.

(2) Menzel and Pekeris: Monthly Notices of the Royal Astronomical Society, V. 96, p. 77, (1935); S. Rosseland, Handbuch der Astrophysik, V. 3' 3 teil.

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grams/cm<sup>3</sup>, (conditions available in stellar interiors) will have on the average 2 K electrons, 1.24 L electrons, 1.10 M electrons, etc. - in all a total average of 4.3 bound electrons. We may expect appreciable numbers of ions with from 2 to 7 bound electron. Moreover of the ions with say 6 bound electrons there will be some with 2K, 4L, others with 2K, 3L, 1M, still others with 2K, 2L, 2M, and so on. Each configuration of these ions gives a rather complex line spectrum - the total number of lines from the assemblage will be enormous. Mixtures of elements will give even a richer line spectrum.

Among the causes for line broadening are 1) Natural breadth; 2) Collision breadth; 3) Stark breadth; 4) Doppler breadth. Each of these is much more important at high temperatures and densities than at ordinary conditions. Because many electrons are in excited orbitals a large number of emission transitions can destroy the initial state of an ion. In addition the intense temperature radiation present can induce absorption transitions. Both effects enhance the natural breadth. At high temperatures collisions with free electrons will frequently occur - a process almost entirely excluded under ordinary conditions. Moreover the high velocity of the ions creates an appreciable Doppler broadening. It also enables relatively high charged ions to approach so close that enormous fields are available to cause Stark broadening. In many cases the lines will be so broadened as to form a virtually continuous absorption band, very effective in producing high opacity.

It will be realized that it is the high excitation of the material, combined with the pervading electrostatic interactions that makes line absorption so important a feature in opacity calculations. Previous treatments of the problem essentially neglected all these interactions except those between a nucleus and its own bound electron. It was felt worthwhile to include these interactions in some moderately satisfactory form in order to insure the accuracy of the calculations of the line absorption. This problem is treated at some length in Chapter IV of this paper.

An immediate byproduct of the statistical mechanical calculation which is there performed, is the thermodynamic properties and the equation of state of material. It is generally assumed in work on stellar interiors that the material obeys a perfect gas equation of state with an effective number of particles equal to the sum of all the electrons and nuclei in the system. In Appendix I, the appropriate modification of the equation taking into account the presence of bound electrons, electrostatic interactions, and a small correction for relativity effects is given.

The complexity of the line spectrum precludes any straightforward attack on the problem. Teller, however, when he proposed considering the line absorption, also suggested the use of a statistical method of finding the contribution to the opacity. The method is developed in detail in Chapter V which constitutes the significant new contribution to the study of opacity.

During our reexamination of the opacity problem, Dr. Maria Mayer noticed that the scattering contribution has always been treated by analogy with the absorption-emission contribution. This proves to be incorrect, although the numerical error is small. The difference between the two types of process lies in the effects of induced emission and induced scattering. The presence of induced emission strengthens a beam in its passage through matter, thus tending to reduce the opacity. In the scattering process, on the other hand, the induced scattering out of a beam compensates for the induced scattering into the beam. The correct calculation of opacity due to scattering therefore gives a result greater (actually 5% greater) than the conventional one.

Although there are many features in common, the treatment of the opacity of heavy elements, is different in many details from the treatment for light elements. This results because the relativistic effects completely change the nature of the line spectrum of heavy compared to light elements. A companion paper to this by Boris Jacobsohn<sup>(3)</sup>, gives specific attention to the calculation of opacities for the

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(3) Dissertation, University of Chicago, Dept. of Physics, 1947.

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heavy elements.

The author wishes to thank Dr. Maria Mayer and Dr. Edward Teller for suggesting the problem and for much valuable assistance in attacking it. It is a sincere pleasure, moreover, to acknowledge my indebtedness to Dr. Boris Jacobsohn for many discussions on every phase of this problem, and to Mr. Rudy Sternheimer for his valuable work on line broadening without which this paper would have little practical significance.



## II. THE PROCESSES CONTRIBUTING TO THE OPACITY

Any process capable of removing quanta from an incident beam, or emitting quanta into that beam must be considered in the opacity problem. The most important of these processes is simple absorption and its inverse. In this case a quantum is absorbed by an atomic system, its energy being transferred to excitation of the electrons. We may distinguish with profit three different types of absorption. In the first an electron in a bound state of the atom is excited to another bound state. This is the familiar line absorption. In the second the bound state electron is removed from the atom, going into one of the continuum of free states available, the usual photoelectric effect. In contrast to line absorption, this process is possible for any energy of the incident quantum greater than the ionization energy of the electron. Lastly, an electron in a free state may absorb energy by a transition to another free state. Any amount of energy whatever may be absorbed in this process. The inverse processes to the three mentioned are, in order: line emission, electron capture, and Bremsstrahlung.

A second absorption process is pair production with its inverse process annihilation.

The last group of processes is scattering. Here an incident quantum is deviated from its original path by an atom or electron. If the atom remains in its initial state after the scattering, we have ordinary coherent scattering; if it does not, the phenomenon is known as Raman scattering. A special case occurs if the frequency of incident radiation is equal to the frequency of an absorption line of the atom. Scattering by free electrons is termed Compton scattering.

The remainder of this chapter gives the transition probabilities for these processes.

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### 1. Line Absorption

The three types of simple absorption - line absorption, photoelectric absorption, and absorption due to free-free transitions differ only in the nature of the initial and final states of the atom. It is therefore possible to develop the treatment of all three at once up to an advanced point and there introduce the differences.

The transition probability for the absorption of a quantum of energy  $h\nu$  from an incident beam is

$$(2.1) \quad w_{ba} \, d\Omega = \frac{e^2}{\hbar_0} \bar{n}_\nu \, d\Omega \overline{\left| \sum_j (\vec{\alpha}_j \cdot \vec{\mathcal{E}}_e^{i\vec{k} \cdot \vec{r}_j}) \right|_{ab}^2} \vec{\mathcal{E}}, \vec{k}$$

In this formula  $\vec{\alpha}_j$  is the Dirac velocity matrix for the  $j$ th electron,  $\vec{\mathcal{E}}$  is the direction of polarization of the incident light beam which has the wave number vector  $\vec{k}$  in the direction of propagation. The matrix element connects the initial state of the atom  $b$  with the final state  $a$  and is averaged over all directions of polarization and orientations of the atom - which latter is the same as the average over directions of propagation of the light. The incident beam has on the average  $\bar{n}_\nu$  quanta in each radiation oscillator, that is the intensity of the beam directed within a solid angle  $d\Omega$  is

$$(2.2) \quad I(\nu) \, d\nu \, d\Omega = h\nu c \bar{n}_\nu \, 2 \frac{\nu^2 \, d\nu \, d\Omega}{3}$$

It is convenient to introduce the electron number defined by

$$(2.3) \quad f_{ba} = \frac{2\pi e^2}{h\nu_{ab}} \overline{\left| \sum_j \left( (\vec{\alpha}_j \cdot \vec{\mathcal{E}})_e^{i\vec{k} \cdot \vec{r}_j} \right) \right|_{ab}^2} \vec{\mathcal{E}}, \vec{k}$$

where

$$(2.4) \quad h\nu_{ab} = (E_a - E_b).$$

This definition reduces to the usual one for one electron atoms in non-relativistic approximation, when  $e^{i\vec{k} \cdot \vec{r}}$  is replaced by unity - the conventional dipole approximation. Combining (1), (2), and (3) we get the transition probability as

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$$(2.5) \quad w_{b \rightarrow a} d\Omega = \frac{\pi e^2}{mc} \frac{\nu_{ab}}{\nu} f_{ba} \frac{I(\nu)}{h\nu} d\Omega .$$

In any actual physical system the absorption is not confined to a single frequency, but it is possible for a range of frequencies in the neighborhood of  $\nu_{ab}$ . We shall therefore introduce the dispersion factor for line absorptions  $b_{ba}(\nu)$  by the definition that the probability of absorbing light of frequency between  $\nu$  and  $\nu + d\nu$  by the transition  $b \rightarrow a$  is

$$(2.6) \quad w_{ba}(\nu) d\nu d\Omega = \frac{\pi e^2}{mc} \frac{\nu_{ab}}{\nu} f_{ba} \frac{I(\nu)}{h\nu} b_{ba}(\nu) d\nu .$$

The dispersion factor will have a sharp maximum at  $\nu = \nu_{ab}$  and furthermore

$$(2.7) \quad \int_0^{\infty} b(\nu) d\nu = 1.$$

The absorption cross-section of this transition per atom for light of frequency  $\nu$  is then

$$(2.8) \quad \phi_{ba}(\nu) = \frac{\pi e^2}{mc} f_{ba} b_{ba}(\nu),$$

where we have put  $\nu = \nu_{ab}$  in the slowly varying function of frequency multiplying  $b(\nu)$ . From the cross-section we get immediately the absorption coefficient or inverse mean free path for line absorption

$$(2.9) \quad \mu_{\nu}(\nu) = \sum_{ba} \frac{N^b}{V} \phi_{ba}(\nu) = \frac{\pi e^2}{mc} \sum_{ba} \frac{N^b}{V} f_{ba} b_{ba}(\nu) ,$$

where  $N^b$  is the number of atoms in initial state  $b$ , and the summation extends over all transitions which may absorb the frequency  $\nu$ .

The inverse process, line emission, is the sum of two terms, one for spontaneous and one for induced emission. The transition probability for the spontaneous emission of a quantum  $h\nu$  within a solid angle  $d\Omega$  due to an atomic transition from state  $b$  to  $a$  is

$$(2.10) \quad w_{ab}^s(\nu) d\nu d\Omega = \frac{2\pi e^2}{mc^3} \nu^2 \left| f_{ab} \right| b_{ab}(\nu) d\nu d\Omega ,$$

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while the probability for induced emission is

$$(2.11) \quad w_{ab}^i(\nu) d\nu d\Omega = \frac{\pi e^2}{mc} \left| f_{ab} \right| \frac{I(\nu)}{h\nu} b_{ab}(\nu) d\nu d\Omega.$$

The quantum theory moreover gives the general result required by thermodynamics that

$$(2.12) \quad \left| f_{ab} \right| = f_{ba} \quad ; \quad b_{ab}(\nu) = b_{ba}(\nu);$$

so that

$$(2.13) \quad \frac{w_{ab}(\nu)}{w_{ba}(\nu)} = 1 + \frac{2h\nu^3}{c^2} \frac{1}{I(\nu)} \cdot$$

An adequate discussion of the electron numbers is given by Jacobssohn<sup>(1)</sup>. He considers an ion with only one electron and treats different order terms arising from the expansion of the factor  $e^{i\vec{k}\cdot\vec{r}}$  in (2.3). The leading term gives the major fraction of the electric dipole strength. Numerical calculations for this term in the non-relativistic case which extend and correct similar calculations by Bethe<sup>(2)</sup> are presented in Table 1 of Jacobssohn's paper and are reproduced here in Table 1. It should be noted that the  $f$  number in these tables is the average from a level ( $n\ell$ ) to a level ( $n'\ell'$ ) found by summing over all states in the final level. In order to divide the  $f$  number properly between the transitions  $n\ell j \rightarrow n'\ell' j'$  we use the relations

$$(2.14) \quad \begin{aligned} f_{n\ell k \rightarrow n'\ell' k+1} &= f_{n\ell \rightarrow n'\ell'} \cdot \\ f_{n\ell k \rightarrow n'\ell' k-1} &= \frac{(k-1)(2k+1)}{k(2k-1)} f_{n\ell \rightarrow n'\ell'} \cdot \\ f_{n\ell k \rightarrow n'\ell' (-k)} &= \frac{1}{k(2k-1)} f_{n\ell \rightarrow n'\ell'} \cdot \end{aligned}$$

where  $|k| = j + \frac{1}{2}$  and  $k = \ell$  or  $-(\ell + 1)$ ,  $k$  being the quantum number which replaces  $\ell$  in the Dirac theory. Jacobssohn also presents some formula and tables for the relativistic electric dipole and non-relativistic electric quadrupole oscillator strength.

(1) Op. Cit.

(2) H. Bethe, Handbuch der Physik (2nd Ed.) 2 V, Part 1, pp. 443.

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For approximate calculations, and to preserve the analogy between treatments of line absorption and continuous absorption, we may use an asymptotic expansion for the dipole  $f$  number (energy of transition  $h\nu$ ) of a hydrogenic atom averaged over all initial states in a shell of the principal quantum number  $n$ . This is<sup>(3)</sup>

$$(2.14a) \quad \bar{f}_{n \rightarrow m} = \frac{2^6}{3\pi\sqrt{3}} \left\{ \frac{1}{n^2} - \frac{1}{m^2} \right\}^{-3} \frac{1}{n^3 m^3} \frac{g_b}{2n^2}$$

where  $m$  is the principal quantum number of the final,  $n$  of the initial state, and

$$(2.14b) \quad g_b \sim 1 - 0.1728 \left( \frac{h\nu}{RhoZ^2} \right)^{1/3} \cdot \left[ \frac{2}{n^2} \frac{RhoZ^2}{h\nu} - 1 \right] + \dots$$

This expansion becomes better as both  $n$  and  $m$  increase.

The dispersion is due to the finite breadth of the atomic-states in the system caused by the interactions with light and with other particles. This problem has been treated in a thorough going fashion in an unpublished paper by R. Sternheimer. For dispersion caused by the interactions with the radiation field, the line has a natural breadth  $\frac{\delta_{ba}}{2\pi}$  and a dispersion

$$(2.15) \quad b_{ba}(\nu) = \frac{\frac{\delta_{ba}}{2\pi}}{4\pi^2(\nu - \nu_0)^2 + \frac{\delta_{ba}^2}{4}} \cdot$$

We note that when  $2\pi(\nu - \nu_0) = \frac{\delta_{ba}}{2}$ , the cross-section has fallen off to half its maximum value. Interactions with fast electrons will cause collision broadening of the lines with the same dispersion form as (2.15). However, interactions with slow moving particles like neighboring nuclei are best treated by an adiabatic approximation and the dispersion curve then falls off exponentially with distance from the line centers. Another cause of exponential type dispersion is the Doppler-Effect which gives

$$(2.16) \quad b(\nu) = \left\{ \frac{Mc^2}{2\pi kT} \left( \frac{1}{2} \right) \right\}^{\frac{1}{2}} \exp \left\{ - \frac{Mc^2}{2kT} \frac{(\nu - \nu_{ab})^2}{\nu_{ab}^2} \right\} \cdot$$

$M$  being the mass of the absorbing atoms and  $T$  the absolute temperature.

<sup>(3)</sup> Menzel and Pekeris. Op. Cit.

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2. Photo-electric absorption.

In the case of line absorption we found a non-zero probability for absorption of frequencies differing slightly from that of the atomic transitions due to the splitting of the atomic states into a continuum by interactions with, for example, the radiation field. For boundfree absorption (photoelectric absorption) the final state is already a member of a continuum, and we will therefore have a finite absorption probability for a continuum of incident frequencies. The probability of absorbing light with frequency between  $\nu$  and  $\nu + \Delta\nu$  is from (2.5)

$$(2.17) \quad w_{bf}(\nu) \Delta\nu = \frac{\pi e^2}{mc} \frac{I(\nu)}{h\nu} \sum_{\substack{\text{all } i \\ \text{in } \Delta\nu}} f_{bfi}.$$

The cross section may therefore be written as

$$(2.18) \quad \phi_{bf}(\nu) = \frac{\pi e^2}{mc} \frac{d}{d\nu} f_{bf},$$

where by  $\frac{df_{bf}}{d\nu}$  we mean

$$(2.19) \quad \frac{df_{bf}}{d\nu} = \sum_{\substack{\text{all } i \\ \text{in } \Delta\nu}} \frac{f_{bfi}}{\Delta\nu} \quad \text{for } \Delta\nu \text{ small.}$$

The absorption coefficient is, then

$$(2.20) \quad \mu_{bf}(\nu) = \sum_b \frac{n^b}{V} \phi_{bf}(\nu),$$

where the summation is extended over all states  $b$  which can absorb the frequency  $\nu$ . Naturally precisely the same expression (2.13) as in line absorption relates the probability of the inverse process of electron capture with photoelectron absorption.

We shall follow historical precedent in transforming (2.18) and (2.20). When Kramers first attacked the problem of the photoelectric effect using the machinery of the old Bohr theory, he found the cross-section for a complete shell of principal quantum number  $n$  to be

$$(2.21) \quad \varphi_{nf}(\nu) = \frac{2^5}{3\sqrt{3}} \frac{he^2}{mc} \frac{n}{h\nu} \left(\frac{I_n}{h\nu}\right)^2$$

where  $I_n$  is the ionization energy of an electron bound in the  $n$  shell. Later workers, Gaunt<sup>(4)</sup> and Stobbe<sup>(5)</sup>, computing the cross section with the new wave mechanics, expressed their result in terms of Kramer's formula (2.21), corrected by a factor, the so-called Gaunt factor  $g$ . It is useful to retain this notation, since Menzel & Pekeris<sup>(6)</sup> have shown that the Gaunt factor  $g$  per electron is close to unity when averaged over a complete shell for transitions to free states near the ionization limit (the region of interest in opacity calculations). To rewrite our cross-section (2.18) in terms of this notation, we define the Gaunt factor by

$$(2.22) \quad \epsilon_{bf}(\nu) = \frac{3\sqrt{3}\pi}{2^4} n \left(\frac{h\nu}{I_n}\right)^2 \nu \frac{df_{bf}}{d\nu}.$$

Thus (2.20) becomes

$$(2.23) \quad \mu_{bf}(\nu) = \sum_b \frac{N^b}{V} \frac{2^4}{3\sqrt{3}} \frac{he^2}{mc} \frac{1}{n} \frac{1}{h\nu} \left(\frac{I_n}{h\nu}\right)^2 \epsilon_{bf}(\nu).$$

As defined here, the  $f$  number, and hence the Gaunt factor refer to atomic transitions and  $N^b$  is the atomic occupation number. It is frequently more convenient to use  $f$  numbers and hence Gaunt factors per electron. The atomic occupation  $N^b$  must then be replaced by  $n_i$ , the number of electrons in the initial state capable of absorbing the frequency  $\nu$ . The transition probabilities must then be multiplied by a factor  $q$ , the probability that the final state will be available. For non-degenerate free electrons this is practically unity.

A discussion of the Gaunt factors with numerical tables is given by Jacobsohn. He shows that for absorption by  $L$  electrons, the dipole Gaunt factors for individual transitions varies considerably from transition to transition and moreover vary with frequency, especially in the region near the ionization edge. The average Gaunt

(4) J. A. Gaunt, Phil Trans. A 229 pp. 163 (1930)

(5) M. Stobbe, Ann. d. Phys. 2 pp. 661 (1930)

(6) Op. Cit.

factor per electron is, however, close to unity. Moreover using relativistic wave functions, while it drastically effects the results for individual transitions, has little effect on the average, even for the very heavy elements. The Gaunt factors for quadrupole transitions are smaller than those for dipole transitions by the factor  $.13(Z\alpha)^2$  for the L shell at the ionization limit ( $\alpha = \frac{1}{137} =$  fine structure constant), and even smaller for the higher shells. For many cases, therefore, it will be a sufficient approximation to replace  $g$  per electron by unity.

### 3. Free-Free Absorption.

The ability of an electron to absorb light depends on its binding to a nucleus, for a free electron cannot conserve momentum in absorption. Hence we expect a tightly bound electron to have a much larger photoelectric cross-section than a loosely bound one, and therefore the free-free transitions should be a small effect. There are two factors which nevertheless make it worthwhile to consider the process. In our highly ionized medium a great portion of the electrons are free--in extreme cases there may be no bound electrons at all. Furthermore, absorption by a bound-free transition can only take place for frequencies higher than the ionization potential for removal of the electron in question. For low frequencies the free-free transition may be the only possible one, or at least can compete favorably with a bound-free transition of a very loosely held bound electron.

The transition probability from one definite initial free state  $f$  to a range of final free states with the absorption of light of frequency between  $\nu$  and  $\nu + \Delta\nu$  is of course the same as (2.16) for the bound-free transitions. However, the same frequency can be absorbed by starting from any initial free state. Hence, to find the absorption coefficient, we must multiply the cross section (2.17) by the number of electrons per unit volume  $\frac{n(\mathcal{E}_f)}{V} d\mathcal{E}_f$  occupying a range of free states between  $\mathcal{E}_f$  and  $\mathcal{E}_f + d\mathcal{E}_f$  and integrating over all energies, keeping  $\nu$  constant.



$$(2.24) \quad \mathcal{M}_{ff'}(\nu) = \int_{\mathcal{E}_f} \frac{n(\mathcal{E}_f)}{V} \frac{\pi e^2}{mc} \frac{df_{ff'}}{d\nu} d\mathcal{E}_f.$$

Menzel and Pekeris<sup>(7)</sup> derive an asymptotic expression for  $\frac{df_{ff'}}{d\nu}$  whose leading term is that given by the Kramer's formula. We can see heuristically what the result must be by analogy with their asymptotic expansion (2.14a,b) for bound-bound transitions. If the initial free state is specified by a quantum number  $f$ , and the final free state after absorption of light energy  $h\nu$  is specified by  $k$ , then

$$(2.25) \quad (a) \quad h\nu = \mathcal{E}_k - \mathcal{E}_f; \quad (b) \quad \mathcal{E}_f = \frac{RhcZ^2}{f^2}; \quad (c) \quad \mathcal{E}_k = \frac{RhcZ^2}{k^2}$$

where  $Z'$  is the effective nuclear charge. The  $f$  number for this transition is obtained from (2.14a) by replacing  $n$  by  $if$ ,  $m$  by  $ik$ , the degeneracy  $2n^2$  by  $o_f$ , the density of initial states per  $df$ , and the bound Gaunt factor  $g_b$  by a free-free factor  $g_{ff}$ . Using the relations (2.25) we obtain

$$(2.26) \quad f_{fk} = \frac{2^6}{3\sqrt{3}\pi} \frac{(Rhc)^{3/2} Z'^3}{(h\nu)^3} \frac{\mathcal{E}_f^{3/2}}{k^3} \frac{g_{ff}}{o_f}$$

where

$$(2.27) \quad g_{ff} \approx 1 + 0.1728 \left( \frac{h\nu}{RhcZ'^2} \right)^{1/3} \left[ 1 + \frac{2\mathcal{E}_f}{h\nu} \right] + \dots$$

Then

$$(2.28) \quad \frac{df}{d\nu} = f_{fk} \frac{dk}{d\nu} = \frac{2^5}{3\sqrt{3}\pi} \frac{(Rhc)^{1/2} Z'^3}{(h\nu)^3} \frac{(\mathcal{E}_f)^{3/2}}{o_f} g_{ff}$$

It might be thought at first that a factor of 2 is lacking from the above equation, since the number of states within a frequency  $d\nu$  is  $2 \frac{dk}{d\nu} d\nu$ , since each level  $k$  may have an electron with either of two spins. But for a dipole one electron transition, the  $f_{fk}$  would be zero for a change of spin direction, so we need count only the states of one spin.

We now substitute (2.28) into (2.24). We shall later show (see Chapter IV) that  $n(\mathcal{E}_f) = o(\mathcal{E}_f) \left\{ \alpha^* + \beta \mathcal{E}_f + \gamma \right\}^{-1}$ , where  $o(\mathcal{E}_f)$  is the density of states of the free

(7) *ibid.*

electron per unit energy interval and  $\beta = 1/kT$ . We obtain from (3.25b)

$$o(\epsilon_f)/c_f = \frac{N_Z}{2} d\epsilon_f/d_f = \frac{N_Z}{2} (Rhc)^{1/2} Z^2 / \epsilon_f^{3/2}$$

where  $N_Z$  is the number of nuclei of atomic number  $Z$  in our system and the factor 2 takes care of electron spin. Gathering together the terms gives

$$(2.29) \quad \mu_{ff'}(\nu) = \sum_Z \frac{2^4}{3\sqrt{3}} \frac{hc^2}{mc} \frac{(Rhc)Z^2}{(h\nu)^3} \frac{N_Z}{V} \int_0^\infty \frac{\epsilon_f^3 q d\epsilon_f}{\left( \alpha^{*2} + \frac{\epsilon_f}{\epsilon_{ff}} + 1 \right)}$$

where a factor  $q$  for the availability of the final state has been added. For non-degenerate free electrons we may safely neglect the term 1 in the denominator and put  $q=1$ . Then the integral gives  $\frac{1}{\beta} e^{-\alpha^*}$  so that

$$(2.30) \quad \mu_{ff'}(\nu) = \frac{2^4}{3\sqrt{3}} \frac{hc^2}{mc} \frac{Rhc}{(h\nu)^3} \frac{NkT}{V} \sum_Z \frac{N_Z}{N} Z^2 e^{-\alpha^*} \bar{\epsilon}_{ff}$$

where

$$(2.31) \quad \bar{\epsilon}_{ff} = 1 + .1728 \left( \frac{kT}{RhcZ^2} \right)^{1/3} \left( \frac{h\nu}{kT} \right)^{1/2} \left[ 1 + \frac{2kT}{h\nu} \right]$$

and  $\alpha^*$  is given by (4.41a) below.

Just as with photoelectric absorption we have the relation (2.13) for the probability of the inverse process.

#### 4. Pair Production.

To produce a free electron-positron pair requires incident quanta of energy at least  $2mc^2$ , while even the production of a bound electron and a positron requires energies greater than  $mc^2$ . In all our discussions the temperature will be so low that the amount of radiation of such high energies is negligible. We may, therefore, safely neglect pair production. Moreover there will be practically no positrons in equilibrium at these temperatures and so we may neglect the inverse process of annihilation.

5. Scattering.

The cross-sections for scattering - coherent, Raman, and Compton - may be found, for example, in Heitler<sup>(8)</sup>. There, however, the case in which initially only one quantum is in the radiation oscillator of the incident beam and none at all in the scattered beam is considered. In order to find the transition probability we must multiply these cross-sections by the incident intensity and by a factor  $(1 + \bar{n}_b)$ ,  $\bar{n}_b$  being the average number of quanta in the radiation oscillator of the scattered beam. The term in  $\bar{n}_b$  is the induced scattering.

Consider then an incident beam in the direction specified by the vector  $\vec{l}$ , having specific intensity  $I_\nu(\vec{l})$ . The probability that a transition will take place, scattering a quantum of energy  $\nu'$  in a direction specified by  $\vec{l}'$  within  $d\Omega'$  is

$$(2.32) \quad w_{\nu, \nu'; n_0} d\nu d\Omega d\Omega' = d\phi(\nu, n_0, \sigma) \frac{I(\nu, \vec{l})}{h\nu} d\nu d\Omega \left\{ 1 + \frac{c^2}{2h\nu'^3} I_{\nu'}(\vec{l}') \right\},$$

where  $n_0$  specifies the initial state of the scattering particle,  $\sigma$  is scattering angle and  $d\phi$  is the usual differential scattering cross section. The scattering coefficient, i.e., the inverse mean free path for scattering is then

$$(2.33) \quad \mu_s(\nu) = \sum_{n_0} \frac{N}{V}^{(n_0)} \int_{\Omega'} w_{\nu, \nu'; n_0} d\Omega' \frac{h\nu}{I_\nu(\vec{l})},$$

where the sum extends over all states which can scatter this frequency.

For Compton scattering from free electrons initially at rest, the differential cross section is

$$(2.34) \quad d\phi(\nu, \sigma, \theta) = \frac{r_0^2}{2} d\Omega' F(\gamma, w),$$

$$F(\gamma, w) = \frac{1+w^2}{[1+\gamma(1-w)]^2} \left\{ 1 + \frac{\gamma^2(1-w)^2}{(1+w^2)(1+\gamma[1-w])} \right\},$$

$$w = \cos \theta,$$

$$\gamma = h\nu/mc^2, \text{ and } r_0 = e^2/mc^2 = \text{classical electron radius.}$$

(8) W. Heitler, Quantum Theory of Radiation, pp. 129-157.

To first order in  $\gamma$ , this reduces to

$$(2.35) \quad d\phi(\nu, \theta, \sigma) = \frac{r_0^2}{2} d\Omega' (1+w^2) [1-2\gamma(1-w)]$$

which is sufficiently accurate for our purposes. To get the cross section for scattering from an electron moving with velocity  $\vec{v}$ , we simply apply a Lorentz transformation. The result, to the same order as (2.35) is

$$(2.36) \quad d\phi(\nu, \vec{v}, \theta) = \frac{r_0^2}{2} d\Omega' (1-w^2) \left\{ [1 - 2\gamma(1-w)] + \frac{v}{c} \cos \alpha + (\frac{v^2}{c^2}) [(\cos^2 \alpha + \frac{1}{2}) + (\cos \alpha - \cos \alpha')^2 (1-w^2) - 1] \right\}$$



Another relation we shall need is the connection between incident and scattered frequencies

$$(2.37) \quad \frac{h\nu'}{h\nu} = \frac{1}{1+\gamma(1-w)} ; \quad \frac{h\nu}{h\nu'} = \frac{1}{1-\gamma(1-w)} ; \quad \gamma' = h\nu'/mc^2 .$$

The Kramer's-Heisenberg formula for coherent or Raman scattering gives a cross-section which, except for frequencies near a resonance line of the atom, is of the same order of magnitude as (2.35). This formula gives the scattering contribution of bound electrons. Now there are usually many more free electrons than bound so that the major part of the scattering will be of the form (2.36). Moreover, the scattering cross-section for bound electrons is generally small compared to the photo-electric cross-section. We will, therefore, never commit a serious error if we use the cross-section (2.36) as if it held for all the electrons, bound and free.

The question of resonance scattering must now be disposed of, for the cross-sections then become exceedingly large and it would be improper to use the simple formula (2.36). Heitler discusses just this question and he concluded that if the atom is irradiated by a continuous spectrum "the resonance fluorescence behaves with regard to the shape of the line absorbed and reemitted exactly as if two independent processes, an absorption and a subsequent emission took place." We must not regard absorption and resonance scattering as two independent fates which may overtake an atom, but rather consider that an atom may be excited to an intermediary state, and either remain there, in which case we have true absorption, or else returns to a lower state in which case we have resonance fluorescence. In calculat-

ing the total cross-section for all processes, we see that resonance fluorescence has been included in the term for line absorption.

### III. THE OPACITY COEFFICIENT

The opacity coefficient is a particular weighted average of the absorption coefficient discussed in the previous chapter. This relation results from a consideration of the equation for energy transport by radiation. A very complete treatment of this equation of radiative transfer and the solution appropriate to stellar interiors is given in Chandrasekhar<sup>(1)</sup>. Chandrasekhar's discussion, however, is restricted to simple absorption and emission processes. Other workers<sup>(2)</sup> in the field of stellar opacities have, by analogy, used the same relations for the scattering process, or combinations of scattering and absorption. It was pointed out by Dr. Maria G. Mayer that this is only approximately true: for pure scattering, the error made overestimates the mean free path for radiation by  $5\frac{1}{2}\%$ . Although the difference is small, it is necessary to see how it arises. We shall, therefore, repeat<sup>the</sup> conventional derivation of the opacity coefficient, including the scattering terms.

We shall first write the equation of radiative transfer in terms of the quantum mechanical cross-sections or transition probabilities discussed in Chapter II. We consider a beam of photons having  $cn_{\nu} d\nu d\Omega d\sigma$  quanta of frequency between  $\nu$  and  $\nu + d\nu$  travelling within the solid angle  $d\Omega$  of a specific direction, and normally incident per unit time upon a surface element  $d\sigma$ . The specific intensity of the beam is then  $I(\nu) = h\nu c n_{\nu}$ . In traversing a length  $ds$  in the direction of propagation some photons will be absorbed or knocked out of the beam, while others will be added to the beam by emission or scattering. The number absorbed from the beam in unit time is

$$(3.1) \quad \text{Absorbed} = \sum_{ba} w_{ba}(\nu) d\nu d\Omega \frac{N^b}{V} ds d\sigma.$$

The sum is over all transitions, bound-bound, bound-free, or free-free, which can absorb the frequency  $\nu$ . The number emitted into the beam per unit time is

(1) S. Chandrasekhar, *Stellar Structure*, pp. 198-213

(2) *Morse Astrophysical Journal*, 92, p. 30, 1940.

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$$(3.2) \quad \text{Emitted} = \sum_{ab} w_{ab}(\nu) d\nu d\Omega \frac{N^a}{V} ds d\sigma.$$

The number per unit time scattered out of the beam is

$$(3.3) \quad \text{Scattered out} = \int_{\vec{v}} \int_{\Omega'} \frac{n(\vec{v})}{V} d\vec{v} w_{\nu\nu'} d\nu d\Omega d\Omega' ds d\sigma,$$

where  $n(\vec{v}) d\vec{v}$  is the number of electrons with velocity vector between  $\vec{v}$  and  $\vec{v} + d\vec{v}$ . The number scattered into the beam is

$$(3.4) \quad \text{Scattered in} = \int_{\vec{v}} \int_{\Omega'} \frac{n(\vec{v})}{V} d\vec{v} w_{\nu''\nu} d\nu'' d\Omega d\Omega' ds d\sigma.$$

Adding up the 4 contributions (3.1) to (3.4) with the proper signs gives the net gain in number of photons  $d \left\{ \frac{\partial N_\nu}{\partial s} d\nu d\Omega d\sigma \right\}$  in the beam as it traverses  $ds$  in the steady state. Then

$$(3.5) \quad \frac{\partial N_\nu}{\partial s} = \sum_{ba} w_{ba}(\nu) \frac{N^b}{V} \left[ -1 + \frac{N^a}{N^b} \frac{w_{ab}(\nu)}{w_{ba}(\nu)} \right] + \int_{\vec{v}} \frac{n(\vec{v})}{V} d\vec{v} \int_{\Omega'} (w_{\nu''\nu} \frac{d\nu''}{d\nu} - w_{\nu\nu'}) d\Omega'.$$

We now introduce the assumption that, at each point in our medium local thermodynamic equilibrium exists. Then

$$(3.6) \quad \frac{N^a}{N^b} = e^{-\frac{E_a - E_b}{kT}} = e^{-\frac{h\nu_{ab}}{kT}} = e^{-u_{ab}}.$$

Furthermore introducing the relation (2.13), the terms involving absorption processes give

$$\begin{aligned} & \sum_{ba} w_{ba}(\nu) \frac{N^b}{V} \left\{ e^{-u_{ab}} - 1 + \frac{2h\nu^3}{c^2} \frac{e^{-u_{ab}}}{I(\nu)} \right\} \\ & = \sum_{ba} \frac{\phi_{ba}(\nu)}{h\nu} \frac{N^b}{V} (1 - e^{-u_{ab}}) \left\{ \frac{2h\nu^3}{c^2} \frac{e^{-u_{ab}}}{1 - e^{-u_{ab}}} - I(\nu) \right\} \end{aligned}$$

Since  $\phi_{ba}(\nu)$  has a sharp maximum at  $\nu = \nu_{ab}$ , it is permissible to put  $u_{ab} = u$  in all places in the sum except in  $\phi_{ba}(\nu)$ .

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With the use of definitions like (2.9), (2.20), we then get

$$(3.7) \quad \frac{dI_\nu}{ds} (\text{absorption}) = \mu_{\text{abs}}(\nu) (1 - e^{-u}) (B_\nu - I_\nu),$$

where

$$(3.8) \quad B_\nu = \frac{2h\nu^3}{c^2} \frac{e^{-u}}{1 - e^{-u}};$$

$$(3.8a) \quad u = \frac{h\nu}{kT}.$$

The terms involving scattering may now be simplified by replacing the transition probabilities by (2.32). This gives

$$(3.9) \quad \frac{dI_\nu}{ds} (\text{scattering}) = \int_{\vec{v}} \frac{n(\vec{v})}{V} d\vec{v} \int_{\Omega'} \left\{ \frac{d\phi(\nu, \vec{v}, \theta')}{d\Omega} I_\nu'(\vec{\ell}') \right. \\ \left. - \frac{d\nu'}{d\nu} \frac{\nu'}{\nu} (1 + \sigma^2) \frac{I_\nu(\vec{\ell})}{2h\nu^3} \right. \\ \left. - \frac{d\phi(\nu, \vec{v}, \theta)}{d\Omega'} I_\nu(\vec{\ell}) \left( 1 + \frac{\sigma^2 I_\nu'(\vec{\ell}')}{2h\nu'^3} \right) \right\} d\Omega'.$$

It is worthwhile to note that since the cross-sections involve  $\theta$  only in the form  $w = \cos \theta$ , and since  $\theta' = -\theta$ , it is permissible to replace  $\theta'$  by  $\theta$ . For the simple case of Thomson scattering from electrons at rest - the most important case in practice, we get

$$(3.10) \quad \frac{dI_\nu}{ds} (\text{scattering}) = \frac{n}{V} \frac{r_0^2}{2} \int_{\Omega'} \left\{ (1 + w^2) I_\nu(\vec{\ell}') \left( 1 + \frac{I_\nu(\vec{\ell}) \sigma^2}{2h\nu^3} \right) \right. \\ \left. - (1 + w^2) I_\nu(\vec{\ell}) \left( 1 + \frac{I_\nu(\vec{\ell}') \sigma^2}{2h\nu'^3} \right) \right\} d\Omega'.$$

It can be seen immediately that the terms in induced scattering cancel exactly, leaving

$$(3.11) \quad \frac{dI_\nu}{ds} (\text{scat.}) = \frac{n}{V} \left\{ -\frac{8\pi}{3} r_0^2 I_\nu(\vec{\ell}) + \frac{r_0^2}{2} \int_{\Omega} (1 + w^2) I_\nu(\vec{\ell}') d\Omega' \right\}.$$

The exact solution to the equation of transfer for absorption alone may be worked out. The result can then be expanded, the zero order term giving isotropic



radiation, and the first order term giving the diffusion theory type of approximation. It is only in this type of approximation that the Rosseland mean opacity appears - however, the approximation is an excellent one in systems we shall consider. We, therefore, employ this expansion to solve the combined equation (3.7) + (3.11), by putting

$$(3.12) \quad I_{\nu} = I_{\nu}^0 + l_{\nu} \frac{\partial}{\partial s} I_{\nu}^0 + l_{\nu} \frac{\partial}{\partial s} l_{\nu} \frac{\partial I_{\nu}^0}{\partial s} + \dots$$

Substituting this expansion in (3.7) and (3.11), and collecting terms not containing  $\frac{\partial}{\partial s} I_{\nu}^0$  gives

$$0 = \mu_{\text{abs}} (1 - e^{-u})(B_{\nu} - I_{\nu}^0),$$

since the scattering terms cancel to this order. Hence we must have

$$(3.13) \quad I_{\nu}^0 = B_{\nu}.$$

The terms in  $\frac{\partial}{\partial s} I_{\nu}^0$  give

$$(3.14) \quad \frac{\partial I_{\nu}^0}{\partial s} \left(1 - \frac{\partial l_{\nu}}{\partial s}\right) = \mu_{\text{abs}}(\nu)(1 - e^{-u}) l_{\nu} \frac{\partial I_{\nu}^0}{\partial s} \left(1 - \frac{\partial}{\partial s} l_{\nu}\right) \\ + l_{\nu} \frac{\partial I_{\nu}^0}{\partial s} \left(1 - \frac{\partial}{\partial s} l_{\nu}\right) \frac{n}{V} \frac{8\pi}{3} r_0^2,$$

since the contribution of the integral in (3.11) is negligible to this order. In order to satisfy (3.14)  $l_{\nu}$  must be

$$(3.15) \quad l_{\nu} = \frac{1}{\mu_{\text{abs}}(\nu)(1 - e^{-u}) + \mu_s(\nu)}$$

where

$$(3.16) \quad \mu_s(\nu) = \frac{n}{V} \phi_0; \quad \phi_0 = \frac{8\pi}{3} r_0^2$$

Thus we see that in this approximation scattering and absorption must be treated in different fashion. The physical reason for this is that the stimulated scattering tending to weaken the beam is exactly compensated by stimulated scattering tending

to strengthen the beam. On the other hand the stimulated emission strengthens the beam and nothing can compensate for this. The effective absorption coefficient must, therefore, be reduced by the factor  $(1 - e^{-u})$ .

Using the zero and first order terms in (3.12) we can compute the flux of energy of frequencies between  $\nu$  and  $\nu + d\nu$

$$(3.17) \quad \hat{n} \cdot \vec{F}(\nu) d\nu = \int_{\Omega} \hat{n} \cdot I(\nu) d\nu d\Omega = -\frac{4\pi}{3} l_{\nu} \hat{n} \cdot \text{grad } B_{\nu} d\nu$$

$$= -\frac{4\pi}{3} l_{\nu} \frac{dB_{\nu}}{dT} d\nu \hat{n} \cdot \text{grad } T,$$

where  $\hat{n}$  is a unit vector normal to the surface over which the flux is desired, and we have assumed that the spatial variations in the conditions of the system are solely due to a temperature gradient. The integrated flux is then  $\vec{F} = \int_0^{\infty} \vec{F}(\nu) d\nu$ . By introducing a mean free path properly averaged over all frequencies--the so-called Rosseland mean

$$(3.18) \quad \Lambda = \frac{\int_0^{\infty} l_{\nu} \frac{dB_{\nu}}{dT} d\nu}{\int_0^{\infty} \frac{dB_{\nu}}{dT} d\nu}$$

the integrated flux can be written

$$(3.19) \quad \vec{F} = -\frac{4\pi}{3} \Lambda \text{grad } T \frac{dB}{dT},$$

where

$$(3.20) \quad B = \int_0^{\infty} B_{\nu} d\nu = \frac{2\pi^5 k^4}{15c^2 h^3} T^4.$$

The energy density may be found from (3.12) since

$$(3.21) \quad u_{\nu} = \int_{\Omega} \frac{I_{\nu}}{c} d\Omega = \frac{B_{\nu}}{c} d\Omega \dots = \frac{4\pi}{c} B_{\nu},$$

whence

$$(3.22) \quad u = \int_0^{\infty} u_{\nu} d\nu = \frac{4\pi}{c} B.$$

The first order term in  $l_{\nu}$  in both these equations vanishes identically, so that (3.21) and (3.22) are correct to the same order as (3.19). Combining (3.22) with (3.19), we have

$$(3.23) \quad \vec{F} = -\frac{c}{3} \Lambda \text{grad } u.$$

By introducing the expression (3.8) for  $B_{\nu}$  and (3.20) for  $B$ , the expression (3.18) simplifies to

$$(3.24) \quad \Lambda = \frac{15}{4\pi^4} \int_0^{\infty} l_{\nu} u^4 e^u (e^u - 1)^{-2} du.$$

The effective mean free path for radiation may be alternatively expressed in terms of the mean opacity coefficient per unit mass  $\kappa$  by the relation

$$(3.25) \quad \kappa = \frac{1}{\rho \Lambda}.$$

$\rho$  being the density. It is this quantity which is usually used in astronomical discussions.

The effect of the present treatment of scattering, compared to the usual practice in opacity discussions is now clear. If there is no absorption, our treatment gives

$$(3.26) \quad \Lambda = \frac{1}{\rho \kappa} = \frac{15}{4\pi^4} \int_0^{\infty} \frac{V}{n\phi_0} u^4 e^u (e^u - 1)^{-2} du = \frac{V}{n\phi_0} = \mu_{\text{scatt}},$$

while the conventional treatment gives

$$(3.26a) \quad \Lambda = \frac{15}{4\pi^4} \int_0^{\infty} \frac{V}{n\phi_0} u^4 e^{2u} (e^u - 1)^{-3} du = \frac{1.055}{\mu_{\text{scatt}}}.$$

In most cases of astrophysical interest, scattering is not the most important process involved and the error is correspondingly much less.

We can now see in outline the steps needed to carry out the calculation of the opacity coefficient. We must first determine the absorption and scattering coefficients. This requires a knowledge of the cross-sections listed in Chapter II and the occupation number - the subject of the next chapter. The averaging process indicated by (3.24) must then be carried out.

#### IV. STATISTICAL MECHANICS OF IONIZED ATMOSPHERES

##### 1. Introductory.

The methods of statistical mechanics will furnish the occupation numbers needed in the calculation of the absorption coefficient. The succeeding sections develop a convenient method for performing this calculation to good approximation. In addition, statistical mechanics gives a description of phenomena related to the breadth and dispersion of spectral lines. This angle is discussed in sections 6 and 7. Lastly, it is a simple matter to calculate the thermodynamic functions of our material once the occupation numbers have been treated. While this is not actually needed in a calculation of the opacity coefficient, it is an extremely useful by-product. We carry out this treatment in the Appendix I.

##### 2. Quantum Mechanical Description of the System.

We assume that the system we deal with is in thermodynamic equilibrium at a temperature  $T$  and occupies a volume  $V$ . Although our entire system is not in such an equilibrium, the gradients of the thermodynamic variables are so small, that we may consider that at each point such a local thermodynamic equilibrium does exist. Furthermore, the temperatures we discuss will be so low that we may completely ignore nuclear reactions and pair production. Then we may describe our system as composed of  $N$  nuclei of which  $N_Z$  have atomic number  $Z$ , associated with  $n$  electrons just sufficient in number to make  $N$  neutral atoms. That is

$$(4.1) \quad N = \sum_Z N_Z, \quad n = \sum_Z Z N_Z.$$

Clearly we have a system of many particles with strong interactions. Following the usual method of separating out the effects of the nuclear motions, we then express the electronic wave function of the system as a properly antisymmetrized product of one electron functions obeying the Hartree-Fock Equations<sup>(1)</sup>.

<sup>(1)</sup> F. Seitz, *Modern Theory of Solids*, pp. 243 ff.

The essential features of the one electron wave functions are apparent from physical considerations, and may also be derived by inspection of the Fock Hamiltonian. For large energies, the kinetic energy term in the Hamiltonian dominates, and the wave functions approach those of a free electron. They are, therefore, independent of the positions of the nuclei. For low energies, on the other hand, the interaction term with the nuclear potential becomes of equal importance to the kinetic energy term. Because of the singularity in the potential at the position of each nucleus, the behavior of the wave function at any position is largely conditioned by the field of the nearest nucleus, secondarily by the nearest neighbors, and is hardly affected by more distant nuclei. We, therefore, expect that near a nucleus, the one electron function will approximate the shape of the atomic wave function of the isolated ion. In this extreme the wave functions depend only on the distance from the nearest nucleus - and are independent of the relative position of the nuclei, just as for the free electron extreme.

A model which embodies these essential features is the crystalline solid. At first sight this appears to be a violent distortion of the actual state of the system, since we should not expect any long range crystalline order at the high temperatures with which we deal. The model will, however, provide the proper qualitative features of the wave functions for a system of many nuclei throughout which the electrons are free to roam. Naturally, any features characteristic of the strict periodicity of the lattice are simply introduced artificially by our model. Those features of the crystal model, however, which depend on near neighbors only should apply to our system, for there will be a local ordering effect corresponding to that present in ordinary liquids.

Precisely, as in the usual theory of metals, we can use the Bloch approximation of periodic wave functions for the electrons. In the low energy case the energy levels will correspond closely to those in the isolated ion, except that a single ionic state is  $N_Z$  fold degenerate. This results because we can

construct  $N_Z$  independent periodic Bloch functions from the  $N_Z$  zero order function, each of which corresponds to the electron being on any one of  $N_Z$  different ions. This degeneracy is removed by interactions with neighboring nuclei, so that finally we shall have in our crystal a narrow band of  $N_Z$  states in the neighborhood of each state of the isolated ion. The wave functions are of the form

$$(4.2) \quad \chi_k = \frac{1}{\sqrt{N_Z}} \sum_{n=1}^{N_Z} e^{2\pi i \vec{k} \cdot \vec{r}_n} u(\vec{r} - \vec{r}_n) ,$$

where  $u(\vec{r} - \vec{r}_n)$  is an atomic wave function with origin at the nucleus located at  $\vec{r}_n$ . As the energy is increased, the atomic wave functions of neighboring ions overlap more and more, thus widening the band. Eventually, the band widths will exceed the distance between atomic levels, and we shall have a quasi-continuum of states. At about this energy the approximation of localized atomic type wave functions breaks down, for the functions overlap several nuclei. Moreover, atomic functions from several levels must be considered in building up a good approximation from (4.2). The transition stage of the onset of the continuum leads naturally into the stage when the atomic wave functions become constant throughout the crystal. For high enough energies the functions (4.2) are of the free-electron type.

The nature of the eigenfunctions in the transition region is complicated. We are fortunate, therefore, that in our system (in contrast to the usual metallic state) only a very small fraction of the electrons will populate states in this region. This results because the Boltzmann factor in the probability of occupation of these states is rather small compared to that of the closely bound low energy states, while the a priori probability factor is not yet so large as in the high energy free states. The contribution of these transition states to the partition function of the system is, therefore, small, and for the thermodynamic properties of the system we may treat them roughly. The approximation we shall use in our statistical mechanics is to ignore the details of these transition states completely. For the low energy states, we shall use atomic wave functions

and hence term them bound states. For energies greater than a certain limit which we term the cut-off energy, we shall use the eigenfunctions for free electrons. Since the transition states are statistically unimportant, the exact position of the cut off energy is not critical. We shall return later to the question of fixing the cut off energy.

The circumstance that the transition states do not affect the thermodynamic properties of our system is no guarantee that they will not seriously affect the optical properties. We shall see later that the most critical element in the Rosseland mean opacity is the presence or absence of absorption in certain frequency regions. We must, therefore, examine whether the onset of a continuum of one electron energy states will lead to a continuous absorption spectrum. In the Bloch scheme an examination of the transition probabilities proves this to be the case. This is not necessarily true in other approximation schemes. The irregularities in our lattice, however, will undoubtedly provide the continuous absorption we assume.

There is still another and more serious short-coming of our one-electron approximation. This is the neglect of correlations between electrons positions, except for that dictated by the Pauli principle. These correlation energies are so small that they do not affect the occupation numbers of the one electron states. They are, however, decisive in determining the line absorption contribution to the opacity. This is so because the number of bound energy levels in our complicated crystal, is, in the one electron function approximation, exactly the same as in an isolated one electron atom. The spectrum would then appear to consist of just a very few very strong lines. Taking correlations into account would split these into very many lines of the same total absorption strength. The next chapter shows that having the absorption strength distributed among many lines very much enhances their effect on the opacity. The treatment of these correlations by

the "ionic" method is the topic of section 5.

Another feature of our approximation which bears watching is the "missing" bound states which have been excluded by the cut off. Of course, these are not missing at all but have been merged with the continuum. The absorption strength of the cut off bound states should be distributed at the beginning of the free states.

With this quantum mechanical approximation, we now proceed to examine the statistical mechanics of our idealized model.

### 3. Statistical Mechanics - Independent Electron Approximation.

The object of this section is to use the methods of statistical mechanics to find the number of electrons in each electronic state in equilibrium at the temperature  $T$ . We shall here assume for simplicity that the electrons are completely independent of each other. The next section will treat the electronic interactions, but the final results can be thrown into essentially the same form as for independent electrons.

The nature of the energy levels and the density of states has been discussed in the previous sections. If  $c_{iZ}$  is the degeneracy of the  $i^{\text{th}}$  ionic level, energy  $\epsilon_{iZ}$ , of a nucleus of charge  $Z$ , there will be a band of  $N_Z c_{iZ}$  states at this energy in the system. Such bands will persist for all energies  $\epsilon_{iZ} < \epsilon_0$  less than the cut off. Since electrons obey the Fermi-Dirac statistics, the number of electrons in the  $i_Z^{\text{th}}$  level will then be

$$(4.3) \quad n_{iZ} = \frac{N_Z c_{iZ}}{\alpha + \beta \epsilon_{iZ} + 1} ; \quad \epsilon_{iZ} < \epsilon_0$$

where  $\beta = \frac{1}{kT}$  and  $\alpha$  is the normalization constant with the physical interpretation that  $\mu = -kT \ln \alpha$  is the free energy of the electrons.



For energies greater than  $\xi_0$ , the density of state will be that of a free electron with kinetic energy  $\xi - \xi_0$ . This is, in the relativistic case

$$(4.4) \quad \rho_f(\xi) = \frac{8\pi V}{(oh)^3} \left\{ 2(\xi - \xi_0)mc^2 + (\xi - \xi_0)^2 \right\}^{\frac{1}{2}} \left\{ (\xi - \xi_0) + mc^2 \right\},$$

or expanding for kinetic energies small compared to  $mc^2$

$$(4.4a) \quad \rho_f(\xi) = \frac{8\pi Vm}{h^3} \left\{ 2(\xi - \xi_0)m \right\}^{\frac{1}{2}} \left\{ 1 + \frac{5}{4} \frac{\xi - \xi_0}{mc^2} + \dots \right\}.$$

Then the number of free electrons with energies between  $\xi$  and  $\xi + d\xi$  is

$$(4.5) \quad n_f(\xi)d\xi = \frac{\rho_f(\xi)d\xi}{\alpha \xi + 1}.$$

The total number of bound electrons is found from (4.3)

$$(4.6) \quad n_b = \sum_Z \sum_1 n_{1Z}$$

while the total number of free electrons is from (4.5)

$$(4.7) \quad n_f = \int_{\xi_0}^{\infty} n_f(\xi)d\xi.$$

Of course, the total number of electrons in the system is the sum of bound and free

$$(4.8) \quad n = n_b + n_f$$

and it is this condition which determines the normalization constant  $\alpha$  of (4.3) and (4.5).

To use these occupation numbers (4.3) and (4.5) we must determine  $\alpha$ . We note that (4.7) is the equation for a free electron gas, except for the one fact that  $n_f$  is not a constant given by the physical nature of the system, but instead varies with the temperature and volume.  $n_f$  may, however, be a rather insensitive function, and we may then employ the following scheme of successive approximations to determine  $\alpha$ . Assume a trial  $n_f$ ; usually we may start by taking  $n_f = n$  the

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total number of electrons. Then use (4.7) to calculate  $\alpha$ . For the case in which relativistic and degeneracy effects are small corrections - the region of greatest interest - a suitable expansion of (4.7) gives

$$(4.9) \quad \alpha^* = \ln \frac{2V}{n_f} \left( \frac{2\pi mkT}{h^2} \right)^{3/2} + \frac{15}{8} \frac{kT}{mc^2} - \frac{e^{-\alpha^*}}{2^{3/2}},$$

where

$$(4.10) \quad \alpha^* = \alpha + \beta E_0.$$

Knowing  $\alpha$ , the sum in (4.6) must be carried out explicitly, giving  $n_b$  and by (4.8) a second approximation to  $n_f$ . The cycle is very rapidly convergent.

If a long series of computations must be made, it is more convenient to fix  $\alpha$  to start. Then using (4.6) we find  $n_b/N$  while (4.7) gives  $n_f/V$ . (Here  $N$  is the total number of atoms in the system). Then we may find out to what value of  $n/V$ ; i.e., to what density; the value of  $\alpha$  corresponds.

#### 4. Statistical Mechanics - Dependent Electrons.

We now treat our system including the electronic interactions by the method of the canonical ensemble. A state of the entire system, symbolized by  $J$ , will be determined if we know the number of electrons in each one-electron orbital of the Hartree-Fock set of equations. Although each of these non-degenerate orbitals may have either one electron or none at all, we find it more convenient to group degenerate or nearly degenerate orbitals together and such groups we will designate by small subscript  $i$  or  $j$  or  $l$ . The number of such orbitals in the  $i^{\text{th}}$  energy group; i.e. the degeneracy; we denote by  $o_i$ . The energy of the state  $J$  is

$$(4.11) \quad E_J = \sum_i n_{Ji} \left\{ \epsilon_{Ji} + \frac{1}{2} \sum_{j \neq i} n_{Jj} v_{Jij} + \frac{1}{2} (n_{Ji}-1) v_{Jii} \right\}.$$

$n_{Ji}$  is the number of electrons occupying orbitals in the energy interval when the system is in the state  $J$ . Now the partition function will involve sums over all

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states  $J$  of the system, but only states near the equilibrium value will contribute heavily. Since the dependence on  $J$  of the interactions  $\mathcal{E}_{Ji}$  and  $V_{Jij}$  is not pronounced, we may insert some average value  $\bar{\mathcal{E}}_i$  and  $\bar{V}_{ij}$  independent of  $J$  instead. Moreover, we introduce the set of numbers  $\bar{n}_j$ , at present wholly arbitrary but later destined to represent some average occupation of the region. Then (4.11) becomes

$$(4.12) \quad E_J = \sum_i n_{Ji} \left\{ \left[ \bar{\mathcal{E}}_i + \frac{1}{2} \sum_{j \neq i} \bar{n}_j V_{ij} + \frac{1}{2} (\bar{n}_i - 1) \bar{V}_{ii} \right] + \left[ \frac{1}{2} \sum_{j \neq i} (n_{Jj} - \bar{n}_j) V_{ij} + \frac{1}{2} (n_{Ji} - \bar{n}_i) V_{ii} \right] \right\}.$$

The first term in square brackets in (4.12) is independent of the occupations and may be regarded as the zero order approximation to the effective energy of the electron. The second term in square brackets gives the difference between the detailed interaction between electrons and the average interaction. We may expect this to be small and hence treat it as a perturbation.

Now according to the canonical ensemble treatment, the probability of finding our entire system in an energy level between  $E_J$  and  $E_J + \Delta E_J$  is

$$(4.13) \quad P_J = \Omega_J e^{-\alpha' - \beta E_J},$$

where

$$(4.14) \quad \Omega_J = \prod_i \frac{c_i!}{n_{Ji}! (c_i - n_{Ji})!}$$

is the number of states in the energy interval  $\Delta E_J$  and  $\alpha'$  is the normalization constant determined so that

$$(4.15) \quad \sum_J P_J = 1.$$

Hence in equilibrium in our system the number of electrons in the  $\ell^{\text{th}}$  region will be

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$$(4.16) \quad n_l = \sum_J n_{Jl} P_J.$$

Substitute in (4.16) the appropriate expressions from (4.12), (4.13), (4.14), introduce the quantity  $\alpha''$  by the relation

$$(4.17) \quad \alpha' = n\alpha'' = \alpha'' \sum_i n_{Ji}$$

and carry out the indicated operations to first order terms in the  $V_{ij}$ . The treatment is characteristic of the grand ensemble method. The manipulations are tedious and somewhat tricky but the result is comparatively simple, namely

$$(4.18) \quad n_l = c_l p_l \left\{ 1 - \beta q_l \left[ [(\bar{n}_l - 1) - 2(c_l - 1)p_l] \frac{V_{ll}}{2} + \frac{1}{2} \sum_{i \neq l} n_i V_{li} - \sum_{i \neq l} c_i p_i V_{il} \right] \right\}.$$

where

$$(4.19) \quad q_l = 1 - p_l.$$

$$(4.20) \quad p_l = \left\{ 1 + \exp \left\{ \alpha'' + \beta \left[ \epsilon_l + \frac{1}{2} \sum_{j \neq l} \bar{n}_j \bar{V}_{lj} + \frac{1}{2} (\bar{n}_l - 1) \bar{V}_{ll} \right] \right\} \right\}^{-1}.$$

We now choose the arbitrary parameters so that the first order terms in (4.18) vanish identically. This gives

$$(4.21) \quad \bar{n}_i = 2 c_i p_i \quad i \neq l$$

$$\bar{n}_l = 1 + 2(c_l - 1) p_l$$

Although the two equations in (4.21) seem contradictory, this really is not so, for there is absolutely nothing which forbids us to use a different set  $\bar{n}_j$  for each  $n_l$  in (4.16). Substituting (4.21) into (4.18) and (4.20) gives our answer

$$(4.18a) \quad n_l = c_l p_l$$

$$(4.20a) \quad p_l = \left\{ 1 + \exp \left( \alpha'' + \beta \bar{\epsilon}_l \right) \right\}^{-1}$$

$$(4.22) \quad \bar{\epsilon}_l = \epsilon_l + \sum_{j \neq l} \sigma_j p_j v_{lj} + (\sigma_l - 1) p_l v_{ll}$$

Comparing our results of the last three equations with those of the independent electron treatment, (4.3) for example, shows them to be of the same form, except the energy  $\epsilon_{1z}$  of the independent electron case is replaced by an effective energy  $\epsilon_l$  of (4.22). We have, therefore, justified using an independent electron approximation with each electron subject to some averaged potential of its neighbors, and we have found that potential correct to first order.

We can considerably simplify the result (4.22). Suppose  $l$  represents a bound level. Then the interaction  $v_{lj}$  between the two bound levels can be shown to be exactly the same as that calculated using atomic wave functions which localize both the  $l$  and  $j$  orbitals on one particular ion. The terms in (4.22) due to the interaction of a bound electron with the other bounds is, therefore,

$$\sum_j \frac{n_{jz}}{N_z} v_{lj} + \frac{p_l}{N_z} (\sigma_l - 1) v_{ll},$$

where now the  $v$ 's are the ordinary coulomb and

exchange interactions of atomic theory. By far, the largest contribution comes from the spherically symmetric part of the coulomb integral, usually denoted by  $F^0(i,j)$  in theoretical spectroscopy. It is more convenient, however, to use screening constants  $O_{i,j}$  instead of the  $F^0$ 's, defined by

$$(4.23) \quad O_{i,j} = \frac{F^0(i,j)}{-\left. \frac{d\epsilon_i^0}{dz} \right|_z}$$

The interaction energy of a bound electron with the frees can likewise be approximated by the interaction of an atomic wave function with the charge density of the free electrons in the neighborhood of one particular ion. Suppose, therefore, we break up our crystal into polyhedra, each containing a nucleus and of sufficient size to enclose a negative charge  $Z'e$  where  $Z' = Z - \frac{n_{Zb}}{N_z}$  is the average charge of the nucleus and its bound electrons. Approximate the polyhedra by spheres of the same volume, with radius  $a_{z'}$ . We then have

$$(4.24) \quad \sum_Z \frac{4}{3} \pi a_Z^3 N_Z = V.$$

If the electrons are really completely free, the charge density will be uniform throughout the crystal, and therefore

$$(4.25) \quad \frac{4}{3} \pi a_Z^3 = \frac{Z' V}{n_f}.$$

Moreover, there will be an electrostatic potential

$$(4.26) \quad \phi_f = \frac{Z' e}{2a_Z} \left\{ \frac{r^2}{a_Z^2} - 3 \right\}$$

within each sphere due to the free electrons, and we obtain for the bound  $l$  to free interaction energy

$$(4.27) \quad - \int |\psi_l|^2 \phi_f d\tilde{z} = \frac{Z' e^2}{2a_Z} \left\{ 3 - \left( \frac{r}{a_Z} \right)^2 \right\}^l$$

where  $\overline{r^2}^l$  is the value of  $r^2$  averaged over the  $l$  bound wave function. For a bound state  $l$ , then, the energy  $\overline{\mathcal{E}}_l$  becomes

$$(4.28) \quad \overline{\mathcal{E}}_l = \mathcal{E}_{lZ}^0 - \frac{d\mathcal{E}_l}{dZ} \Big|_Z \left\{ \sum_j \frac{n_{jZ}}{N_Z} \sigma_{l,j} + \frac{PlZ}{N_Z} (\sigma_{lZ} - 1) \sigma_{l,l} \right\} \\ + \frac{Z' e^2}{2a_Z} \left\{ 3 - \left( \frac{r}{a_Z} \right)^2 \right\}^l.$$

To first order in  $\frac{d\mathcal{E}_l}{dZ}$ , this is the same as

$$(4.29) \quad \overline{\mathcal{E}}_l = \mathcal{E}_l^0(Z_l^*) + \frac{Z' e^2}{2a_Z} \left\{ 3 - \left( \frac{r}{a_Z} \right)^2 \right\}^l$$

where

$$(4.30) \quad Z_l^* = Z - \sum_{j \neq l} \frac{n_{jZ}}{N_Z} \sigma_{l,j} - \frac{n_{lZ}}{N_Z} \left( 1 - \frac{1}{\sigma_{lZ}} \right) \sigma_{l,l}$$

We now must rewrite (4.22) for the case that  $l$  represents a free electron. For this purpose, we assume the bound electrons are localized at the nucleus. This is generally an excellent approximation. The free electrons move in the potential

field, which is in each ionic sphere

$$(4.31) \quad \phi = \frac{Z'e}{2a_{Z'}} \left\{ \frac{2a_{Z'}}{r} - 3 + \frac{r^2}{a_{Z'}^2} \right\}.$$

This is due to the nucleus and bound electrons, and the free. The energy  $\mathcal{E}_l$  of (4.22) in this case includes the kinetic energy  $\mathcal{E}_f$  and the interaction with the nuclei, while the other terms in (4.22) give the interactions with other bound and free electrons. All these interactions are just  $-e\bar{\phi}, \bar{\phi}$  being averaged over the volume of the ion. Hence, for a free electron

$$(4.32) \quad \bar{\mathcal{E}}_f = \mathcal{E}_f - \frac{3}{5} \sum_Z \frac{N_Z}{n_f} \frac{Z'^2 e^2}{2a_{Z'}}.$$

We note that the interactions have raised the energies of the bound electrons from the zero order approximation of interaction with the nucleus alone, while for free electrons the energy has been lowered from the different zero order approximation of no interactions. We now shift the zero of energy, so that a free electron with zero kinetic energy has zero total energy, by adding the constant  $\frac{3}{5} \sum_Z \frac{N_Z}{n_f} \frac{Z'^2 e^2}{2a_{Z'}}$ . This will have the advantage that the density of states for the free electrons takes the simple form  $o(\bar{\mathcal{E}}_f)d\bar{\mathcal{E}}_f = o(\mathcal{E}_f)d\mathcal{E}_f$  and hence (4.23) becomes

$$(4.33) \quad n(\bar{\mathcal{E}}_f)d\bar{\mathcal{E}}_f = \frac{o(\mathcal{E}_f)d\mathcal{E}_f}{\alpha^* + \beta\mathcal{E}_f + 1}.$$

Of course, changing the zero of energy has no effect on the occupation numbers, since it merely replaces  $\alpha''$  by another normalization constant

$$\alpha^* = \alpha'' - \frac{3}{5} \beta \sum_Z \frac{N_Z}{n_f} \frac{Z'^2 e^2}{2a_{Z'}}. \quad \text{With this change in zero of energy, (4.29)}$$

becomes

$$(4.34) \quad \bar{\mathcal{E}}_{lZ} = \mathcal{E}_l^{\circ}(Z_l^*) + \frac{Z'e^2}{2a_{Z'}} \left\{ 3 - \left( \frac{r}{a_{Z'}} \right)^2 \right\} + \frac{3}{5} \sum_Z \frac{N_Z}{n_f} \frac{Z'^2 e^2}{2a_{Z'}}.$$

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Now we shall somewhat arbitrarily place our division into bound and free states at the zero in our new energy scale. This means that whenever  $\bar{E}'_{lZ}$  of (4.34) is positive, that state is not bound. In most cases the higher states of an ion have their electrons rather uniformly distributed in the ions sphere and, therefore,  $\left(\frac{r}{a_{Z'}}\right)^{2l} \sim 3/5$ . We can, therefore, generally "out off" the bound states at about

$$(4.35) \quad -E'_l(z_l^*) = 3 \frac{z_l'^2 e^2}{2a_{Z'}} \cdot$$

The relevant equations for calculating the occupation numbers will now be summarized in final form.

$$(4.36) \quad \frac{n_{lZ}}{N_Z} = \frac{\sigma_{lZ}}{\alpha^* + \beta \bar{E}'_{lZ} + 1} \cdot$$

$$(4.37) \quad \bar{E}'_{lZ} = E'_l(z_l^*) + \frac{z_l'^2 e^2}{2a_{Z'}} \left\{ 3 - \left(\frac{r}{a_{Z'}}\right)^{2l} \right\} + \frac{3}{5} \sum_Z \frac{N_Z}{n_f} \frac{z_l'^2 e^2}{2a_{Z'}} \cdot$$

$$(4.38) \quad z_l^* = z - \sum_{j \neq l} \frac{n_{jZ}}{N_Z} \sigma_{l,j} - \frac{n_{lZ}}{N_Z} \left(1 - \frac{1}{\sigma_{l,l}}\right) \sigma_{l,l} \cdot$$

$$(4.39) \quad n(\bar{E}'_f) d\bar{E}'_f = \frac{8\pi V m}{h^3} (2m \bar{E}'_f)^{\frac{1}{2}} \left\{ 1 + \frac{5}{4} \frac{\bar{E}'_f}{mc^2} + \dots \right\} \cdot$$

$$\frac{\alpha^* + \beta \bar{E}'_f + 1}{\alpha^* + \beta \bar{E}'_f + 1}$$

$$(4.40) \quad n_b = \sum_Z N_Z \sum_l n_{lZ} \quad \text{sum for all } \bar{E}'_{lZ} < 0,$$

$$(4.41) \quad n_f = \int_{\bar{E}'_f=0}^{\infty} n(\bar{E}'_f) d\bar{E}'_f \cdot$$

$$(4.42) \quad n = n_b + n_f \cdot$$

$$(4.43) \quad \frac{4\pi}{3} a_{Z'}^3 = \frac{z_l' V}{n_f} ; \quad (4.43a) \quad V = \frac{4\pi}{3} \sum_Z a_{Z'}^3 N_Z$$



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$$(4.44) \quad Z' = Z - \sum_{\ell} \frac{n_{\ell} Z}{N_Z}$$

and as an explicitly equivalent of (4.41)

$$(4.41a) \quad \alpha^* = \ln \frac{2V}{n_f} \left( \frac{2\pi mkT}{h^2} \right)^{3/2} + \frac{15}{8} \frac{kT}{mc^2} - \frac{15}{16} \left( \frac{kT}{mc^2} \right)^2$$

$$\frac{e^{-\alpha^*}}{2^{3/2}} \left( 1 - \frac{15}{16} \frac{kT}{mc^2} \right) + e^{-3\alpha^*} \left( \frac{1}{3^{3/2}} - \frac{1}{16} \right) + \dots$$

This set of equations is somewhat deceptively simple in form, for it must actually be solved by a somewhat lengthy series of successive approximations. If we are given the temperature  $T$  and volume  $V$ , we must assume a set of  $n_{\ell} Z$ , and  $\alpha^*$ , and a set of  $a_{Z'}$  satisfying (4.43). (The latter is, of course, trivial if our system has only one element.) We then calculate  $Z_{\ell}^*$  by (4.38) and by interpolation in a table of energy levels find  $\mathcal{E}_{\ell}^0(Z_{\ell}^*)$ . Meanwhile, by (4.44) calculate  $Z'$ . We can then immediately get  $\mathcal{E}_{\ell}^1$  and by (4.36) a new set of  $n_{\ell} Z$ . By (4.40) we get  $n_b$  which with (4.42) gives  $n_f$ . Employing  $n_f$  in (4.41a) we arrive at a new  $\alpha^*$ . Moreover, using (4.43a) gives a new set of  $a_{Z'}$ . Continuing this cycle, we can establish our final occupation numbers. The tables of screening constants  $\sigma_{i,j}$ , energy levels, and  $r^{\frac{1}{2}\ell}$  needed for the calculation are presented here as Table 2, 3, and 4 respectively.

One approximation made in the foregoing set of equation is the assumption of the uniform charge distribution of the free electrons. An improvement on this approximation, which also demonstrates the range of its validity, is given in Appendix II.

## 5. Ionic Occupation Numbers.

A somewhat different model for our system was mentioned briefly in the last section - the ionic model. We shall now describe the basis for this model somewhat more fully, show its relevancy to the opacity problem, and indicate how our previous results may be applied in this case.

We know that if an electron is in a state of sufficiently low energy, it will be temporarily bound to one nucleus. Because of the high coulomb barrier between neighboring nuclei, it will remain bound for a considerable time - indeed it would be improper to use atomic wave functions for the electron unless it remained bound for times long compared to the time of revolution of its Bohr orbit. Naturally, several electrons may be bound to the same nucleus at the same time. The interactions between the electrons will not be expressible in terms of the treatment we have hitherto used, for the correlations which were neglected are now of decisive importance. For example, a nucleus with two bound K electrons will behave much differently, particularly with regard to its spectrum, than one with 2K and four bound L electrons. We can take these correlations into account by abandoning our simple "product of one electron functions" approximation and using instead functions which depend upon all the coordinates of the bound electrons of each nucleus. This is equivalent to describing our system as composed of many different ions in a dynamic equilibrium in a sea of free electrons. Applying the statistical mechanics appropriate for systems undergoing "chemical" reactions, we can get, for example, the number of ions of each type in our system, and the distribution of the ions among ionic quantum states. Essentially the same result is obtained by the use of the canonical ensemble treatment for dependent particle systems if we appropriately express the energy of the system as the sum of ionic energies, free electron energies, and interaction energies between these components. The latter method has the advantage that we are able to take into account, to first order at any rate, the interactions of the free electrons and ions. This model, which is certainly to be preferred to that of the previous section, gives the spectrum of our system as the superposition of the many different ionic spectra. It is precisely this very rich line spectrum which causes the lines to be so important in the opacity problem.

Despite the apparent dissimilarity of the ionic and "one-electron function" models, we can show an intimate relationship between the two. In our ionic model we may use for each ion the conventional treatment of many electron ions. This consists in expressing the wave function of the ion as antisymmetrized products of one-electron functions and then carrying out perturbation calculations - usually only to first order. Suppose we then neglect all but the spherically symmetric coulomb interaction. This makes many of the ionic levels degenerate, of course, but the energy changes are so slight as not to change the ionic occupations. If we then take the average number of electrons in a particular orbital throughout all the ions in our system, we get, to first order, the results of section 4. The useful point about this relationship is that we can use the occupation numbers of section 4, giving the average occupation, to find the ionic occupations to good accuracy without the need of starting off afresh in a laborious calculation from the ionic model. Thus the work of the previous section gave the number of electrons  $\frac{n_l Z}{N_Z}$  in the  $l^{\text{th}}$  level of an ion of nuclear charge  $Z$ , or alternatively  $P_{lZ} = \frac{n_l Z}{n_l Z}$  the probability of occupation of the states of that level. From this

we calculate the probability of finding an ion in our system with several bound electrons arranged to give some particular quantum state of the ion. For example, the probability of having an ion with electron configuration  $(1s)^2 (2s \frac{1}{2}) (3p_{3/2})$  in the K, L and M shells, whatever the configuration of the higher shells may be, is

$$(4.45) \quad P_{1s}^2 \times 2P_{2s} q_{2s} \times q_{2p_{\frac{1}{2}}}^2 \times q_{2p_{3/2}}^4 \times q_{3s}^2 \times q_{3p_{\frac{1}{2}}}^2 \times 4P_{3p_{3/2}} q_{3p_{3/2}}^3 \times q_{3d_{3/2}}^4 \times q_{3d_{5/2}}^6$$

where

$$(4.46) \quad q_l = (1 - p_l).$$

In general the probability of having an ion with  $n_l$  electrons in the  $l^{\text{th}}$  level regardless of the occupation of the other levels is given by the binomial distribution

$$(4.47) \quad P_{\nu l} = \frac{c_l!}{\nu l! (c_l - \nu l)!} p_l^{\nu l} q_l^{c_l - \nu l}$$

As is well known, for large  $c_l$  and small  $p_l$ , (which is the case for the higher bound levels of an ion) this reduces to the Poisson distribution

$$(4.48) \quad P_{\nu l} \sim \frac{\bar{\nu l}^{\nu l}}{\nu l!} e^{-\bar{\nu l}}; \quad \bar{\nu l} = c_l p_l.$$

The ionic model gives a simple physical interpretation to the rather surprising looking formulae of section 4. Consider, for example, the term

$$-\frac{d\epsilon_l}{dz} \frac{n_{jZ}}{N_Z} \sigma_{l,j}' \quad \text{in (4.28) the energy } \bar{\epsilon}_l. \quad \text{The factor } -\frac{d\epsilon_l}{dz} \sigma_{l,j} \text{ is the inter-}$$

action between the  $j^{\text{th}}$  and the  $l^{\text{th}}$  bound electron levels in an ion. Averaging over all the ions of the system, some having no electrons in the  $j^{\text{th}}$  level, others having one, others having two, etc. gives precisely the term we are considering.

Again consider the ions which definitely have one electron in the  $l^{\text{th}}$  level. The average occupation among these ions of the other  $c_{lZ}-1$  states in the level is

$$p_{lZ}(c_{lZ}-1). \quad \text{The average interaction energy between one particular } l \text{ electron and the others then is just } p_{lZ}(c_{lZ}-1) \sigma_{l,l} \left( \frac{d\epsilon_l}{dz} \right). \quad \text{This is precisely the}$$

third term in (4.28). We see that the energies involved in the dependent electron treatment are averages over the ions of the system. Going a little further, we can show that (4.28) is actually the average ionization energy of an  $l^{\text{th}}$  level electron in our ionic system. To prove this, we note that if an ion has  $x_j$  electrons in the  $j^{\text{th}}$  level, its energy to first order is approximately

$$E(x_1, x_2, \dots, x_l, \dots) = \sum_j x_j \epsilon_{jZ}^0 + \frac{1}{2} \sum_i \left( \sum_{j \neq i} x_i x_j F^0(i, j) + \sum_i x_i \frac{x_i - 1}{2} F^0(i, i) \right)$$

so that the ionization energy of the  $l^{\text{th}}$  electron is

$$E(x_1, x_2, \dots, x_l, \dots) - E(x_1, x_2, \dots, x_{l-1}, \dots) = \epsilon_{lZ}^0 + \sum_{j \neq l} x_j F^0(l, j) + (x_l - 1) F^0(l, l).$$

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Averaging this ionization energy over all the ions having at least one bound *l* electron gives (4.28) except for the terms involving the interactions with the free electrons.

This completes our discussion of the occupation numbers in our system, which are needed to get the absorption coefficient.

#### 6. The Influence of Nuclear Motion.

Thus far we have considered the nuclei as fixed in a lattice position. This is justified, since neither the bound nor free wave functions depends appreciably on the relative position of nuclei. All our occupation numbers are, therefore, correct. There are two phenomena, however, which depend on the nuclear motion: 1) the total energy of the system has a contribution from the kinetic and potential energies of the nuclei; 2) in their motion, nuclei will exert varying electric fields upon the bound electrons of neighbors, thus causing Stark effect shifts and splittings of the spectral lines. The first effect is of some small importance in the thermodynamic properties of our system, while the second may be very important in influencing the effect of lines on the opacity.

The result of separating the wave equation for our entire system so as to give the electronic energy separately, describes the motion of the nuclei as if proceeding in a potential determined by the electronic energy. This potential is in our case approximately the classical potential of an assembly of positive ions moving in a uniform charge density due to the free electrons. We treat this potential in two limiting cases. Assume first that the nuclei are at lattice positions, which configuration represents the zero of potential energy. For small deviations from this position the potential increases. For example, the change in potential energy, if a single ion of effective charge  $Z^+$  is at a small distance  $r$  from its equilibrium position is

$$(4.49) \quad Z'e \left[ \phi_f(r) - \phi_f(0) \right] = \frac{Z'^2 e^2}{2a_{Z'}} \frac{r^2}{a_{Z'}^2} = \mathcal{E}(r),$$

where  $\phi_f$ , given by (4.26), is the electrostatic potential of the free electrons. So long as (4.49) holds, the nuclei will perform simple harmonic vibrations about their position of equilibrium. The heavy mass of the nuclei will make the frequency so low that the contribution to the energy of the system is classical

$$(4.50) \quad E_{\text{nuclei}} = 3NkT.$$

Continuing the treatment of this approximation, we consider the Stark effect due to this motion. The number of ions with displacement  $r$  to  $r+dr$  is

$$(4.51) \quad N(r)dr = N_Z \frac{4\pi r^2 \exp(-\mathcal{E}(r)/kT) dr}{\int_0^{a_{Z'}} 4\pi r^2 \exp(-\mathcal{E}(r)/kT) dr},$$

where  $\mathcal{E}(r)$  is given by (4.49). Carrying out the integration gives

$$(4.52) \quad \frac{N(r)dr}{N_Z} = \frac{\left(\frac{sr}{a_{Z'}}\right)^2 \exp\left(-\left(\frac{sr}{a_{Z'}}\right)^2\right) d\left(\frac{r}{a_{Z'}}\right)}{\sqrt{\frac{\pi}{4}} \operatorname{erf} s - (s/2) \exp - s^2}.$$

where

$$(4.52a) \quad \operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy,$$

and

$$(4.53) \quad s^2 = \frac{Z'^2 e^2}{2kT a_{Z'}}.$$

One important result of this formula is obvious: the Stark effect dispersion will fall off exponentially with distance from the line center.

To examine the range of applicability of this approximation, we calculate the average displacement

$$(4.54) \quad \frac{\bar{r}}{a_{Z'}} = \int_0^{a_{Z'}} \frac{r}{a_{Z'}} \frac{N(r)dr}{N_{Z'}} = \frac{1}{2s} \frac{\left\{ 1 - e^{-s^2(s^2+1)} \right\}}{\frac{\sqrt{\pi}}{4} \operatorname{erf} s - (s/2)e^{-s^2}} .$$

For  $s \gg 1$  this becomes

$$(4.54a) \quad \frac{\bar{r}}{a_{Z'}} \sim \frac{2}{\sqrt{\pi} s} ,$$

while for  $s \ll 1$

$$(4.54b) \quad \frac{\bar{r}}{a_{Z'}} = \frac{3}{4} \left( 1 - \frac{s^2}{1s} \right) .$$

The expansion shows that for  $s \ll 1$ , that is high temperature, low density (large  $a_{Z'}$ ) or small nuclear charge, the average displacement of the nuclei will be  $3/8$  of the average internuclear distance. This is the result if the nucleus could be with equal probability at any point in the sphere. In this case we could scarcely speak of harmonic vibrations and the method of treatment is not applicable. For large  $s$  however, that is low temperature, high density, and/or high nuclear charge, (4.54a) shows our approximation to be adequate. Figure 2 shows the behavior of the  $\bar{r}/a_{Z'}$  as a function of  $s$ .

For the cases where the approximation is valid, the electric field on a nucleus situated at  $r$  is directed toward the lattice point and has magnitude

$$(4.55) \quad \left| \vec{E} \right| = \frac{d}{dr} \phi_f = \frac{Z'e}{a_{Z'}^2} \frac{r}{a_{Z'}} .$$

The distribution of nuclear positions will lead to a distribution of electric field magnitudes, and hence a continuous dispersion of the observed spectral lines of the assembly of ions. The fraction of ions of effective charge  $Z'$  which will be subject to a field of between  $|\vec{E}|$  and  $|\vec{E} + d\vec{E}|$  is

$$(4.56) \quad \frac{N_{Z'}(|\vec{E}|) d|\vec{E}|}{N_{Z'}} = \frac{s^3 \left( \frac{a_{Z'}^2}{Z'e} \right)^3 |\vec{E}|^2 d|\vec{E}| \exp \left[ -s^2 \left( \frac{a_{Z'}^2}{Z'e} \right)^2 |\vec{E}|^2 \right]}{\frac{\sqrt{\pi}}{4} \operatorname{erf} s - s/2 e^{-s^2}} .$$

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Fermula (4.55), while correct in order of magnitude, does not tell the whole story, for neighboring ions will be displaced from their equilibrium <sup>position</sup> and give rise to a dipole field. The resultant of all dipoles will give a field of the same order as (4.55). Moreover, in applications to Stark effect, it should be remembered that the field (4.55) is radial, not linear as in the usual considerations.

We now turn to the case where  $S \ll 1$  and harmonic vibrations do not describe the motion. Here the nuclei may wander rather freely about, except when one nucleus makes a very close approach to another. The energy contribution will be essentially that of a perfect gas

$$(4.57) \quad E_{\text{nuclei}} = 3/2 NkT.$$

The spatial distribution of the ions will be determined by their mutual potential energy for close approaches. To good approximation this is simply

$$(4.58) \quad \mathcal{E}(r_{12}) = \frac{Z'Z''e^2}{r_{12}} \quad \text{for } r_{12} < \frac{a_{Z'} + a_{Z''}}{2}$$

$$\mathcal{E}(r_{12}) = 0 \quad \text{elsewhere.}$$

Then

$$(4.59) \quad N(r_{12})dr_{12} = \frac{N_{Z'}}{V} e^{-\mathcal{E}(r_{12})/kT} 4\pi r_{12}^2 dr_{12}.$$

The electric field felt by the ion  $Z''$  as it approaches  $Z'$  is

$$(4.60) \quad |\vec{\mathcal{E}}| = \frac{Z'e}{r_{12}^2},$$

so that the number of ions in fields between  $|\vec{\mathcal{E}}|$  and  $|\vec{\mathcal{E}}| + d|\vec{\mathcal{E}}|$  is

$$(4.61) \quad \frac{N_{Z''}(|\vec{\mathcal{E}}|) d|\vec{\mathcal{E}}|}{N_{Z''}} = \frac{2\pi}{V} \frac{(Z'e)^{3/2}}{|\vec{\mathcal{E}}|^{5/2}} d|\vec{\mathcal{E}}| \exp - \frac{|\vec{\mathcal{E}}|^{1/2}(Z'e)^{3/2}}{kT}.$$

Here again we can see that the Stark effect dispersion will fall off exponentially.



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## 7. Fluctuations.

The quantum mechanical treatment we have used did not actually find the stationary energy levels of our system. The approximations which we were forced to introduce had the result that we treated the ions as if they were independent systems, and then we introduced interactions between other ions and the free electrons as perturbations. The true stationary states, of course, will resemble the zero order approximation except that interactions will have removed some of the degeneracy. This splitting is very important as a source of line breadth. To include this splitting we can consider the interactions as time dependent perturbations or fluctuations.

One of these fluctuations is caused by the nuclear motions just discussed in section 6. The nuclei being so massive can be thought of classically. Since they have in equilibrium the same energy as the electrons, their velocity will be a factor  $\sqrt{\frac{m}{M}}$  smaller. ( $M$  is the nuclear mass,  $m$  the electronic mass). The motion will be so slow compared to that of the electrons that we may use the adiabatic approximation for the interactions. The result is that electronic levels are shifted by a Stark effect when two nuclei approach, but no electronic transitions are induced.

If we thought of the free electrons classically, they would be randomly distributed in space. We would then obtain considerable density fluctuations in the neighborhood of each ion and it might be imagined these effects must be considered. Our quantum mechanical treatment of the free electrons, however, is much closer to the truth. We must really consider the wave function of a free electron to extend throughout the solid. This eliminates the density fluctuations. But, because we have neglected correlations, there is another effect we have missed. This is the collision of free electrons with the ions. Since this is a fast process, it will induce transitions from one ionic state to another, giving the states a collision breadth. It is well known that such breadth gives the same form of dispersion as the natural breadth.

V. EFFECT OF LINES ON OPACITY.METHODS FOR TREATING LINE CONTRIBUTION.1. Separation of Line Contribution

The Rosseland mean opacity  $K$  as is shown in Chapter III (3.24) and (3.15) is a weighted average absorption coefficient given by

$$(5.1) \quad \Lambda = \frac{1}{\rho K} = \int_0^{\infty} \frac{W(u)}{\mu u^3} du,$$

where

$$(5.2) \quad W(u) = \frac{15}{4\pi^4} u^7 e^{2u} (e^u - 1)^{-3},$$

and

$$(5.3) \quad \mu = \mu_{\text{abs}} + \mu_{\text{scatt}} (1 - e^{-u})^{-1}.$$

It is usually convenient to consider the absorption coefficient resolved into two terms

$$(5.4) \quad \mu = \mu_0 + \mu_l.$$

$\mu_0$  being the absorption due to continuous processes alone, and  $\mu_l$  the absorption due to the lines. The reason for this division is that  $\mu_0$  is a moderately smooth function of frequency except at the location of an absorption edge, while  $\mu_l$  is a very ragged function with sharp maxima at the frequency of each absorption line.

Substituting (4) in (1) and introducing the notation

$$(5.5) \quad r = \frac{\mu_l}{\mu_0}; \quad P = \frac{1}{1+r},$$

we get for the mean free path

$$(5.6) \quad \Lambda = \frac{1}{\rho K} = \int_0^{\infty} P \frac{W(u) du}{\mu_0 u^3} = \Lambda_0 - \Lambda_l.$$

where

$$(5.7) \quad \Lambda_c = \int_0^{\infty} \frac{w(u) du}{\mu_c u^3} \quad .$$

and

$$(5.8) \quad \Lambda_l = \int_0^{\infty} \frac{\kappa}{1+\kappa} \frac{w(u) du}{\mu_c u^3} \quad .$$

The latter form of (5.5) shows how the lines reduce the mean free path from the value  $\Lambda_c$  obtained by considering continuous processes alone. The contribution  $\Lambda_c$  of the continuous processes has been treated by all workers in the field of stellar opacities with varying degrees of completeness, but the contribution of lines has hitherto been ignored.

## 2. Effect of a single line

To understand the effect lines make on the opacity, and to help in developing methods of treating lines, we start by considering the simplest case of a spectrum with only one line. The line absorption coefficient in that case is (c.f. equation (2.9))

$$(5.9) \quad \mu_l(\nu) = \frac{\pi e^2}{mc} \frac{N^l}{V} f_{ba} b_{ba}(\nu) \quad .$$

where  $b(\nu)$ , the dispersion factor shows the frequency dependence of the absorption.  $b(\nu)$  has a sharp maximum at  $\nu = \nu_0$ , the frequency of the center of the absorption line, and is so normalized that

$$(5.10) \quad \int_0^{\infty} b(\nu) d\nu = 1 \quad .$$

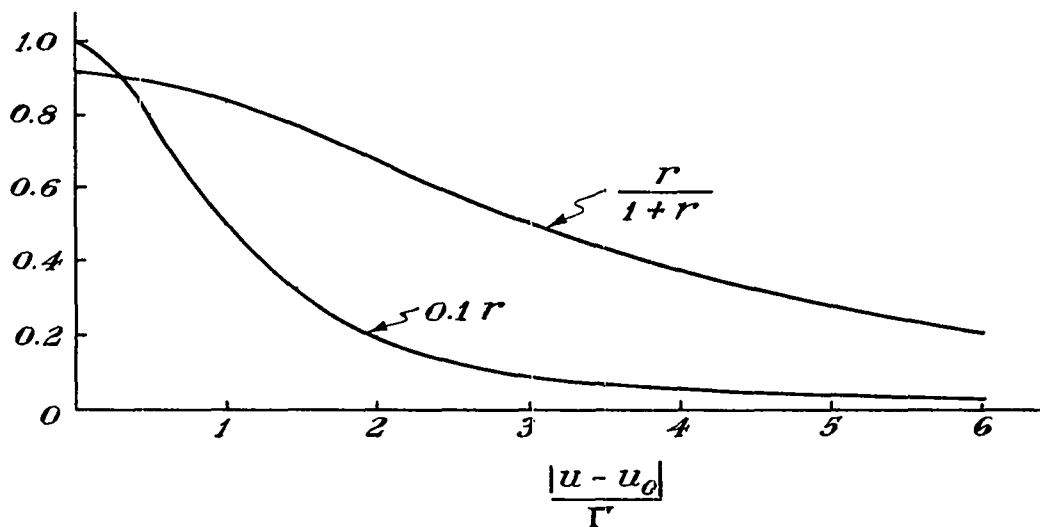
Without considering further details, we can see qualitatively what is the contribution of this single line to the opacity. Dropping the subscripts for the moment, we have

$$(5.11) \quad \frac{\kappa}{1+\kappa} = \frac{1}{1 + \frac{S}{N f b'}} \quad .$$

where

$$(5.11a) \quad S = \frac{kT}{h} \frac{mc}{\pi e^2} \nu \mu_0 ; \quad b'(u) = \frac{kT}{h} b(\nu).$$

The frequency variation of this function for a typical case is shown in the accompanying figure. It is seen that this function



approaches unity when  $r$  is a maximum at the frequency of the center of the line, decreases slowly with displacement from the center until it becomes  $\frac{1}{2}$  when the line absorption is equal to the continuous absorption background. The variation of the function in the neighborhood of  $\frac{1}{2}$  is rapid, the transition from values near unity to values near zero occurring within a small frequency range. For greater displacements the function falls off rapidly, soon behaving simply as  $r$ . The contrast between the function  $r$  which one might naively expect to determine the line effect and  $r/(1+r)$  is marked. Whereas  $r$  drops to  $\frac{1}{2}$  its value at  $(u-u_0) = \Gamma$ , we find that  $r/(1+r)$  drops to half its value only at  $(u-u_0) \sim 3\Gamma$ .

The integral (5.8) giving the contribution of the line is approximately

$$(5.12) \quad \Delta l = \int_0^{\infty} \frac{r}{1+r} du \left. \frac{W(u)}{\mu_0 u^3} \right|_{u=u_0},$$

since the integrand is negligible except for frequencies near  $\nu = \nu_0$ . What is

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important then is  $\int_0^{\infty} \frac{r}{1+r} du$ . The greatest part of the contribution to this integral comes in the range where  $r/(1+r) \cong 1$ ; practically nothing is contributed by regions where  $r/(1+r) < \frac{1}{2}$ . Thus if  $w$  is the distance between  $u_0 = h\nu_0/kT$  and the frequency  $u = h\nu/kT$  at which  $r=1$ , the integral is approximately

$$(5.13) \quad \Delta = \frac{W(u)}{c u^3} \Big|_{u=u_0} \times 2w.$$

The quantity  $2w$  we shall term the wingspread of the line upon its continuous background. It is this quantity, as is shown by (5.13), rather than the dispersion breadth of the line which determines the contribution of the line to the opacity. We may actually think of the line, according to (5.13), as leaving the transmission of light unaffected throughout the spectrum except in the region of its wingspread, where it completely blocks the transmission.

The wingspread of the line is determined by the condition

$$(5.14) \quad \frac{Nf}{S} b'(w-u_0) = 1;$$

thus it depends on the ratio of line strength  $Nf$  to continuous background, and the dispersion. Even a line which has very small dispersive breadth may have a considerable wingspread if it is strong enough. On the other hand, a broad line may have very small or zero wingspread if it is weak compared to its background. Arguments for neglecting line contributions because of the small dispersive breadths alone are, therefore, incorrect. Another important conclusion we may draw is the following. Since the wingspread does not depend on the position of the line, the line contribution in the case of an isolated line is not sensitive to position.

Suppose we consider first an artificial example of a line with a rectangular shaped dispersion

$$(5.15) \quad \begin{cases} b(\nu) = \frac{1}{2\Delta\nu} & \text{for } \nu_0 - \Delta\nu \leq \nu \leq \nu_0 + \Delta\nu, \\ b(\nu) = 0 & \text{otherwise.} \end{cases}$$

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Then

$$(5.16) \quad \int_0^{\infty} \frac{r}{1+r} du = \int_{u_0 - \Delta u}^{u_0 + \Delta u} \frac{du}{1 + \frac{S}{Nf} 2 \Delta u} = \frac{1}{\frac{1}{2 \Delta u} + \frac{S}{Nf}} .$$

If the line absorption is very strong, compared to the continuous absorption, we obtain the obvious result that

$$(5.17) \quad \Delta_{\ell} = \left. \frac{W(u)}{\mu_0 u^3} \right|_{u=u_0} \times 2 \Delta u,$$

that is, the line eliminates the entire transmission of the frequency intervals  $2 \Delta u$ . It seems at first sight a little amazing that this result does not depend on  $Nf$ , the line strength, for this implies that a line 10 times as strong as another will have just the same effect on opacity. But a little reflection shows that if a line completely absorbs the radiation in an interval, it already has a maximum effect in reducing the transmission. A stronger line can do no more. On the other hand, if the line absorption coefficient is weak compared to the continuous background, that is

$$(5.18) \quad \frac{Nf}{2 \Delta u S} \ll 1,$$

we get

$$(5.19) \quad \Delta_{\ell} = \left. \frac{W(u)}{\mu_0 u^3} \right|_{u=u_0} \frac{Nf}{S} .$$

Here we get the important result (in contrast to (5.17) above) that the effect of the line is directly proportional to its integrated strength  $Nf$ , but is independent of the dispersion interval  $2 \Delta u$ . As an immediate consequence of this, we have that  $\Delta_{\ell}$  is independent of the dispersion shape whatever that may be, so long as the analogue to (5.18) is fulfilled. This is a very important result, for weak lines; that is, lines for which  $Nf b'_{\max}(u)/S \ll 1$  always give the contribution (5.19) and it is unnecessary to inquire into the details of the dispersion. Since most of the lines in a spectrum are of this nature, (5.19) solves a great deal of the problem.

Proceeding now to the actual types of dispersion we shall encounter, the specific case of natural and/or collision breadth has the dispersion formula (c.f. (2.15)),

$$(5.20) \quad b(\nu) = \frac{\gamma}{4\pi^2(\nu - \nu_0)^2 + \gamma^2/4} ; \quad b'(u) = \frac{1}{\pi} \frac{\Gamma}{(u-u_0)^2 + \Gamma^2} ,$$

where  $\gamma/4\pi$  is the half breadth, and

$$(5.21) \quad \Gamma = \frac{h\gamma}{4\pi kT} .$$

The wingspread  $w$  is obtained from (5.14) giving

$$(5.22) \quad w = \left\{ \frac{Nf\Gamma}{\pi S} - \Gamma^2 \right\}^{\frac{1}{2}} = \left\{ \frac{Nf\Gamma}{\pi S} \right\}^{\frac{1}{2}} ,$$

the latter approximation being valid if

$$(5.23) \quad \frac{\pi S \Gamma}{Nf} \ll 1 ,$$

i.e. if  $\Gamma \ll w$ , a condition which is frequently the case. The wingspread is then proportional to  $\Gamma^{\frac{1}{2}}$  and to the square root of the line strength  $(Nf)^{\frac{1}{2}}$ . Carrying out the integration of (5.12), we get

$$(5.24) \quad \Delta \ell = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} \pi \left( \frac{Nf\Gamma}{\pi S} \right)^{\frac{1}{2}} \left\{ 1 + \frac{\pi S \Gamma}{Nf} \right\}^{-\frac{1}{2}} .$$

In the case where  $\pi S \Gamma / (Nf) \ll 1$  we may put the last factor equal to 1. In just this case the wingspread is given by the simplified form of (5.22) and the result is

$$(5.25) \quad \Delta \ell = \frac{\pi}{2} \times 2w \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} .$$

The fact that the line blacks out a frequency interval  $\pi/2$  times the wingspread is a confirmation of the general qualitative result in (5.13). The reason the numerical factor is so different (1.57 instead of 1) is that the natural breadth dispersion gives appreciable absorption even rather far from the line center. We shall generally speak of the extra contribution to the opacity of regions

beyond the wing spread as a "tail" effect, because it is due to the tail ends of the dispersion curve.

In the other extreme case of weak lines (5.24) reduces to

$$(5.26) \quad \Delta \nu = \frac{W(u)}{u^3} \Big|_{u=u_0} \frac{Nf}{S} \cdot$$

This result is precisely the same as (5.19) for the case of step-like dispersion, and is a special illustration of the general validity of the weak line formula, regardless of type of dispersion or breadth.

Turning next to the case of Doppler broadening, the dispersion is

$$(5.27) \quad b(\nu) = \frac{h}{kT} \left\{ \frac{Mc^2}{2\pi kTu_0^2} \right\}^{\frac{1}{2}} \exp - \left\{ \frac{Mc^2}{2kT} \frac{(u-u_0)^2}{u_0^2} \right\} \cdot$$

The half breadth is given by the value  $\gamma$  which makes

$$(5.28) \quad b(\gamma - \nu_0) = \frac{1}{2} b(\nu_0).$$

We see from (5.28) and (5.27) that

$$(5.29) \quad \gamma = \frac{h\gamma}{kT} = u_0 \left\{ \frac{2kT}{Mc^2} \ln 2 \right\}^{\frac{1}{2}} \cdot$$

The wingspread, however, is given by the condition that

$$\frac{Nf}{S} \left\{ \frac{Mc^2}{2\pi kTu_0^2} \right\}^{\frac{1}{2}} \exp - \left\{ \frac{Mc^2 w^2}{2kTu_0^2} \right\} = 1 \cdot$$

whence

$$(5.30) \quad w = \left\{ \frac{2kTu_0^2}{Mc^2} \ln \left[ \frac{Nf}{S} \left( \frac{Mc^2}{2\pi kTu_0^2} \right)^{\frac{1}{2}} \right] \right\}^{\frac{1}{2}} \cdot$$

Thus

$$(5.31) \quad w = \gamma \left\{ 1.443 \ln \left[ .4696 \frac{Nf}{S\gamma} \right] \right\}^{\frac{1}{2}} \cdot$$

Aside from the logarithmic factor, the expressions for the wingspread (5.30) and the dispersion breadth agree. This is, of course, due to the exponentially falling off of the dispersion curve with distance from the line center; as a conse-



quence, the line has effective absorption only in the region of its dispersion breadth.

The actual contribution of the line with Doppler breadth to the opacity is from (5.11), (5.12), and (5.27)

$$(5.32) \quad \chi_{\ell} = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} \int_0^{\infty} \frac{du}{1 + \frac{\sqrt{\pi} SB^{-\frac{1}{2}}}{Nf} e^{\frac{1}{2}3(u-u_0)^2}}$$

where

$$(5.33) \quad B = \frac{Mc^2}{2kTu_0^2}$$

We can express the integral as

$$(5.34) \quad \chi_{\ell} = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} \frac{\sqrt{\pi}}{a} \sum_{n=1}^{\infty} (-1)^{n-1} \left(\frac{B^{\frac{1}{2}}}{a}\right)^{n-1} \frac{1}{n^{\frac{3}{2}}}; \quad a = \frac{\sqrt{\pi} S}{Nf}$$

which for small values of  $B^{\frac{1}{2}}/a$  develops as

$$(5.35) \quad \chi_{\ell} = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} \frac{Nf}{S} \left\{ 1 - \frac{Nf}{S} \frac{1}{\sqrt{2\pi}} \left(\frac{Mc^2}{2kTu_0^2}\right)^{\frac{1}{2}} + \dots \right\}$$

The leading terms of this expansion is the weak line result (5.19) as should indeed be expected, for the condition

$$(5.36) \quad \frac{B^{\frac{1}{2}}}{a} = \frac{Nf}{S} \left(\frac{Mc^2}{2\pi kTu_0^2}\right)^{\frac{1}{2}} \ll 1$$

means that the lines are weak.

For large values of  $B^{\frac{1}{2}}/a$ , the analytic form (5.34) is inconvenient for calculation. We then develop the integral from (5.32) as

$$\int_0^{\infty} \frac{x^{-\frac{1}{2}} dx}{\frac{1}{B^{\frac{1}{2}}} + e^x} = \int_0^{\ln \frac{B^{\frac{1}{2}}}{a}} \frac{x^{-\frac{1}{2}} dx}{\frac{B^{\frac{1}{2}}}{a} (1 + \frac{B^{\frac{1}{2}}}{a} e^x)} + \int_{\ln \frac{B^{\frac{1}{2}}}{a}}^{\infty} \frac{x^{-\frac{1}{2}} dx}{e^x (1 + \frac{B^{\frac{1}{2}}}{a} e^{-x})}$$

The leading term in the development is  $2(a/B^{\frac{1}{2}}) \sqrt{\ln B^{\frac{1}{2}}/a}$

whence

$$(5.37) \quad \Lambda_{\ell} = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u_0} \times 2w.$$

The higher order terms constitute a tail effect.

It is instructive to compare the effect of two lines having the same total strength and the same half breadth, although the dispersion in one is caused by natural and/or collision breadth, while in the other it is caused by Doppler breadth. For weak lines (5.19) tells us the result is identical. For strong lines, we have

$$(5.38) \quad \frac{\Lambda_{\ell} \text{ natural}}{\Lambda_{\ell} \text{ Doppler}} = 1.57 \left\{ \frac{Nf}{\pi S \Gamma} \right\}^{\frac{1}{2}}.$$

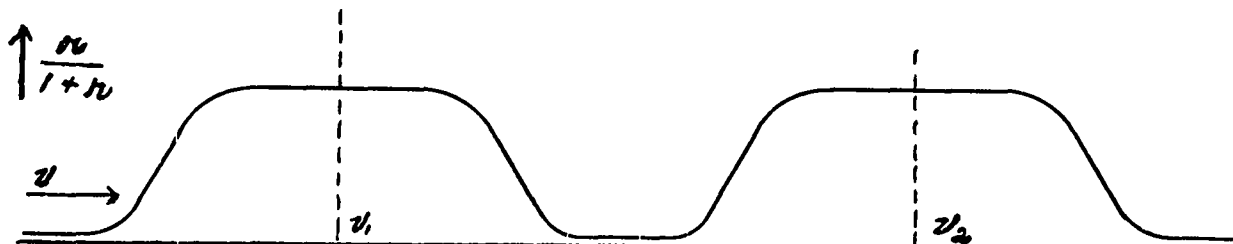
For the case of strong lines this ratio is always much greater than unity. We can, therefore, conclude that the natural breadth dispersion is always as effective as or more effective than Doppler dispersion in increasing the opacity.

### 3. Effect of Two Lines.

Now that we understand the contribution of a single line to the opacity, we can investigate the effect of a line spectrum. It is characteristic of this problem that the superposition principle does not hold in general, i.e. the effect of lines is not simply additive. Instead, it depends upon the relative positions of the lines. To illustrate this most clearly, we shall consider the contribution of two lines to the opacity. The line absorption coefficient will then be

$$(5.39) \quad \mu_{\ell} = \sum_{j=1}^2 \frac{\pi e^2}{mc} \frac{N_j f_j}{\nu} b_j(\nu)$$

where  $j$  denotes the number of the line. Suppose first that the lines are very far away from each other compared to their wingspread (not their breadth). Then the function  $\frac{x}{1+x^2}$  in the integrand of (5.8) will have two widely separated humps, as illustrated in the accompanying figure.



Since the individual line absorption coefficients in the regions outside the wingspread of a line are very small compared to the continuous absorption, we will have, as suggested by (5.19) and demonstrated later on, that the contributions to the integral of this region are almost precisely additive. Moreover, they are small, so it is not necessary to worry about the very slight deviations from additivity. Within the wingspread of each line, the contribution to  $r$  of the neighboring line is small; the ratio  $r/(1+r)$  is almost unity. Increasing  $r$  slightly will have even less effect on  $r/(1+r)$ . Thus, within the wingspread each line makes the same contribution to the opacity whether its neighbor is present or not. Hence, the overall effect of the two lines is very nearly additive.

The additivity feature breaks down as soon as the wingspread of the lines overlap appreciably. Going to the extreme case of overlapping, we consider two identical lines at the same frequency. The line absorption coefficient will then be

$$(5.40) \quad \mu_2 = 2\mu_1$$

where  $\mu_1$  indicates the line absorption coefficient of the single line.

The ratio  $r/(1+r) = 2r_1/(1+2r_1)$ . Now within the wingspread of the line (if the line is strong  $r_1 \gg 1$ ) we have that  $2r_1/(1+2r_1) \sim 1 \sim r_1/(1+r_1)$ . Hence, the two lines together have no more effect on the transmission than the single line. This result was again foreshadowed by (5.17). The tails of the two lines go as  $2r_1$  compared to  $r_1$  for a single line, and additivity will characterize their contribution. However, the tail effect is usually small, so roughly we have the result that two strongly overlapping lines do not increase the opacity much beyond that resulting from the stronger of the two lines.

Naturally for cases of intermediary overlapping we shall have the situation between the extremes of strict additivity for no overlapping, and no added effect for complete overlapping. Thus, we conclude that the relative position of the

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two lines is critical, although their absolute position is not.

We shall now reinforce these qualitative conclusions with examples for the case of stepwise dispersion, natural breadth dispersion, and Doppler dispersion.

For the case of stepwise dispersion we take

$$(5.41) \quad \begin{cases} b_1(\nu) = \frac{1}{2\Delta\nu_1} & \text{for } \nu_1 - \Delta\nu_1 \leq \nu \leq \nu_1 + \Delta\nu_1, \\ b_1(\nu) = 0 & \text{otherwise,} \end{cases}$$

and similarly with  $b_2(\nu)$ . Then

$$(5.42) \quad \chi = \int_0^\infty \frac{W(u)}{\mu_0 u^3} \frac{r}{1+r} du = \int_0^\infty \frac{W(u)}{\mu_0 u^3} \frac{du}{1 + \frac{S}{\sum_j N^j f_j b_j'(u)}}.$$

If the two steps do not overlap, that is  $\nu_2 - \nu_1 > \Delta\nu_1 + \Delta\nu_2$ , we can break up the integral  $\int_0^\infty = \int_0^{\nu'} + \int_{\nu'}^\infty$  where  $\nu'$  is any frequency  $\nu_1 + \Delta\nu_1 < \nu' < \nu_2 - \Delta\nu_2$  between the steps. In each integral, the integrand is exactly the same as for the case of each line taken alone. Thus

$$(5.43) \quad \int_0^{\nu'} \frac{W(u)}{\mu_0 u^3} \frac{du}{1 + \frac{S}{\sum_j N^j f_j b_j'}} = \int_0^{\nu'} \frac{W(u)}{\mu_0 u^3} \frac{du}{1 + \frac{S}{N^1 f_1 b_1}}$$

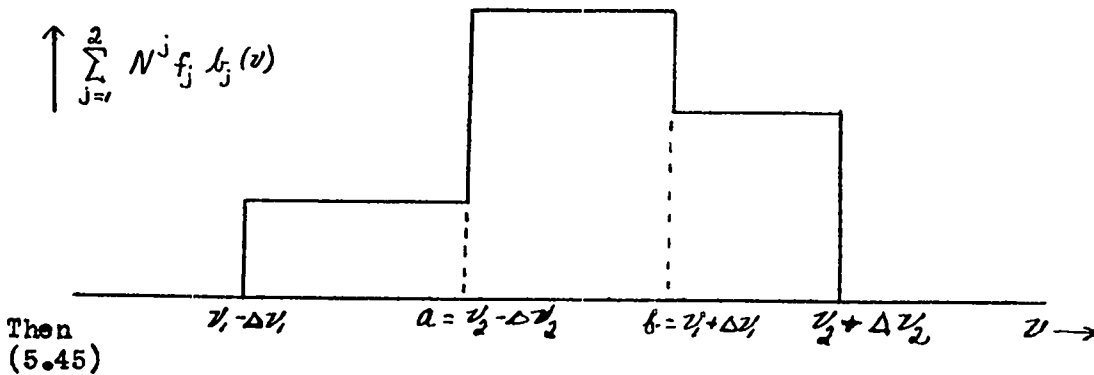
where we have extended the upper limit from  $\nu'$  to  $\infty$  because the integrand is zero in that region. We thus obtain exact auditivity for the no overlapping case.

Suppose now there is some overlapping. Then  $\sum_{j=1}^2 N^j f_j b_j(\nu)$  will behave as

follows:

$$(5.44) \quad \left\{ \begin{aligned} \sum_{j=1}^2 N^j f_j b_j(\nu) &= 0; & \nu < \nu_1 - \Delta\nu_1. \\ &= \frac{N^1 f_1}{2\Delta\nu_1}; & \nu_1 - \Delta\nu_1 \leq \nu \leq a. \\ &= \frac{N^1 f_1}{2\Delta\nu_1} + \frac{N^2 f_2}{2\Delta\nu_2}; & a \leq \nu \leq b. \\ &= \frac{N^2 f_2}{2\Delta\nu_2}; & b < \nu \leq \nu_2 + \Delta\nu_2. \\ &= 0; & \nu_2 + \Delta\nu_2 \leq \nu \leq \infty. \end{aligned} \right.$$

The function is illustrated in the accompanying figure.



$$\Lambda_L \approx \frac{W(u)}{u_c u^3} \Big|_{u=u^*} \left\{ \frac{u_2 - \Delta u_2 - (u_1 - \Delta u_1)}{1 + \frac{S}{N^1 f_1} 2\Delta u_1} + \frac{(u_1 + \Delta u_1) - (u_2 - \Delta u_2)}{1 + \frac{S}{\frac{N^1 f_1}{2\Delta u_1} + \frac{N^2 f_2}{2\Delta u_2}}} + \frac{u_2 + \Delta u_2 - (u_1 + \Delta u_1)}{1 + \frac{S}{N^2 f_2} 2\Delta u_2} \right\}$$

where  $u^*$  is some mean frequency of the two lines whose value is not critical.

In the case where the lines are weak compared to the background, we can neglect the unity in each of the three denominators. We then get

$$(5.46) \quad \Lambda_L \approx \frac{W(u)}{u_c u^3} \Big|_{u=u^*} \left\{ \frac{N^1 f_1}{S} + \frac{N^2 f_2}{S} \right\}$$

that is the contributions are still exactly additive despite the overlapping.

Incidentally this shows that the contributions of any set of weak absorptions upon a strong continuous background are additive, for any line absorption coefficient can be approximated by a series of step functions. In particular the contribution of overlapping line tails are usually additive.

If the lines are strong compared to the background we may neglect the second term in each denominator giving

$$(5.47) \quad \Lambda_L \approx \frac{W(u)}{u^3 u_c} \Big|_{u=u^*} \left\{ u_2 + \Delta u_2 - (u_1 - \Delta u_1) \right\}$$

Here we can definitely see the non additivity of the line contribution but it is even more striking if the lines exactly overlap. Then we get

$$(5.48) \quad \Lambda_L \approx \frac{W(u)}{\mu_c u^3} \Big|_{u=u^*} 2 \Delta u,$$

which is precisely the same as the effect of either line alone.

The general conclusions about additivity hold for the case of natural and/or collision breadth dispersion, but are somewhat influenced by the pronounced tail in this type of dispersion. For the case of two identical lines when the wings spreads do not overlap, the contribution to the opacity is  $\Lambda_L = 2 \Lambda_{L1}$ , where  $\Lambda_{L1}$  is the contribution of each line individually. But suppose the lines are exactly superposed. Then from (5.24) we get

$$(5.49) \quad \Lambda_L = \frac{W(u)}{\mu_c u^3} \Big|_{u=u^*} \pi \left\{ \frac{2Nf_1}{\pi S} \right\}^{1/2} \left\{ 1 + \frac{\pi S \Gamma}{2Nf} \right\}^{-1/2}.$$

For strong lines the last factor is unity and we can see that  $\Lambda_L = \sqrt{2} \Lambda_{L1}$ . The factor  $\sqrt{2}$  is easy to understand, since the contribution of the region inside the wingspread is the same in the case of two lines as with one, while the tail region is additive. Referring to (5.25) we see that the tail contributes  $(\frac{\pi}{2} - 1)$  times the contribution within the wingspread. Thus

$$(5.50) \quad \Lambda_L = \left\{ 2 \left( \frac{\pi}{2} - 1 \right) + 1 \right\} 2w \frac{W(u)}{\mu_c u^3} \Big|_{u=u^*} = 1.364 \Lambda_{L1}.$$

The numerical factor 1.364 is quite close to  $\sqrt{2} = 1.414$ .

For weak lines, on the other hand we may neglect 1 compared to  $\pi S \Gamma / (2Nf)$ , and we get

$$(5.51) \quad \Lambda_L = \frac{W(u)}{\mu_c u^3} \Big|_{u=u^*} \frac{2Nf}{S} = 2 \Lambda_{L1},$$

and thus the contributions are additive.

#### 4. Effect of many line spectrum

From the preceding discussion of the contribution of two lines, the features and difficulties of the treatment of many lines appears. The most critical factor is whether or not the wingspread of the lines overlap. If there is no overlapping the contributions are additive. The case of weak lines which are always additive is really included in the category of non-overlapping wingspread, because the wingspread of a weak line is zero. When overlapping exists no simple treatment is readily available, but we may say the contribution of the lines is less than in the non-overlapping case.

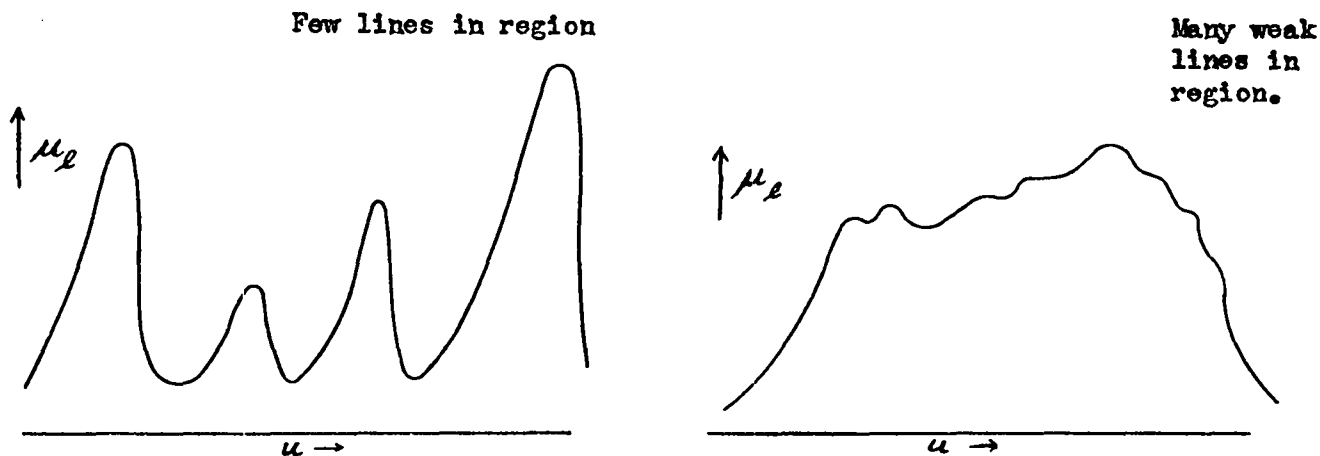
In general, even if the contributions of the lines are additive, the result is still not simple enough to permit ready calculation for a complicated line spectrum, because the effect of thousands of individual lines has to be computed and then summed. This requires knowing the strengths, positions and dispersions of every line. Such a calculation is practical only for a very simple spectrum like that characteristic of a one-electron ion. However, such cases are of some practical importance for often we shall have an assemblage of ions having either no bound electrons at all, or only 1 bound K electron. Even the case of 2 bound K electrons is simple enough, as is also the case of a single bound electron outside a closed shell. The weak line case, however, is much more readily adapted to computation. We can see by our consideration of the step type dispersion that the contribution of the line is independent of the dispersion interval. Generalizing, since any dispersion curve may be made up by superposing steps, we conclude that the effect of weak lines is independent of the dispersion shape and breadth as well. This is confirmed by the specific results for natural breadth dispersion and Doppler dispersion. Hence the  $j$ th weak line gives a contribution (5.19) and if

we take a group of lines in the neighborhood of a particular frequency  $u^*$ , we get

$$(5.52) \quad \lambda_{\ell} = \sum_j \lambda_{\ell j} = \frac{W(u)}{\mu_0 u^3} \Big|_{u=u^*} \sum_j \frac{N_j^r}{S},$$

since the contributions are additive and the continuous absorption  $\mu_0$  and the weighting factors  $W(u)/u^3$  do not alter much from one member of the group to another. The important point about this formula is that only the total strength  $\sum_j N_j^r$  of the group of lines enters. Thus, we need not calculate strengths of individual lines, for often the total strength is given directly by the theory of the spectrum. There is also no need to calculate the dispersion. The resulting simplification of calculation is enormous. Since most of the lines are weak, equation (5.52) solves a great deal of our problem in a simple manner.

Because of its importance, we shall present another derivation of (5.52) which emphasizes a different aspect of its physical interpretation. Consider a group of many lines with centers in the interval  $u^* - \Delta u$  to  $u^* + \Delta u$ , none of which very much exceeds the average in strength. Assume also that the lines are distributed fairly uniformly and thickly over the region. Then the absorption coefficient for all these lines will no longer be a very jagged function; for, although it still may have many maxima and minima, and even more inflections, the variations from a smoothed average curve will be small. This is illustrated in the accompanying figure



Since the contribution to the opacity is determined by an integral, it is only some



sort of average which is important. The average absorption coefficient may be obtained by considering the total strength of the group of lines  $\sum_j N_j^2 f_j$  uniformly "smeared out" over the interval  $2\Delta u$  centered at  $u^*$ . Then

$$(5.53) \quad \mu_l = \frac{\pi e^2}{m c} \frac{\sum_j N_j^2 f_j}{2\Delta u} \cdot$$

The line opacity is then given in analogy with (5.16) as

(5.54)

$$\Lambda_l = \frac{W(u)}{u^3 \mu_c} \Big|_{u^*} \cdot 2\Delta u \cdot \frac{\kappa}{1+\kappa} \cdot$$

If the entire absorption due to the group of lines is weak this reduces to (5.52).

If we compare the contribution of continuous processes in the same interval we get from (5.7) simply  $\frac{W(u)}{u^3 \mu_c} \Big|_{u^*} \cdot 2\Delta u$ . Comparing with (5.54) we see that a fraction  $1/(1+\kappa)$  of the continuous transmission of the region remains.

Because of this derivation we shall call (5.54) the "smearing out" approximation.

We should emphasize some of the limitations of this approximation. First, all the absorption strength has been artificially confined to the region  $u^* - \Delta u$  to  $u^* + \Delta u$ . Because of the dispersion, there is a tail effect of some absorption outside this region. If the region within which the strengths were smeared out has been made very black, the inclusion of some extra absorption which should properly go into the tails will not change the contribution of this region. The absence of absorption in the tails, may, however, considerably over estimate the transmission there. The tail effect has thus caused us to underestimate the opacity. Balancing this is the fact that smearing out overestimates the opacity due to the contribution of lines in the smeared out regions. Furthermore when the total absorption coefficient due to lines is small compared to the background, the contributions are strictly additive, and not including the tails is exactly compensated by putting the extra strength into the interval  $2\Delta u$ . We conclude that it is generally better to for-

get about the tail effect, unless something is also done to improve the smearing out approximation.

A second limitation of this approximation occurs if one or a few lines carry the bulk of the strength. While smearing out is valid for the greater number of lines, the few strong lines should not be smeared out. A possible procedure to follow in this case is to smear out the weak lines and calculate their contribution to the line absorption coefficient  $\mu_{lw}$ . Add this to the continuum  $\mu_c$  to form a new background, and superimposed the strong lines upon this. The strong line contribution will be given by (5.6) except that  $r$  now has the significance  $\kappa = \frac{\mu_{l \text{ strong}}}{\mu_c + \mu_{l \text{ weak}}}$ .

The opposing extreme to the smearing out approximation occurs when many lines very clearly overlap. This case is also extremely frequent because practically every line in a spectrum is accompanied by many close shadows - its fine structure components for example. In general it will be sufficient to determine the wingspread of the group of closely spaced lines and assume that the transmission is zero within the wingspread. For natural breadth dispersion this estimate must be increased by the factor  $\pi/2$  to account for the pronounced tail effect. We may contrast the results in the case of natural breadth for the two situations 1) the total strength  $\Sigma Nf$  of the lines is equally distributed among  $M$  non-overlapping lines giving a strength  $Nf$  to each 2) the  $M$  lines are coincident. In 1) the contributions are additive and

$$(5.55) \quad \Lambda_{\ell} = M \Lambda_{\ell_1},$$

while in 2) we find

$$(5.56) \quad \Lambda_{\ell} = M^{1/2} \Lambda_{\ell_1}.$$

Intermediary cases will lie between the two extremes.

While we cannot carry out the treatment for the intermediary cases in detail except by a device, soon to be discussed, which treats the lines statistically, we can make an approximate treatment correct to first order terms. Suppose we have a group of several lines all with about the same dispersion and all at almost the same frequency. Then if we consider the line absorption contribution to the opacity and expand the result in powers of the deviations of the lines from some average position, we get the result that the zero order term is precisely the same as would result if we had a single line with the total strength of the group located at the average position. The first order term may be made to vanish by appropriately choosing this average position. Calculations show that the proper method of averaging is to weight each line position and breadth by  $Nf\Gamma$ , the product of strength and breadth of the line. Indeed the principle of a strength-breadth weighted average is general.

The foregoing considerations will enable us to make rough estimates of the contribution of lines to the opacity. In many cases this will suffice, since the line contribution is small, or else may be of the type given by the extremes considered here. But we should examine the more general problem of an arbitrary array of lines. The line absorption coefficient is then

$$(5.57) \quad \mu_{\ell} = \frac{\pi e^2}{mc} \sum_{j=1}^N \frac{N^j f_j}{\nu} b_j(\nu)$$

and we merely need carry out the operations indicated in (5.6). But let us note what this requires. We need the following data for each individual line. 1) position, 2) strength, 3) dispersion. Then we have to perform a very complicated numerical integration. In principle all this may be done, - in practice the complexity of the calculations makes the job prohibitively long unless we wish to treat a small spectral region with few lines.

5. General Statistical Features of Lines,  
Statistical Treatment of Line Spectra.

The very complexity of a line spectrum may be the means of providing a simple method of calculating its effect on opacities. For, if the enormous number of lines precludes an individual treatment, it makes possible a statistical approach. This approach will be developed in general in the succeeding paragraphs and then applied later in the special cases of interest.

Now the line absorption coefficient  $\mu_l$  and consequently  $r$  is the sum of contributions from every line in the spectrum. The  $i$ th line gives an absorption coefficient  $\mu_{l_i}$  which has a sharp maximum at the frequency  $u = u_i$  of the center of the line and approaches zero for frequencies far from the center. The sum  $r = \sum_i r_i = \sum_i \frac{\mu_{l_i}}{\mu_0}$  therefore appears as a very irregular function of  $u$  with many maxima, which it is practically hopeless to calculate. We see, however, that in order to calculate the mean opacity, it is not strictly necessary to know all the details of the line absorption coefficient itself as a function of frequency, but it would suffice to know the average value. At first sight, however, the calculation of the proper average would seem to involve evaluation of the very same integral (5.6) as needed to find the opacity. Here it is that the statistical approach proves useful. Suppose in (5.6) instead of the actual value of  $P$ , we insert a statistical average  $\bar{P}$ , averaged over certain distributions of line position, strength, and breadth. It may turn out that this average is rather easily susceptible to calculation compared to  $P$  itself. While the two functions may not have the same detailed dependence on frequency, we may hope that, if a sensible statistical average is used, the integral (5.6) itself will not be very much altered by the substitution of  $\bar{P}$  for  $P$ .

To understand the physical basis for the statistics we shall use, let us consider the very idealized case of a line spectrum having just two lines, separated sufficiently so that there is very little overlap of the dispersion curves of each line. Of course, in this case we can calculate  $P$  and, therefore, the opacity  $K$ . We can also calculate the opacity if the two lines were a little further apart or a little closer together, and we would get substantially the same result, since the integral is insensitive to the position of each line, except for the overlap which is assumed small. We can indeed pick a number of different distributions of the positions of the two lines, which will not give very different values of  $1/(\rho K)$ , calculate these values, and average them. The average will naturally agree rather closely with the true value, since every member of the group averaged agreed rather closely by itself. It will not affect the average very much even if we include a few distributions (for example, one in which the centers of both lines coincide), whose resultant opacity is quite different from the true value. Now, it is immaterial whether we calculate  $P$  for each distribution, integrate each one, and then average, or invert the order of averaging and integration, thus finding the average  $\bar{P}$  for all the distributions and then integrating to find the averaged opacity.

The question now arises as to what distribution should be included in our average. To answer this, we look at a line spectrum composed of several groups of two lines, each group in a slightly different frequency range so that lines in different groups do not overlap to any extent. Some of these groups undoubtedly will have the two lines far apart and others will have them closer together. We can treat each group separately by the averaging procedure because of the non-overlap between groups. If in the distributions we averaged, we never included any in which the two lines strongly overlap, we would estimate the opacity due to the groups with overlap too high, while we would be substantially correct for all the groups without overlap. It is better to make compensating errors by including in our average some distributions with strong overlap. For

then, while we would estimate the opacity of a group having little overlap too low, we would on the other hand estimate too high for the groups with strong overlap. If the proportion of strong to weak overlap distributions included in our averages is the same as the proportion of strong to weak overlap groups in the actual spectrum, the errors will exactly compensate. This principle is of course applicable to the general case of a line spectrum, as well as to the specific example discussed here.

Now there are laws which tell, in any actual spectrum, exactly where each line must be. These are extremely complicated, and because of this fact the distribution of line positions in the groups of a complicated spectrum is very nearly random, that is, considering all groups, a line has about equal probability of occurring anywhere within the frequency range covered by the group. It is just this distribution of line positions then which we shall use in our statistical average. Now if the  $i$ th line of a spectrum can with equal probability lie anywhere in the region  $u_i^* - \Delta_i$  to  $u_i^* + \Delta_i$ , the expected average of  $P(u; u_1, u_2, \dots, u_i, \dots)$  over all distributions of line positions consistent with this probability is

$$(5.58) \quad \bar{P}(u; u_1^*, \dots, u_i^*, \dots; \Delta_1, \dots, \Delta_i, \dots) = \frac{1}{\prod_i 2\Delta_i} \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} \dots \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} P(u; u_1, \dots, u_i, \dots) du_i, \dots du_i, \dots$$

This iterated integral is even more hopelessly complicated than (5.6) but it yields its value to any desired degree of approximation by the use of an extremely ingenious device suggested by Dr. Edward Teller. Develop the function  $P = 1/(1+x)$  as an exponential series

$$(5.59) \quad P = \frac{1}{1+x} = \sum_n a_n e^{-bnx} = \sum_n a_n e^{-bn \sum_i^* h_i} = \sum_n a_n \prod_i e^{-bn h_i}$$

By properly choosing the  $a_m$  and  $b_m$ , it is possible to get good numerical agreement (2 or 3%) between the series  $\sum_m a_m e^{-b_m \nu}$  and the function  $1/(1+\nu)$  in the range  $0 \leq \nu \leq 100$ , taking only four terms. This range of  $\nu$  will usually be sufficient; in any case the contributions to the opacity of regions where  $\nu > 100$  will be negligible. The series we shall use is

$$(5.60) \quad \frac{1}{1+\nu} = .470 e^{-.170\nu} + .370 e^{-.35\nu} + .120 e^{-.10\nu} + .040 e^{-.015\nu}$$

Inserting (5.59) into (5.58) reduces the iterated integral to a product of single integrals each of the same type.

$$(5.61) \quad \bar{P} = \sum_m a_m \prod_i \frac{1}{2\Delta_i} \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} e^{-b_m \nu_i} d\nu_i$$

Although the essential simplification has now been made, (5.61) can be transformed into more convenient form, as follows:

$$(5.62) \quad \bar{P} = \sum_m a_m \prod_i \left\{ 1 - \frac{j_m i}{2\Delta_i} \right\} = \sum_m a_m \exp \left\{ \sum_i \ln \left( 1 - \frac{j_m i}{2\Delta_i} \right) \right\},$$

where

$$(5.63) \quad \frac{j_m i}{2\Delta_i} = \frac{1}{2\Delta_i} \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} \left\{ 1 - e^{-b_m \nu_i} \right\} d\nu_i$$

Further defining

$$(5.64) \quad E_m = -\frac{1}{b_m} \sum_i \ln \left( 1 - \frac{j_m i}{2\Delta_i} \right),$$

equation (5.62) becomes

$$(5.65) \quad \bar{P} = \sum_m a_m e^{-b_m E_m}$$

The quantity  $\bar{P}$ , a function of frequency  $\nu$ , may now be inserted into (5.6) in place of  $P$ , with the expectation that the integral itself will not be very much altered. A straightforward numerical integration will then give the opacity.

We now examine the quantity  $E_n$ , the essential factor in  $\bar{P}$ , more closely. It involves a sum over all lines in the entire spectrum. It appears then that we are up against the same difficulty which prevented the calculation of  $\kappa = \sum_i \kappa_i$  itself, before we introduced the statistical approach, namely too many lines to calculate individually. But closer examination shows we have made some progress. First,  $E_n$  does not require knowledge of the exact position of every line, but only the limiting frequencies of the region within which it may be found in the statistical treatment. Many lines have these same limits, and we thus have eliminated very much of the data required for the opacity calculation. Second, it is generally possible to group lines into classes such that the sum over the lines in a class is simple. As one important example of such a case, suppose the  $M_k$  lines  $\nu_1, \nu_2, \dots, \nu_k, \dots, \nu_{M_k}$  which both fall into the same frequency region and have the same value for the integral  $\int_{\nu_i} \nu_i$  are treated together.

Then

$$(5.66) \quad -\frac{1}{\ln} \sum_{\nu_k=1}^{M_k} \ln \left( 1 - \frac{\int_{\nu_i} \nu_i}{2D_i} \right) = -\frac{M_k}{\ln} \ln \left( 1 - \frac{\int_{\nu_k} \nu_k}{2D_k} \right) \equiv E_{nk},$$

and part of the sum occurring in  $E_n$  has been performed by reducing it to one term. Other ways of grouping lines into classes may also be used, the common feature of all such devices being the reduction of the sum over all lines  $E_n$  to a sum over classes of lines  $\sum_k E_{nk}$ , the sum over the lines in each class being already performed. Thus we no longer treat individual lines, but classes with tens, hundreds or thousands of lines. Furthermore, it may be possible to use overall properties of a class, for example the total absorption strength of all the lines in the class, or again the average breadth, instead of requiring detailed calculation of this data for each line. Looking further ahead we may even find features among the classes which facilitate summing over them. For the moment we pause to consider the special cases with which we shall be mainly concerned in our applications.



We first consider the case in which natural and/or collision breadth are the determining factors in dispersion. In that case the absorption coefficient for the  $i$ th line is given by (2.15) and (2.9). Inserting the value of  $\nu_i = \mu_i/\mu_c$  into (5.63) we obtain:

$$(5.67) \quad \frac{j_{mi}}{2\Delta_i} = \frac{1}{2\Delta_i} \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} \left\{ 1 - \exp\left( -\frac{b_m N^i f_i \Gamma_i}{\pi S (u - u_i)^2 + \Gamma_i^2} \right) \right\} du_i.$$

Changing variable of integration in (5.67),  $x = \frac{u_i - u}{\Gamma_i}$ , gives

$$(5.68) \quad \frac{j_{mi}}{2\Delta_i} = \frac{\Gamma_i}{2\Delta_i} \int_{\frac{u_i^* - u - \Delta_i}{\Gamma_i}}^{\frac{u_i^* - u + \Delta_i}{\Gamma_i}} \left\{ 1 - \exp\left( -\frac{b_m N^i f_i}{\pi S \Gamma_i} \frac{1}{x^2 + 1} \right) \right\} dx.$$

The result is a definite integral which depends on one parameter and the limits of integration. By defining

$$(5.69) \quad F(a, u) = \frac{2}{\pi a} \int_0^u \left\{ 1 - \exp\left( -\frac{a}{1+x^2} \right) \right\} dx,$$

we can write (5.68) as

$$(5.70) \quad \frac{j_{mi}}{2\Delta_i} = \frac{b_m N^i f_i}{2\Delta_i S} F(a_{mi}, \infty) g'_{mi}(u),$$

where

$$(5.71) \quad g'_{mi}(u) = \frac{F(a_{mi}, \frac{u_i^* - u + \Delta_i}{\Gamma_i}) - F(a_{mi}, \frac{u_i^* - u - \Delta_i}{\Gamma_i})}{2 F(a_{mi}, \infty)},$$

and

$$(5.72) \quad a_{mi} = \frac{b_m N^i f_i}{\pi S \Gamma_i}.$$

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Values of the integral  $F(a, u)$  are presented in Table V; so that it is a comparatively simple matter to compute  $J_{nk}$ .

If, in a certain frequency interval  $u_k^* - \Delta_k$  to  $u_k^* + \Delta_k$ , there are many lines  $M_k$  having the same value of  $J_{nk}$ , such a set of lines can be considered as a class and formula (5.66) applies. This will occur for example if all lines had the same strength, breadth and dispersion. As pointed out previously this means a great simplification. If in addition the  $J_{nk}/2\Delta_k \ll 1$ , we can expand the logarithm obtaining

$$(5.73) \quad E_{nk} = -\frac{M_k}{\ln} \ln \left( 1 - \frac{J_{nk}}{2\Delta_k} \right) \sim \frac{M_k}{\ln} \frac{J_{nk}}{2\Delta_k} = \frac{M_k}{2\Delta_k} \frac{N^j f_j}{S} F(a_{nk}, \infty) g'_{nk}(u).$$

The first set of factors  $M_k N^j f_j / (2\Delta_k S)$  is independent of  $n$ , the term number in the series development of  $1/(u+\nu)$ , and depends only slightly on frequency through the factor  $S$ ; also  $M_k N^j f_j$  is the total absorption strength of all lines in the group. The second factor  $F(a_{nk}, \infty)$  is less than unity, approaching unity as a limit as  $a_{nk} \rightarrow 0$ . In a great many cases this limiting value can be inserted, if not for all values of  $n$ , at least for the higher values. The strong frequency dependence of  $E_{nk}$  is exhibited in the factor  $g'_{nk}(u)$  which is close to unity within the region  $u_k^* - \Delta_k \leq u \leq u_k^* + \Delta_k$  and is close to zero outside this region. Similar to the factor  $F(a_{nk}, \infty)$ , the factor  $g'_{nk}(u)$  depends upon  $n$  only through the appearance of  $a_{nk}$  and if  $a_{nk} \ll 1$ , the dependence on  $n$  disappears entirely. Thus if  $a_{nk} \ll 1$ ,  $E_{nk}$  is independent of  $n$  and we have the interesting result that

$$(5.74) \quad \bar{p} = \sum_n a_n e^{-\ln \sum_k E_{nk}} = \frac{1}{1 + \sum_k E_{nk}}$$

We shall later give an important physical interpretation to this result after we have seen it appear in other connections.

It may happen that in a region there are lines which have the same breadth, but

not the same strength. While the simplification (5.73) does not apply, an even simpler result can be obtained in one important case by use of a treatment due to Boris Jacobsohn. Let the number of lines of the group we are treating as a class which have a strength times breadth  $N_k f_i \Gamma_i$  between  $Q_j$  and  $Q_j + \Delta Q_j$  be  $N_k(Q_j) \Delta Q_j$ . Then

$$(5.75) \quad E_{Mk} = -\frac{1}{\Gamma_k} \sum_{i=1}^{M_k} \ln\left(1 - \frac{j_{Mk} i}{2 D_k \Gamma_k}\right) = -\frac{1}{\Gamma_k} \sum_{Q_j} N_k(Q_j) \Delta Q_j \ln\left(1 - \frac{j_{Mk} i}{2 D_k \Gamma_k}\right),$$

or, if one may expand the logarithm,

$$(5.76) \quad E_{Mk} \cong \frac{1}{\Gamma_k} \sum_{Q_j} N_k(Q_j) \Delta Q_j \frac{j_{Mk} i}{2 D_k \Gamma_k}.$$

If there are very many lines they will form a practically continuous distribution in  $Q_j$ , and the sum over all  $Q_j$  in (5.76) may be replaced by an integral. Referring to (5.68), however, we see that  $j_{Mk} i$  is also an integral, but the variable of integration is related to the frequency  $u_i$  of the center of the line. The order of the two integrations may be reversed and we obtain

$$(5.77) \quad E_{Mk} \cong \frac{1}{\Gamma_k} \frac{\Gamma_k}{2 D_k} \int_{\frac{u_k^* - u - D_k}{\Gamma_k}}^{\frac{u_k^* - u + D_k}{\Gamma_k}} \int_Q \left\{ N_k(Q) - N_k(Q) \exp\left(-\left(\frac{\Gamma_k N_k^* f_k}{\pi S \Gamma_k} \frac{1}{x^2 + 1}\right)\right) \right\} dQ du.$$

Now the essential point of the method is to find a distribution of strengths which occurs frequently in practice, and which enables both integrations in (5.77) to be performed analytically. Such a distribution is

$$(5.78) \quad N_k(Q) = \frac{M_k}{\bar{Q}_k} \exp\left(-\frac{Q}{\bar{Q}_k}\right),$$

where  $M_k$  is the total number of lines in the  $k$ th class and  $\bar{Q}_k$  is the average  $Nf$  of the class. Although it is physically impossible to have any lines of infinite

(1) Op. cit.

strength, the upper limit of the integral over  $Q$  may well be extended to infinity, since because of the exponential nature of the distribution (5.78) the contribution of the very large  $Q$  is negligible. The integrating over  $Q$  from 0 to  $\infty$  gives

$$(5.79) \quad E_{nk} \approx \frac{1}{b_n} \frac{M_k \Gamma_k}{2 \Delta k} \int_{\frac{u^*k-u-\Delta_k}{\Gamma_k}}^{\frac{u^*k-u+\Delta_k}{\Gamma_k}} \frac{b_n \overline{Nf}/(\pi S \Gamma)}{1+x^2 + b_n \overline{Nf}/(\pi S \Gamma)} dx.$$

Integrating now over  $x$ , we have

$$(5.80) \quad E_{nk} \approx \frac{M_k \overline{Nf} k}{2 \Delta k S} \frac{\varepsilon_{nk}(u)}{\sqrt{1+a_{nk}}},$$

where

$$(5.81) \quad a_{nk} = b_n \frac{\overline{Nf} k}{\pi S \Gamma_k}$$

is exactly the same quantity previously defined in connection with a distribution of lines of equal strength and

$$(5.82) \quad \varepsilon_{nk}(u) = \frac{1}{\pi} \left\{ \tan^{-1} \frac{u^*k-u+\Delta_k}{\Gamma_k \sqrt{1+a_{nk}}} - \tan^{-1} \frac{u^*k-u-\Delta_k}{\Gamma_k \sqrt{1+a_{nk}}} \right\}.$$

To facilitate computations of this function, nomographs have been prepared, (Fig. 3a, Fig. 3b, Fig. 4). A comparison of (5.80) and (5.73) shows the extreme similarity of the results for these two different distributions. The first set of factors  $\frac{M_k \overline{Nf} k}{2 \Delta k}$  giving the essential magnitude of  $E_{nk}$  is identical. The second factor  $F(a_{nk}, \infty)$  or  $(1+a_{nk})^{-\frac{1}{2}}$  is less than unity and independent of  $a_{nk}$  as  $a_{nk} \rightarrow 0$ . The last factor in both cases contains the important frequency dependence, and has the same qualitative features. In the limit  $a_{nk} \rightarrow 0$  the two formulae become identical as considerations of the properties of  $F(a, u)$  shows. In that case equation (5.74) applies to this type of distribution also.

To explain why the results are identical in the limit  $a_{nk} \rightarrow 0$ , and what the simple form (5.74) means, we return to the smearing out approximation (5.57).

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Using this approximation gives  $r = \frac{\sum_j N_j^j}{S 2 \Delta u}$  and

$$(5.83) \quad P = \frac{1}{1 + \frac{\sum_j N_j^j}{S 2 \Delta u}} .$$

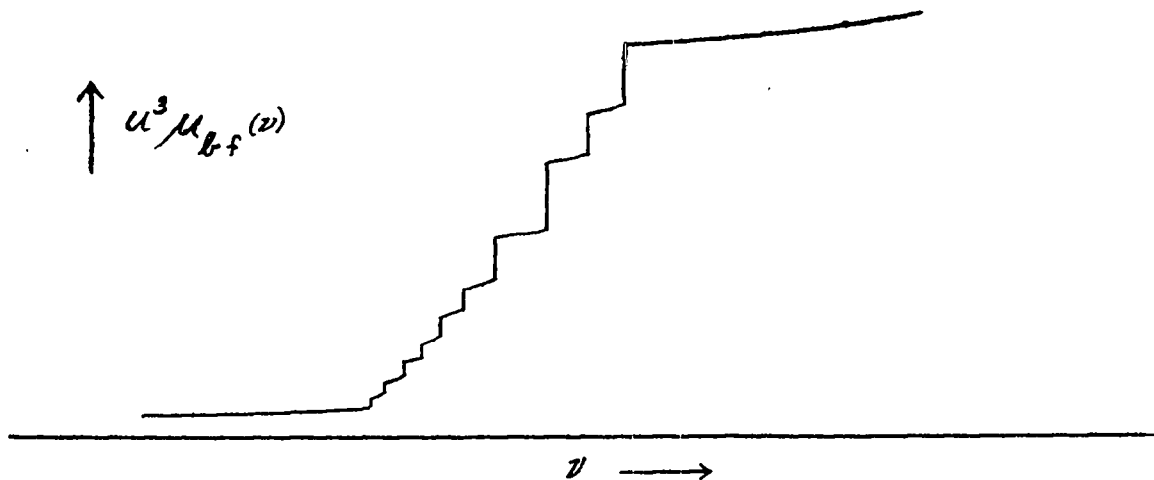
The only difference between (5.83) and (5.74) is the fact that in the latter case  $E_{nk}$  is not quite zero outside the interval  $u_k^* - \Delta_k$  to  $u_k^* + \Delta_k$ , and it is not quite equal to  $r_k$ , differing by the factor  $g_{nk}$  which may be .8 to .98 in typical cases, within the interval. The first difference mentioned, the so-called tail effect, is the more important. Now it is just under the assumptions used in making this derivation that the quantity  $a_{nk} \ll 1$  and  $\frac{j_{nk}}{2\Delta k} \ll 1$ . The approximation (5.74) is thus essentially equivalent to continuously smearing out the absorption strength of the lines in the regions where they occur.

#### 6. Statistical Treatment of Absorption Edges.

The very same type of statistical treatment appropriate for lines should also be used to treat the bound-free (photoelectric) absorptions, for there will be a very large number of absorption edges. In this section we shall develop this method, and also discuss some rather less accurate approximations. The bound-free absorption cross-section given by (2.23) may be rewritten as

$$(5.84) \quad \mu_{bf}(\nu) = \frac{2^4}{3\sqrt{3}} \frac{hc^2}{kTmc} \frac{1}{u^3} \sum_b \frac{N_b^b}{V} \frac{1}{n} \left( \frac{I_n}{kT} \right)^2 \epsilon_{bf}(\nu)$$

In the neighborhood of the ionization potential of an electron shell, say the L shell, the function  $u^3 \mu_{bf}$  will have a large number of small steps due to the appearance of a new term in the sum at each absorption edge. It may well have somewhat the shape indicated by the accompanying figure



Between such groups of edges,  $\mu_{bf}$  and consequently  $\mu_c$ , the continuous absorption, is a smoothly varying function.

By means of a statistical treatment completely analogous to our treatment of lines, the function  $1/\mu_c$ , jagged near each group of edges, is replaced by a smoothly varying average chosen so that the final opacity is not falsified. To do this, we artificially divided the absorption coefficient into three contributions:

$$(5.84a) \quad \mu = \bar{\mu}_c + (\mu_c - \bar{\mu}_c) + \mu_l,$$

where  $\bar{\mu}_c$  is some average function approximately representing the gross aspects of  $\mu_c$ . Then

$$(5.85) \quad \mu = \bar{\mu}_c (1+r')(1+r),$$

where

$$(5.86) \quad r' = \frac{\mu_c - \bar{\mu}_c}{\bar{\mu}_c}; \quad r = \frac{\mu_l}{\mu_c};$$

and introducing

$$(5.87) \quad P = \frac{1}{1+r}; \quad P' = \frac{1}{1+r'},$$

the opacity formula becomes

$$(5.88) \quad \Lambda = \frac{1}{\rho K} = \int_0^{\infty} \frac{PP'N(u)}{u^3 \mu_0} du.$$

We shall endeavor to replace  $P'$  by  $\bar{P}'$  its statistical average. Then since  $1/\mu_0 = P'/\mu_0$  we have approximately

$$(5.89) \quad \frac{1}{\mu_0} = \frac{\bar{P}'}{\mu_0};$$

$$(5.90) \quad r = \frac{\mu_l}{\mu_0} \approx \frac{\mu_l \bar{P}'}{\mu_0}.$$

The entire statistical treatment of lines of the last section can be carried through unaltered but we now interpret  $r$  by (5.90) which involves only the statistical average of  $\mu_0$ , not its small details.

Suppose now that the  $i$ th absorption edge might with equal probability fall anywhere in the interval from  $u_i^* - \Delta_i$  to  $u_i^* + \Delta_i$ . Then by following similar steps to those in the statistical treatment of lines which lead to (5.61), we get

$$(5.91) \quad \bar{P}'(u) = \sum_n a_n \prod_i \frac{1}{2\Delta_i} \int_{u_i^* - \Delta_i}^{u_i^* + \Delta_i} e^{-b_n r_i'} du_i,$$

where  $r_i'$  is the contribution to  $r'$  of the  $i$ th term in the sum (5.54). We thus see that

$$(5.92) \quad \begin{aligned} r_i' &= 0 & \text{for } u < u_i, \\ r_i' &= \rho_i & \text{for } u \geq u_i, \end{aligned}$$

and  $\rho_i$  is a slowly varying function of frequency. Now consider the edges arranged in order of ascending ionization frequency. For the particular frequency  $u$  at which  $\bar{P}'(u)$  is to be evaluated, assume that the edges  $1, 2 \dots j(u)$  all certainly lie below  $u$ , that is

$$(5.93) \quad u_i^* + \Delta_i < u \quad \text{for } 1 \leq i \leq j(u).$$

Also assume that the regions in which edges  $j(u) + 1, \dots, k(u)$  fall include  $u$ , that is

$$(5.94) \quad u_i^* - \Delta_i \leq u \leq u_i^* + \Delta_i \quad \text{for } j(u) + 1 \leq i \leq k(u).$$

Lastly, the other edges will all certainly lie above  $u$ , that is

$$(5.95) \quad u < u_i^* - \Delta_i \quad \text{for } k(u) < i.$$

For the edges of (5.95) the integral in (5.91) is just  $2\Delta_i$ , for those of (5.94) it is  $\left[ u - (u_i^* - \Delta_i) \right] e^{-b_n \rho_i} + (u_i^* + \Delta_i - u)$ , while for those of (5.93) it is  $2\Delta_i e^{-b_n \rho_i}$ .

We, therefore, have for (5.91)

$$(5.96) \quad \bar{P}'(u) = \sum_n a_n \prod_{i=1}^{j(u)} e^{-b_n \rho_i} \prod_{i=j(u)+1}^{k(u)} \left\{ 1 - \frac{u - (u_i^* - \Delta_i)}{2\Delta_i} (1 - e^{-b_n \rho_i}) \right\} \prod_{i=k(u)+1}^{\infty} 1$$

The absorption edges occur in groups with long frequency intervals between groups. Let us follow the variation of  $\bar{P}'(u)$  with  $u$  from a frequency  $u = u_1$ , which is below a particular group of edges--for concreteness say below the L shell ionization edges,--to a frequency  $u = u_2$  above the group edges. At  $u = u_1$ , there will be no terms in the second product, so that

$$\bar{P}'(u_1) = \sum_n a_n \prod_{i=1}^{j(u)} e^{-b_n \rho_i} = \sum_n a_n \exp(-b_n \sum_{i=1}^{j(u)} \rho_i),$$

whence by (5.59)

$$(5.97) \quad \bar{P}'(u_1) = \frac{1}{1 + \sum_{i=1}^{j(u)} \rho_i}.$$

Likewise for  $u = u_2$ , there will be no terms in second product of (5.96) but there will be additional terms in the first product giving

$$(5.98) \quad \bar{P}'(u_2) = \frac{1}{1 + \sum_{i=1}^{j(u)} \rho_i}.$$

The form (5.97) will hold as  $u$  increases from  $u_1$  until  $u$  becomes equal to the limit of the region available to the lowest edge. Then some terms in the second product begin to appear and  $\bar{P}'(u)$  decrease until after  $u$  has passed through the region of the edges, it takes the form (5.98). The variation through the region of the edges



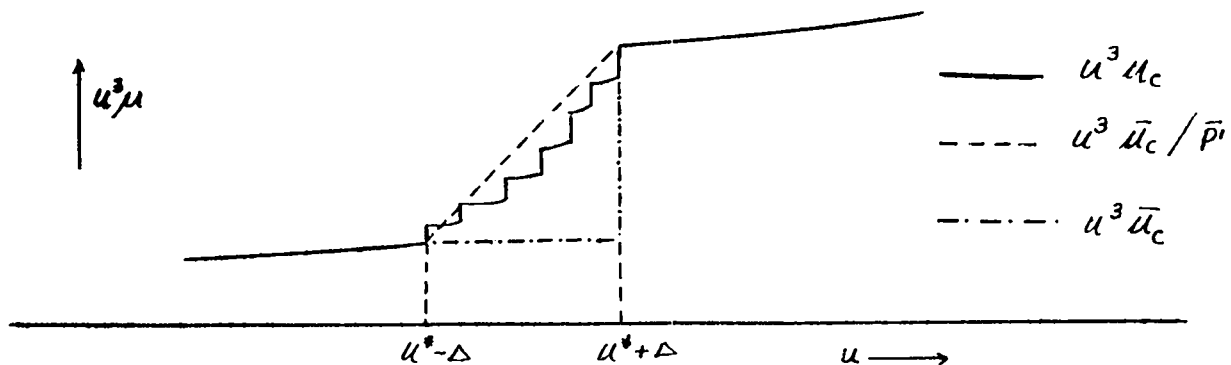
takes a very simple form in the case where there are very many,  $M$ , edges all having the same  $\rho_i = \rho$  and the same region in which they may fall. Then the second product becomes

$$\left\{ 1 - \frac{u-(u^*-\Delta)}{2\Delta} (1-e^{-b_n \rho}) \right\}^M \sim \left\{ 1 - \frac{u-(u^*-\Delta)}{2\Delta} \frac{b_n M \rho}{M} \right\}^M .$$

Now assume that the total strength of the edges remains fixed but  $M$  increases approaching  $\infty$ . Then the second product approaches  $\exp - \frac{u-(u^*-\Delta)}{2\Delta} b_n M \rho$  and (5.96) itself becomes

$$(5.99) \quad \bar{P}'(u) = \frac{1}{1 + \sum_{i=1}^j(u_1) \rho_i + \frac{u-(u^*-\Delta)}{2\Delta} M \rho} .$$

A reasonable choice for  $\bar{\mu}_0$  would be to make  $\bar{\mu}_0 = \mu_0$  between the groups of edges, but to have  $\bar{\mu}_0$  jump in one step from its value before the group to its value after the group at the frequency of the highest edge in the group. The behavior of  $u^3 \mu_0$ ,  $u^3 \bar{\mu}_0$  and  $\bar{\mu}_0 u^3 / \bar{P}'$  in the neighborhood of a group of edges are illustrated schematically in the accompanying figure.



As a crude approximation, one can simply use a single absorption edge to replace a whole group of edges. Whenever this is legitimate, the position of the edge is not critical, and we may place it at the ionization energy of the ion with average occupation, that is at the ionization energies  $\bar{\epsilon}'_{LZ}$  of (4.37). The reason the position of the edge is not critical is that there are always a great number of lines near the edges. Their high absorption coefficient hides any small

alteration in edge absorption. Jacobsohn has worked out a refinement of this treatment placing the effective edge of a group so as to make the average of  $1/\mu_c$  correct throughout the group but it is rarely necessary to use this treatment.

#### 7. Simplified Practical Treatment of Lines.

We have thus far discussed two detailed methods of treating lines. The straightforward approach is exact but impossibly complicated except for a small frequency region. The statistical approach brings the problem within the limits of human computation and should be nearly as accurate as the exact treatment. However, even the statistical approach involves as much as 6 computer-months work to get a single value of the opacity. When flexible rapid electronic computing machines become available, the statistical method will come into its own as a good method of treating the lines. Until such time, we shall have to content ourselves with rougher approximations. It is these rougher treatments which we investigate here.

The clue to the problem is the smearing out approximation. Instead of using the full statistical treatment to give  $\bar{P}$ , we may use the approximate formula.

$$(5.94) \quad \bar{P} = \frac{1}{1 + \sum_k E_{nk}} \approx \frac{1}{1 + \sum_k r_k} \quad .$$

where

$$(5.95) \quad r_k = \sum_{jk} \frac{N^{jk} f_{jk}}{S \ 2 \Delta k} \quad .$$

In the most detailed treatment of this type, we may consider a class as composed of all the lines from a particular ion type arising from the same one electronic transition. We would also incorporate three features which will very much enhance the accuracy of our result; namely, 1) Treat strongest lines individually by superimposing them upon the background absorption of the continuum plus the weak smeared out lines; 2) Incorporate an empirical correction factor to reduce the contribution of each group of lines, since the smearing out treatment overemphasizes line effects.

This factor must be determined by comparing the genuine statistical treatment with the smearing out treatment in several representative cases, 3) Take into account the tail effect neglected by smearing out treatment. Corrections 2 & 3 are of opposite sign and experience may show that it is sufficiently accurate to neglect both.

It may even prove possible to do a much less detailed smearing out treatment by considering a class of lines as composed of all lines from a single or small group of one electron transitions. This treatment should also include an empirical factor designed to force its results to agree with the detailed statistical treatment. By this method the work for computing the line effect could be reduced to 2 computer weeks.

An entirely different approach in modifying the detailed statistical treatment is to use the so-called pattern treatment. This treatment is based on the fact that relative positions of classes of lines are the same for two groups of one electron transitions differing only in the principal quantum number  $n$  of the final state. Moreover, the ratio of strength of each line in one group to that in another is a constant for all lines. Then the value of  $\sum_k E_{nk}$  at one frequency can be obtained from that at another, by the so-called pattern transformation

$$(5.96) \quad \sum_k E_{nk}(u) = \text{const.} \sum_k E_{nk} (u \dagger \text{const.}).$$

VI. SUMMARY OF FORMULAE FOR COMPUTING OPACITIES.

In this Chapter all the formulae essential for opacity calculations are collected in form for computation. Energies are expressed in terms of the Rydberg energy  $Rhc = 13.61$  electron volts and lengths in terms of the first Bohr radius for Hydrogen  $a_0 = .5291 \times 10^{-8}$  cm.

1. Formulae for Occupation Numbers:

The volume  $V$  is related to the density  $\rho$  by

$$(6.1) \quad \frac{V}{Na_0^3} = \frac{\sum Z M_Z \frac{N_Z}{N}}{\rho N_0 a_0^3} .$$

$M_Z =$  gram atomic weight  
 $N_0 = 6.023 \times 10^{23} =$  Avogadro's number.

The radius of the ion spheres is from (4.43),

$$(6.2) \quad \frac{a_{Z'}}{a_0} = \left\{ \frac{3}{4\pi} Z' \frac{V}{Na_0^3} \frac{N}{n_f} \right\}^{1/3} ,$$

where

$$(6.3) \quad Z' = Z - \sum_l \frac{n_l Z}{N_Z} .$$

The number of bound electrons  $n_b$  is from (4.40)

$$(6.4) \quad \frac{n_b}{N} = \sum_Z \frac{N_Z}{N} \sum_l \frac{n_l Z}{N_Z} ,$$

and the number of frees  $n_f$  from (4.42) is

$$(6.5) \quad \frac{n_f}{N} = \frac{n}{N} - \frac{n_b}{N} .$$

The free energy  $-kT\alpha^*$  of the electrons is given by (4.41a)

$$(6.6) \quad \alpha^* = -3.1034 + \ln \frac{V}{Na_0^3} - \ln \frac{n_f}{N} + \frac{3}{2} \ln (kT/Rhc) \\ + \frac{15}{16} \alpha^2 \frac{kT}{Rhc} - \frac{15}{64} \alpha^4 \left( \frac{kT}{Rhc} \right)^2 \\ - .35355 e^{-\alpha^*} \left( 1 - \frac{15}{64} \alpha^2 \frac{kT}{Rhc} \right) + .12995 e^{-2\alpha^*}$$

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where  $\alpha = 1/137.03$  is the fine structure constant.

From (4.38) we get

$$(6.7) \quad z_l^* = z - \sum_{j \neq l} \frac{n_{jZ}}{N_Z} \sigma_{l,j} - \frac{n_{lZ}}{N_Z} \left( 1 - \frac{1}{\sigma_{lZ}} \right) \sigma_{l,l} .$$

Table II gives the screening constants  $\sigma_{l,j}$ . Then from (4.37)

$$(6.8) \quad -\frac{\bar{E}'_{lZ}}{Rhc} = -\frac{\bar{E}'_l(z_l^*)}{Rhc} = z' \frac{a_0}{a_{Z'}} \left\{ 3 - \left( \frac{r}{a_0} \right)^2 \left( \frac{a_0}{a_{Z'}} \right)^2 \right\} = 3/5 \sum_Z \frac{N_Z}{N} \frac{N}{n_{Z'}} z'^2 \frac{a_0}{a_{Z'}} .$$

Table III gives the one electron energy levels  $-\bar{E}'_l(z_l^*)/Rhc$  and table IV gives the average square radius  $(r/a_0)^2$ . Finally, the occupation numbers are (4.36)

$$(6.9) \quad \frac{n_{lZ}}{N_Z} = \frac{\sigma_{lZ}}{\alpha^* - \frac{Rhc}{kT} \left( -\frac{\bar{E}'_{lZ}}{Rhc} \right) + 1} .$$

The ionic occupations are found from (4.47). The probability of having an ion with  $\nu_l$  electrons in the  $l$  level is

$$(6.10) \quad P_{\nu_l} = \frac{c_{l, \nu_l}}{\nu_l! (c_l - \nu_l)!} p_l^{\nu_l} q_l^{c_l - \nu_l} .$$

where

$$(6.11) \quad p_l = n_{lZ}/c_l .$$

$$(6.12) \quad q_l = 1 - p_l .$$

These formulae must be modified if

$$(6.13) \quad \lambda = 2z' \frac{a_0}{a_{Z'}} \frac{Rhc}{kT} > 1$$

and the appropriate change is discussed in Appendix II.

2. Formulae for Thermodynamic Functions c.f. Appendix I.

The total energy of the system E is obtained from (AI 16, 17, 18) and following discussion.

$$(6.14) \quad \frac{E}{NRhc} = \sum_Z \frac{N_Z}{N} \sum_i \frac{N_{iZ}}{N_Z} \frac{\epsilon_i^0}{Rhc} (\bar{z}_i) - \frac{9}{5} \sum_Z \frac{N_Z}{N} z'^2 \left( \frac{a_0}{a_{z'}} \right) \\ + (3/2) \frac{n_f}{N} \frac{kT}{Rhc} \left\{ 1 + \frac{5}{8} \alpha^2 \frac{kT}{Rhc} - \frac{5}{16} \alpha^4 \left( \frac{kT}{Rhc} \right)^2 \dots \right\} \left\{ 1 + .17678 e^{-\alpha^*} \left( 1 - \frac{15}{32} \alpha^2 \frac{kT}{Rhc} \right) \dots \right\} \\ + \left[ \begin{array}{c} 3 \\ \text{or} \\ 3/2 \end{array} \right] \frac{kT}{Rhc} .$$

where c.f. AI.15

$$(6.15) \quad \bar{z}_i = z - \frac{1}{2} \sum_{j \neq i} \frac{n_{jZ}}{N_Z} \sigma_{i,j} - \frac{1}{2} \frac{n_{iZ}}{N_Z} \left( 1 - \frac{1}{\sigma_{iZ}} \right) \sigma_{i,i} = z - \frac{1}{2} (z - z_i^*) .$$

The zero of energy is taken as the state in which all the nuclei and electrons are infinitely separated and at rest. We should use the upper value 3 in the last term when

$$(6.16) \quad z'^2 \frac{a_0}{a_{z'}} \frac{Rhc}{kT} > 11.6$$

and the lower value 3/2 in other cases.

The pressure P is obtained from (AI.20). It is

$$(6.17) \quad \frac{PV}{NkT} = \frac{n_f}{N} \left\{ 1 + .17678 e^{-\alpha^*} \left( 1 - \frac{15}{32} \alpha^2 \frac{kT}{Rhc} \right) \dots \right\} - \frac{3}{5} \sum_Z \frac{N_Z}{N} z'^2 \frac{Rhc}{kT} \frac{a_0}{a_{z'}} \\ + \left[ \begin{array}{c} 3/2 \\ \text{or} \\ 1 \end{array} \right] .$$

where the condition (6.13) requires the use of upper value 3/2 in square bracket when fulfilled, and the lower values when violated.

3. Continuous Opacity Formulae

The continuous transmission  $\Lambda_c$  is defined by (5.7) as being the value of the mean free path found by neglecting line absorption. We write this in the form

$$(6.18) \quad \Lambda \Lambda_c = \int_0^\infty \frac{W(u)}{D(u)} du .$$

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where the weighting function

$$(6.19) \quad W(u) = \frac{15}{4\pi^4} u^7 e^{2u} (e^u - 1)^{-3}$$

is recorded in Table VI, and the reduced absorption D is

$$(6.20) \quad D = \frac{u^3 \mu_c}{A} .$$

The reciprocal length A is introduced to give the quantities in the integral (6.15) simple coefficients and make them dimensionless. It has the value

$$(6.21) \quad A = \frac{2^4}{3\sqrt{3}} \frac{hc^2}{mc} \frac{1}{kT} \frac{N}{V} = 4.762 \times 10^6 \frac{Rhc}{kT} \frac{\rho}{\sum_Z N_Z \frac{N_Z}{N}}$$

where c.g.s. units are used for  $\rho$  and  $N_Z$ . The continuous absorption coefficient and consequently D is the sum of 3 terms,  $D_s$  from scattering,  $D_{ff}$  from free-free transition and  $D_{bf}$  from bound-free transitions

$$(6.22) \quad D = D_s + D_{ff} + D_{bf} .$$

The scattering term is

$$(6.23) \quad D_s = \frac{n}{V} \frac{\mathcal{Q}}{A} \frac{u^3}{1-e^{-u}} = \sqrt{\frac{3}{8}} \alpha^3 \frac{n}{N} \frac{kT}{Rhc} \frac{u^3}{1-e^{-u}} \frac{\mathcal{Q}}{\mathcal{Q}_0}$$

where the scattering cross section is

$$(6.24) \quad \frac{\mathcal{Q}}{\mathcal{Q}_0} = \left( 1 - u \alpha^2 \frac{kT}{Rhc} \right) \left[ 1 + O \left( \frac{kT}{mc^2} \right)^2 \right] .$$

Here, of course,  $\alpha$  is the fine structure constant =  $1/137.03$  and  $\mathcal{Q}_0$  the Thompson cross section  $\mathcal{Q}_0 = \frac{8\pi}{3} (e^2/(mc^2))^2 = .6654 \times 10^{-24} \text{cm}^2$ . The free-free absorption term follows from (2.30),

$$(6.25) \quad D_{ff} = \frac{Rhc}{kT} \sum_Z \frac{N_Z}{N} Z'^2 e^{-\alpha^*} \bar{E}_{ff} .$$

If we neglect small correction terms in  $\alpha^*$ , we obtain from (4.41a)

$$(6.25a) \quad -\alpha^* = \ln \frac{(4\pi)^{3/2}}{2} \frac{n}{N} \frac{Na^3}{V} \left( \frac{Rhc}{kT} \right)^{3/2} = \ln \frac{1}{1.0075} \frac{2n}{MN} \rho \left( \frac{Rhc}{kT} \right)^{3/2}$$

where  $\bar{M} = \sum_Z M_Z \frac{N_Z}{N}$ , and putting this with (6.2) into (6.25) we get

$$(6.26) \quad D_{ff} = 3\sqrt{\pi} \left(\frac{\text{Rho}}{kT}\right)^{5/2} \sum_Z \frac{N_Z}{N} Z^3 \left(\frac{a_0}{a_Z}\right)^3 \bar{\epsilon}_{ff},$$

where

$$(6.27) \quad \bar{\epsilon}_{ff} = 1 + .1728 \left(\frac{kT}{\text{Rho}Z^2}\right)^{1/3} u^{1/2} (1 + 2/u).$$

The bound free absorption term (2.23) gives simply,

$$(6.28) \quad D_{bf} = \sum_b \frac{N_b^b}{N} \frac{1}{n} \left(\frac{I_n}{kT}\right)^2 \epsilon_{bf}(u),$$

the Gaunt factors being defined by (2.22). They are discussed further in Appendix III. Fig. I is a graph of these factors.

In most cases the function  $D(u)$  varies rather slowly with frequency except in the neighborhood of an absorption edge, where  $D_{bf}$  is discontinuous. It is the usual practice among astrophysicists to break up the integration range into intervals within which  $D(u)$  may be considered constant, and thus

$$(6.29) \quad A\Lambda_c = \sum_k \frac{1}{D(u_{k+1/2})} \int_{u_k}^{u_{k+1}} W(u) du = \sum_k \frac{S(u_{k+1}) - S(u_k)}{D(u_{k+1/2})},$$

where  $S(u)$  is the Strömgen function

$$(6.30) \quad S(u) = \int_0^u W(x) dx.$$

Values of this function are given in Table VI. Formula (6.29) is valuable for quickly obtaining approximate results, if we approximate all the absorption edges associated with a one electron ionization by a single edge.

For more accurate results, we should use the statistical treatment of absorption edges discussed in V-6. In this treatment  $D(u)$  of (6.18) is replaced by  $\bar{D}(u)/P'(u)$  where from (5.99)

$$(6.31) \quad \frac{\bar{D}(u)}{P'(u)} = D(u) \left\{ 1 + \sum_{i=1}^{j(u_k)} \rho_i + \frac{u - (u_k^* - \Delta_k)}{2\Delta_k} M_k \rho_k \right\}.$$

In this result, the  $k$ th group of  $M_k$  edges lies between  $u_k^* - \Delta_k$  and  $u_k^* + \Delta_k$ . Each edge has a relative jump, from (5.92), (5.86)



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$$(6.32) \rho_i = \frac{\mu_{ci} - \bar{\mu}_{ci}}{\bar{\mu}_0} ,$$

and  $\bar{\mu}_0$  is a function such that

$$(6.33) \bar{\mu}_0(u) = \mu_0(u) \text{ between groups of edges}$$

$$\bar{\mu}_0(u) = \mu_0(u_k^* - \Delta_k) \text{ for } u_k^* - \Delta_k < u < u_k^* + \Delta_k .$$

The reduced absorption  $\bar{D}(u)$  is

$$(6.34) \bar{D}(u) = \frac{u^3 \bar{\mu}_0}{A} .$$

#### 4. Line Absorption Contribution.

The line absorption coefficient is defined by (5.8) as the reduction in the continuous mean free path, due to the effect of the lines. It is

$$(6.35) A\Delta_\ell = \int_0^\infty \frac{r}{1+r} \frac{\bar{P}'(u)W(u)}{D(u)} du ,$$

where

$$(6.36) r = \mu_\ell / \bar{\mu}_0$$

is the ratio of the line absorption coefficient to the continuous background - statistically averaged in regions of absorption edges. For a line of natural and/or collision breadth dispersion this is o.f. (5.24)

$$(6.37) A\Delta_\ell = \frac{\bar{P}'(u)W(u)}{D(u)} \Big|_{u=u_i} \pi \left( \frac{N^i f_i \Gamma_i}{\pi S} \right)^{\frac{1}{2}} \frac{1}{\left( 1 + \frac{\pi S \Gamma_i}{N^i f_i} \right)^{\frac{1}{2}}} .$$

where

$$(6.38) \Gamma_i = \frac{h\gamma_i}{4\pi kT} , \frac{h\gamma_i}{4\pi} \text{ is the energy half breadth,}$$

$$(6.39) S = \frac{2^4}{3\sqrt{3}\pi} \frac{N\bar{D}(u)}{\bar{P}'(u)} \approx 0.98015 \frac{N\bar{D}(u)}{u^3 \bar{P}'(u)}$$

$N^i$  is the number of ions in the initial state, and  $f_i$  is the electron number for the transition.

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If the absorption strength may be smeared out over the interval  $u^* - \Delta$  to  $u^* + \Delta$ , we get from (5.54)

$$(6.40) \quad A\Delta_{\ell} = \left\{ \frac{\sum_j \frac{N^j f_j}{2\Delta u S}}{1 + \frac{\sum_j N^j f_j}{2\Delta u S}} \right\} \left\{ \frac{S(u^* + \Delta) - S(u^* - \Delta)}{\bar{D}(u^*)/P'(u^*)} \right\}.$$

When recourse is made to the statistical treatment of lines, the following formulae should be used:

$$(6.41) \quad A\Delta = \frac{A}{\rho K} \int_0^{\infty} \bar{P}(u) \frac{\bar{P}'(u)}{\bar{D}(u)} W(u) du.$$

$$(6.42) \quad \bar{P}(u) = \sum_n a_n e^{-b_n E_n(u)}$$

$$= .47 e^{-1.7E_1} + .37 e^{-.35E_2} + .12 e^{-.10E_3} + .040 e^{-.015E_4}.$$

$$(6.43) \quad E_n = \sum_{\substack{i \\ \text{all lines}}} E_{ni} = \sum_k \sum_{\substack{i_k \\ \text{all} \\ \text{classes}}} E_{nik} = \sum_k \sum_{\substack{i_k \\ \text{all lines} \\ \text{in a class}}} E_{nk}.$$

$$(6.44) \quad E_{nk} = -\frac{M_k}{b_n} \ln \left( 1 - \frac{j_{nk}}{2\Delta_k} \right) \sim \frac{M_k}{b_n} \frac{j_{nk}}{2\Delta_k},$$

where  $M_k$  is the number of lines in the  $k$ th class.

For natural breadth type dispersion, if a line may with equal probability fall anywhere in the region  $u_i^* - \Delta_i$  to  $u_i^* + \Delta_i$

$$(6.45) \quad \frac{j_{ni}}{2\Delta_i} = \frac{b_n}{2\Delta_i} \frac{N^i f_i}{S} F(a_{ni}, \infty) \mathcal{E}'_{ni}(u),$$

where

$$(6.46) \quad a_{ni} = \frac{b_n}{\pi^i f_i} \frac{N^i f_i}{S},$$

$$(6.47) \quad \mathcal{E}'_{ni}(u) = \frac{F(a_{ni}, (u_i^* - u + \Delta_i)/\Gamma_i) - F(a_{ni}, (u_i^* - u - \Delta_i)/\Gamma_i)}{2F(a_{ni}, \infty)},$$

and the function  $F(a, u)$  is recorded in Table V.

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If it is valid to use an exponential distribution of strength within a group

$$(6.48) \quad E_{nk} \approx \frac{M_k}{2\Delta_k S} \frac{\bar{Nf}^k}{\sqrt{1+a_{nk}}} \varepsilon_{nk}(u),$$

where  $\bar{Nf}^k$  is the average strength of each line and

$$(6.49) \quad a_{nk} = \frac{b_n}{\pi} \frac{1}{S} \frac{\bar{Nf}^k}{r_k}.$$

A nomograph of the function

$$(6.50) \quad \varepsilon_{nk}(u) = \frac{1}{\pi} \left\{ \tan^{-1} \frac{(u_k^* - u + \Delta_k)}{r_k \sqrt{1+a_{nk}}} - \tan^{-1} \frac{u_k^* - u - \Delta_k}{r_k \sqrt{1+a_{nk}}} \right\}$$

is given in Fig. III to facilitate calculations.

## VII Similarity Properties and Limiting Forms of the Opacity

### 1. Similarity transformations for opacity calculations.

Since the calculation of even a single opacity coefficient is laborious, it is desirable to have approximate similarity transformations, which, if given values of the opacity coefficient for one element at one temperature and density, will predict values for other elements under related conditions. This can be done approximately if line absorption is not too important a factor.

We refer to our summary of formulae, Chapter VII, specialized for the case of a single element. From (6.9) we can see that the occupation numbers will be the same for two cases (subscripts (1) and (2)) provided that  $\alpha^*$  is the same and

$$(7.1) \quad \frac{\bar{E}'_{l_2(1)}}{kT_1} = \frac{\bar{E}'_{l_2(2)}}{kT_2} .$$

The major contribution to these energies is just the interaction with the nuclei, so that (7.1) is essentially equivalent to

$$(7.2) \quad Z_1^2 \frac{Rhc}{kT_1} = Z_2^2 \frac{Rhc}{kT_2} .$$

Magee<sup>(1)</sup> has suggested a refinement which partially takes into account the screening of the nuclei by the bound electrons. He requires that

$$(7.3) \quad \gamma = (Z_1 - \mathcal{L})^2 \frac{Rhc}{kT_1} = (Z_2 - \mathcal{L})^2 \frac{Rhc}{kT_2}$$

where  $\mathcal{L}$  is the screening of the level with probability of occupation 1/2. This forces the occupations of the half filled levels to be the same; the lower energy levels will be completely filled anyway, while the higher ones will have so small an occupation as not to affect the opacity.

(1) John Magee: Similarity Law for Opacity of Light Elements. Unpublished.

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We next examine the continuous opacity of two different elements under conditions such that  $\alpha^*$  and  $\delta$  are the same for each. From (6.25) we can see that the free-free absorptions  $D_{ff}$  will have the same contribution to  $A \Lambda_c$  in each case since (7.4)  $D_{ff} \approx \gamma e^{-\alpha^*}$ .

The same result is also evident for the bound-free transitions, since from (6.28)

$$(7.5) \quad D_{bf} \sim \sum_i \frac{N_i^b}{N} \frac{1}{M^5} \gamma^2$$

(The sum extending over all states with  $I_n/kT \sim \delta/n^2 < u$ ) and  $N_i^b/N$ , the occupation numbers are functions of  $\alpha^*$  and  $\gamma$  alone. The scattering contribution (6.23), however, cannot be written as a universal function of  $\alpha^*$  and  $\gamma$ , and hence spoils the similarity transformation. If there are any bound electrons at all, however, scattering will play only a minor roll, while in the absence of bound electrons, the calculation of the opacity coefficient is simple enough so that no resort need be had to similarity transformations. We can say therefore that in most cases  $A \Lambda_c$  of (6.18) is a function of  $\alpha^*$  and  $\gamma$  alone.

From (6.25a) we see that if  $\alpha^*$  is the same in two cases then we must have approximately

$$(7.6) \quad \frac{Z_1}{M_1} \frac{\rho_1}{T_1^{3/2}} = \frac{Z_2}{M_2} \frac{\rho_2}{T_2^{3/2}},$$

or since  $Z_1/M_1 \sim Z_2/M_2 \sim 2$  for light elements except hydrogen

$$(7.7) \quad \frac{\rho_1}{\rho_2} = \left( \frac{T_1}{T_2} \right)^{3/2}.$$

But if  $\gamma$  is the same in the two cases

$$(7.8) \quad \frac{T_1}{T_2} = \frac{Z_1^2}{Z_2^2}$$

so that

$$(7.9) \quad \frac{\rho_1}{\rho_2} = \frac{Z_1^3}{Z_2^3}.$$

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Using (7.8) and (7.9) we can find the temperature and densities for which two different elements will have the same values of  $A \Lambda_c$ . Moreover since from (6.21)  $A \propto \beta \rho / (Z^2 M)$  we get that, under these conditions,

$$(7.10) \quad \frac{K_{c1}}{K_{c2}} = \frac{Z_2^2 M_2}{Z_1^2 M_1} \sim \left( \frac{Z_2}{Z_1} \right)^3.$$

The line absorption contribution does not lend itself to a similarity treatment. The most important single factor in the effect of lines is the spread of each group. This spread, being due to electrostatic and exchange interaction, is proportional to  $Z$ . If we keep  $Z^2/(kT)$  constant, then, on the frequency scale  $u = h\nu/(kT)$ , the spread of the groups will be inversely proportional to  $Z$ . Hence the line contribution will be more important for light elements than for heavy elements under conditions of similarity for the continuous opacity.

Relativity effects are to first order proportional to  $Z^4$ . This again spoils the similarity transformation, even when lines are unimportant. It also spoils any attempt to scale the line contribution separately. This is just another example of the qualitative difference in opacity calculations between the light and heavy elements.

## 2. Limiting values for the opacity.

At very high temperatures, all the electrons will be ionized so that the only processes contributing to the opacity are the free-free transitions and the scattering. Since scattering is proportional to the number of electrons per unit volume, while the free-free transitions are proportional to the square of the electron density, the former will be dominant at low densities, the latter at high. We examine the results to be expected under these extreme conditions.

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If there are to be no bound electrons, the quantity  $\alpha^* + \beta \bar{\epsilon}'_{LZ}$  must be much greater than unity for all states. Putting  $\bar{\epsilon}'_{LZ} \sim -Z^2 Rhc$  and using (6.6) for  $\alpha^*$ , this condition gives approximately

$$(7.11) \quad \ln \frac{1}{\rho} \left( \frac{kT}{Rhc} \right)^{3/2} - Z^2 \frac{Rhc}{kT} \gg 1.$$

This result clearly indicates that increasing temperature favors increased ionization. But it also predicts that increasing the density always decreases the ionization. This is not altogether true; the reason our result is misleading is our neglect of the interaction terms in  $\bar{\epsilon}'_{LZ}$ . These give a pressure ionization for high densities.

In the low density, high temperature limit, where the only process contributing to the opacity is scattering we get

$$(7.12) \quad \Lambda_{scat} = \frac{1}{\rho \kappa} = \frac{15}{4\pi^4} \int_0^\infty \frac{u^4 e^u (e^u - 1)^{-2} du}{\frac{N}{V} \phi_0 \left(1 - \frac{3kT}{mc^2}\right) \left(1 - 2u \frac{kT}{mc^2}\right)}.$$

The denominator is independent of frequency except for the correction factor  $\left(1 - 2u \frac{kT}{mc^2}\right)$ . We may replace  $u$  by  $u_{max} \sim 4$ , the value maximizing the integrand in (7.12) without fear of serious error. Then

$$(7.13) \quad \Lambda_{scat} = \left\{ \frac{u}{V} \phi_0 \left[1 - \frac{kT}{mc^2}\right] \right\}^{-1},$$

or

$$(7.14) \quad \kappa_{scat} = \frac{1}{\rho \Lambda} = N_0 \phi_0 \left[1 - \frac{kT}{mc^2}\right] \frac{\bar{z}}{M_0}$$

where  $\bar{M} = \sum_Z M_Z \frac{N_Z}{N}$  = ave molecular weight  $\bar{z} = \sum_Z z \frac{N_Z}{N}$  = average atomic number

$\phi_0$  = Thomson cross-section =  $.6654 \times 10^{-24}$  cm<sup>2</sup>.

$N_0$  = Avogadro's number  $6.023 \times 10^{23}$

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In this limit the opacity is independent of density and virtually independent of temperature. Moreover for the light elements  $Z/M_0 \approx 1/2$  so that except for hydrogenous material the opacity is independent of composition.

In the high density high temperature region free-free transitions become the dominant process. Then using (6.13) and (6.25)

$$(7.15) \quad A \Lambda_c = \int_0^{\infty} \frac{W(u) du}{\frac{Rhc}{kT} \sum_1^Z \frac{N_2}{N} Z^2 e^{-\alpha^*} \bar{g}_{ff}}$$

The only frequency dependent factor in the denominator is the slowly varying  $\bar{g}_{ff}$ . We replace  $u$  by  $u_{\max}^2$  in this factor. Then we can use  $\int_0^{\infty} W(u) du = S(\infty)$  giving.

$$(7.16) \quad A \Lambda_c = \frac{196.5}{\frac{Rhc}{kT} e^{-\alpha^*} \sum_1^Z \frac{N_2}{N} Z^2 \left(1 + .588 \left[\frac{kT}{Rhc Z^2}\right]^{1/2}\right)}$$

or putting in the value of  $\alpha^*$  from (6.25a) we get

$$(7.17) \quad k = \frac{1}{\rho \Lambda_c} = \frac{A}{\rho} \frac{4\pi^{3/2}}{196.5} \frac{\bar{Z}}{M} \rho N_0 a_0^3 \left(\frac{Rhc}{kT}\right)^{5/2} \sum_1^Z \frac{N_2}{N} Z^2 \left[1 + .588 \left(\frac{kT}{Rhc Z^2}\right)^{1/2}\right],$$

or inserting the value of  $A/\rho$  from (6.21), we have in c.g.s. units

$$(7.18) \quad k = 4.815 \times 10^{-4} \frac{\bar{Z}}{M^2} \rho \left(\frac{Rhc}{kT}\right)^{7/2} \sum_1^Z \frac{N_2}{N} Z^2 \left[1 + .588 \left(\frac{kT}{Rhc Z^2}\right)^{1/2}\right].$$

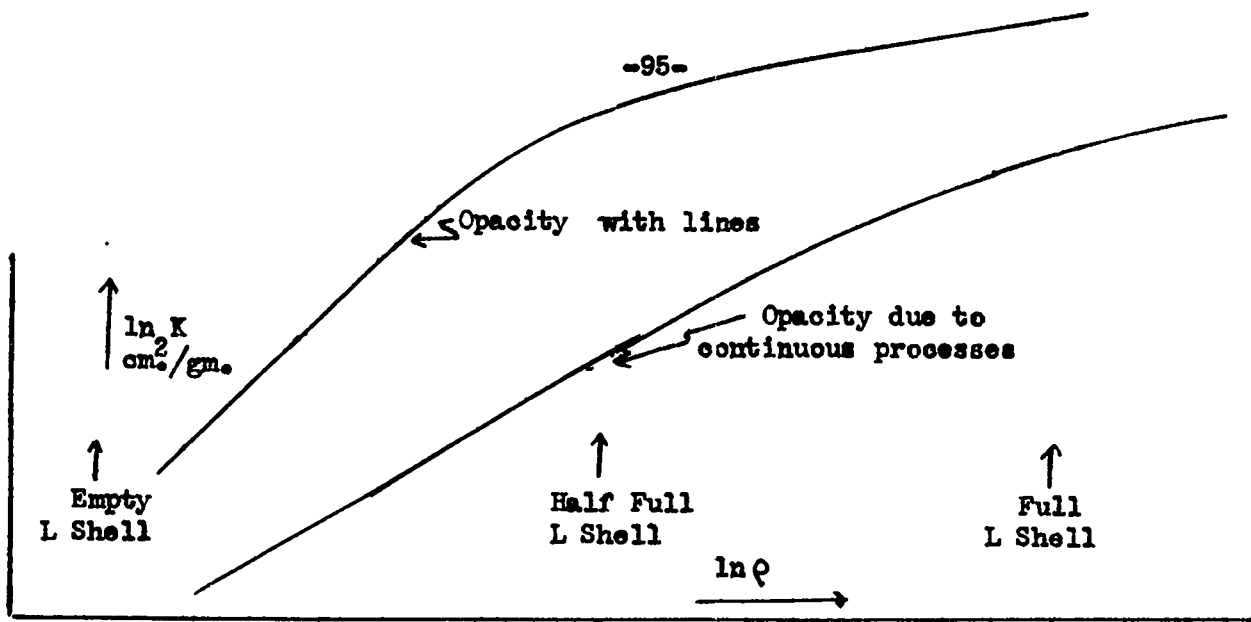
In contrast to the scattering, the free-free opacity is proportional to the density, varies almost as  $T^{-7/2}$  and is also approximately proportional to  $Z$ . It is because of this limiting form that astronomers have used the temperature dependence of the opacity as  $T^{-7/2}$ . But the limitations of this law should be clearly understood.



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### 3. Variation of Opacity with Temperature, Density and Atomic Number.

The qualitative variation of the opacity with various factors is evident to a considerable extent by a consideration of the equations, although the quantitative evaluation requires an immense amount of computation. Consider first the variation of opacity with density. At the lowest density the only important process is scattering. So long as this is true the opacity is independent of density. But as the density increases, the K electrons become bound with appreciable probability, unless the temperature is too high. For temperatures at which the K electrons can become bound  $kT \sim \left( \frac{1}{10} \text{ to } \frac{1}{3} \right) Z^2 \rho$ , the ionization limit of the K electrons is low enough so that their photoelectric absorption will occur in a region where there is considerable radiation. Their absorption will, therefore, be very important in reducing the transmission. For low densities the K occupation will increase proportionally to the density; then  $A \Delta_c \rho^{-1}$  and  $K \rho$ . Superimposed upon this linear variation of the continuous opacity is the effect of lines. So long as only K electrons are bound, this is usually a small effect, since the line spectrum is simple. As the density further increases, the K shell becomes full. The increase in density then can cause no further increase in K occupation. For a short while, therefore, the opacity is again independent of the density. But then the L shell begins to fill. Initially the occupation of this shell again varies as  $\rho$  and it may well be that considerable radiation is in the frequencies which they will absorb photoelectrically. For awhile, therefore, we again have the continuous opacity  $K_c \rho$ . However, eventually the L shell will be filled and then  $K_c$  will be independent of  $\rho$ . In this case, in contrast to the filling of the K shell, the lines are very often of decisive importance. The line spectrum will be very simple for a practically empty L shell, increase to a maximum complexity as 4 or 5 electrons become bound, and then decrease in complexity as the shell fills up full. The interplay of the line and continuous process is shown schematically in the figure.



The ratio  $K/K_0$  will have a broad maximum near the density at which the L shell is half full. This pattern of behavior is repeated but much less distinctly as the higher shells fill in. Finally, however, increasing density "cuts off" more and more bound state. Eventually all the electrons are pressure ionized and the determining process is free-free scattering. The opacity then increases proportional to the density. It is doubtful, however, that the methods outlined in this paper are adequate to cope in detail with the free-free absorptions at such high densities, since they are based upon hydrogenic wave functions for the electrons.

The variation with temperature is much more complicated than with density, because, not only do the occupation numbers change, but the frequency region in which the maximum radiation is present also changes. At usual densities a shell will begin to fill up at a temperature from 1/10 to 1/3 times its ionization energy, and thus the absorption from the latest bound shell is always of decisive importance in determining the opacity. The occupations vary as  $\exp(-I_m/kT)$ , the bound free absorption coefficient as  $D_{bf} \sim (I_m/kT)^2 \exp(-I_m/kT)$  and hence  $A \sim (kT/I_m)^2 \exp(-I_m/kT)$ . Finally  $K_c = 1/(\rho N_c) \propto \frac{I_m^2 R h c}{(kT)^3} e^{-I_m/kT}$ , i.e.  $K_c \propto T^{-3} \exp(-const/T)$ . This variation is quite a bit more rapid than the  $T^{-7/2}$  law for free-free processes. In addition the line contribution must be superposed upon this.

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The variation with atomic numbers is related to that with temperature - indeed we discussed a similarity transformation with the parameter  $Z^2 Rk c / kT$ . Hence roughly  $K_c \propto Z^4 \text{ exp}(-\text{const } Z^2)$ . The line effects are important but too varied to discuss in brief. As was mentioned previously the lines change their qualitative behavior when relativity effects become important, that is for high  $Z > 60$  or  $70$ . A comprehensive discussion of the high  $Z$  phenomena is given by Jacobsohn.

VIII Opacity of Iron

To illustrate the principles of the preceding chapters, the calculation of the opacity of pure iron,  $Z = 26$ , at normal density  $\rho = 7.85$  grams /cm<sup>3</sup> and at a temperature of  $kT = 1$  kilovolt will now be discussed in detail.

1. Occupation Numbers

The data for the calculation are

$$(8.1) \quad \begin{aligned} Z &= 26 \\ \rho &= 7.85 \text{ grams /cm}^3 \\ M &= 55.85 \text{ grams} = \text{molar weight} \\ \frac{kT}{Rhc} &= 73.49 \end{aligned}$$

Using the above data and (6.2) we determine the radius of the ion spheres - a particularly simple job in the case of a pure element. From (6.2)

$$V = \frac{4\pi}{3} N a_0^3, \quad \left(\frac{a_{Z'}}{a_0}\right) = \left(\frac{3}{4\pi} \frac{V}{N a_0^3}\right)^{1/3}$$

But

$$(8.2) \quad \frac{V}{N a_0^3} = \frac{M}{N_0 \rho a_0^3} = 79.75 \quad N_0 = \text{Avogadro's number}$$

Hence

$$(8.3) \quad \frac{a_{Z'}}{a_0} = 2.670$$

The successive approximation procedure must now be used to find the actual occupation number. The last cycle of the approximation is summarized in the accompanying table, Table A. Column (1) gives the orbital (specified by  $\ell$ ), column (2) the degeneracy  $C_{\ell Z}$  and column (3) the assumed values for the occupation. The sum  $\sum_{\ell} \frac{n_{\ell} Z}{N} = \frac{n_b}{N} = 2.925$  at the foot of the column gives the number of bound electrons, and hence  $n_f/N = \frac{n - n_b}{N} = 23.075$ .

$\mathcal{E}_{\ell}^0 (Z^*)$  can be determined by the use of (6.7) and interpolation in Table III, the table of energy levels. This is recorded in column (4). With a knowledge of  $a_{Z'}$  and

$$Z' = Z - \sum_{\ell} \frac{n_{\ell} Z}{N} = 26 - 2.9251 = 23.075 \text{ we can compute the correction terms in (6.8),}$$

and the final value of  $\bar{\epsilon}_{lZ}$ ' is recorded in column (5). Whenever this energy becomes positive we know that the bound state has been out off, and merged with the free states. This happens for levels with  $n > 4$ .  $\mathcal{L}^*$ , determined by (6.6), has the value 4.5826 so that by the use of (6.9) a final set of occupation numbers, listed in column (6), is obtained. The value of  $n_b/N = 2.924$  is in close agreement with  $n_b/N = 2.925$  assumed in column (3) indicating that the successive approximations have satisfactorily converged. It will be noted that only the K shell is substantially occupied under these conditions.

The ionic occupation numbers may now be found. The fraction of ions having electrons in the  $l$ th shell is recorded in Table B following. More important for our later calculations is the number of K electrons in ions of a given configuration. This number is given in Table C.

Table A Occupation Numbers of Iron  $Z = 26$

$\rho = 7.85$  grams /cm<sup>3</sup>

$kT = 1$  kilovolt

Level $l$	Weight $C_{lZ}$	Occupation $\frac{n_{lZ}}{N}$	$-\frac{\epsilon_l^0(Z^*)}{Rhc}$	Ionization energy $-\frac{\bar{\epsilon}'_{lZ}}{Rhc}$	Occupation $\frac{n_{lZ}}{N}$
1s	2	1.9541	643.32	612.22	1.9540
2s	2	.09229	145.09	114.07	.09214
2p <sub>3/2</sub> <sup>1</sup>	2	.03826	141.63	110.64	.03813
2p <sub>1/2</sub> <sup>1</sup>	4	.17403	140.60	109.56	.1738
3s	2	.03113	62.595	31.934	.03110
3p <sub>3/2</sub> <sup>1</sup>	2	.03069	61.564	30.351	.03065
3p <sub>1/2</sub> <sup>1</sup>	4	.06113	61.260	30.547	.06106
3d <sub>3/2</sub> <sup>1</sup>	4	.06063	60.764	29.934	.06055
3d <sub>5/2</sub> <sup>1</sup>	6	.09082	60.666	29.336	.09071
4	32	.34215	33.907	3.979	.3413
Bound Electrons		$\sum \frac{M_{lZ}}{N} = 2.9252$	Bound Electrons		$\sum \frac{M_{lZ}}{N} = 2.924$

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Table B Ionic Occupations of Iron Z = 26 $\rho = 7.85 \text{ grams/cm}^3$ 

kT = 1 kilovolt

Shell	Fraction of ions with the following number of electrons in the shell					
	0	1	2	3	4	5
K	.000529	.04494	.95453			
L	.69616	.25794	.041808	.003873	.000224	neg.
M	.75864	.21117	.027759	.0022894	.000133	neg.
N	.70922	.24509	.041025	.004431	.000347	neg.

Table C Ionic Occupation of Iron Z = 26 $\rho = 7.85 \text{ grams/cm}^3$ 

kT = 1 kilovolt

Shell	Number of K electrons per atom in ions having the following number of electrons in the shell.		
	0	1	2
K	0	.04494	1.9091

2. Thermodynamic Properties

Using the occupation numbers found in the preceding section and the formulae of Appendix I it is a simple matter to compute the energy and the pressure. The various terms are given in the following table.

Table D Energy and Pressure for Iron

$\rho = 7.85 \text{ gm/cm}^3$        $kT = 1 \text{ kilovolt}$

Binding energy of ions	$\frac{E_b}{N Rho} \text{ (AI.17)}$	- 1381.6
Potential energy	$\frac{P.E.}{N Rho} \text{ (AI.17)}$	- 15.56
Kinetic energy of free electrons	$\frac{K.E.}{N Rho} \text{ (AI.18)}$	2550.1
Energy of nuclei	$\frac{E \text{ nuclei}}{N Rho} = \frac{3}{2} \frac{kT}{Rho}$	<u>110.2</u>
Total Energy	$\frac{E}{N Rho}$	1263.1
Free electrons	$\frac{PV}{N Rho} \text{ (AI.20)}$ Kinetic energy term Potential energy term	1695.0 -5.19
Nuclei	$\frac{PV}{N Rho} = \frac{kT}{Rho}$	73.49
Total pressure	$\frac{PV}{N Rho}$	<u>1764.3</u>
	$\frac{PV}{(Z+1)kT}$	,8897

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For this calculation the nuclei were treated as free, because  $\beta = \frac{Z'e}{\sqrt{2kT_m}} = 1.65 \ll 3.4$  (c.f. Appendix I). We note that the material does not behave like a perfect gas of  $(Z+1)N$  particles, but instead behaves as if only 89% of the particles were completely free. Furthermore this percentage will vary rapidly with temperature and somewhat more slowly with density. With regard to the energy, we can see that the potential energy and nuclear energy terms are small corrections; it is not necessary to further refine our treatment of them. To the other terms we may attach a high degree of reliability. It is also worthy of note that the kinetic energy is almost twice the total ionization energy of the remaining bound electrons.

### 3. The Continuous Opacity

The calculation of the scattering and free-free absorption contributions is a straightforward application of (6.23) and (6.25). The bound-free contribution requires some care, however. We first make a preliminary calculation which assumes that all the ions have the same ionization potentials for a particular one electron transition. This is the average ionization potential  $-\bar{\epsilon}_{nZ}$  recorded in Table A column 5. We notice that the subshells  $2s$ ,  $2p_{3/2}^1$ ,  $2p_{3/2}^3/2$  have very nearly the same ionization potential and for simplicity we take an occupation weighted average value  $-\bar{\epsilon}_2^1 = 111.0$  Rho. Similarly for the  $n = 3$  shell, we use  $-\bar{\epsilon}_3^1 = 30.36$  Rho. Table D summarizes the continuous opacity results. In column 1 the frequency  $u = \frac{h\nu}{kT}$  for which the reduced absorption coefficient  $D(u)$  is to be calculated is given. Entries with an asterisk are the ionization frequencies. The contribution of the various absorption processes is given in columns 2 to 7 and the total  $D(u)$  in column 8. Column 9 gives the difference  $\Delta S = S(u_{k+1}) - S(u_k)$  of the Strömgen functions for the interval between the two frequencies. This is a measure of how important the contribution of the region may be. In the final column is given  $\Delta S/D(\bar{u})$ , the contribution to the reduced mean free path  $\Lambda/\Lambda_0$  of the region.

For the very lowest frequencies, the only important process is free-free absorption. It is only above the ionization potential of the L electrons that the bound-free absorptions become of dominant importance. Even here the free-free contribution is 16% while



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the scattering contribution is  $\sim 10\%$  of  $D(u)$ . Since it is the region between the K and L ionization limits which, according to the last column, contributes practically 100% to the mean free path, it is not possible to dismiss scattering and free-free absorption lightly. Above the K ionization limit, however, the bound-free absorption of the K electrons alone is sufficient to black out the region, so the other processes need hardly be considered.

In the K to L window the Gaunt factor for the L electron absorption varies from .875 at the L edge to 1.05 at the K edge. The error made by putting the Gaunt factor exactly equal to unity, that is, by using the old Kramer's formula is not large.

The neighborhood of the K edge is one in which the weighting function  $W(u)$  is particularly large, and in which  $D(u)$  take a very large jump. The details of the absorption in this region will therefore have a considerable effect on the final transmission. We therefore return to our ionic picture for an accurate treatment of this region. The results are summarized in Table E. The first column gives the ion type, that is the number of electrons in each of the K, L, M, and N shells. The second column gives the number of K electrons per atom of the system, which are in the various ions. The fourth column gives the contribution to the absorption coefficient of each ion type at the ionization frequency which is given by column 3. Since the Gaunt factor varies slowly with frequency, we may assume these contributions do not change within the region occupied by the K edges of the various ions. The next column (5) gives the absorption coefficient and the final column  $\Delta S / D(\bar{u})$  the contribution of the region to  $\Lambda \Lambda_0$ , the reduced mean free path. Whereas this region gave a contribution 15.37 in the rough treatment of Table D, we now get .939, reducing the total transmission to  $\Lambda \Lambda_0 = 186.31$  a change of 7.7%. Such a large change is only to be expected for even the few ions which have small ionization potential still have sufficient strength in their K absorption to wipe out most of the transmission left by the weak L absorptions.

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To avoid all the labor of this detailed calculation we could use a statistical treatment of the edges. This gives a transmission in the region of the edges as .565 instead of the accurate result .306. The agreement within the region of the edges cannot be considered too good, but this is unimportant for the error in the total transmission is only 0.13%.

TABLE E

CONTINUOUS OPACITY OF IRON  $Z=26$

Frequency $\nu$	Scattering $D_S$	Free-Free Abs. $D_{ff}$	Bound-Free Absorption Contribution to $D_{bf}$ from the Following Shells				$D(u)$	$\Delta S$	$D(\bar{u})$	$\frac{\Delta S}{D(u)}$	
			K shell	L shell	M shell	N shell					
8 5 0 9 8 8.3305*	negligible negligible negligible negligible negligible	negligible negligible negligible negligible negligible	127.1	.4	negligible	↑ negligible ↓	127.7	3.492	130	.02686	} .67
			115.5	.4	negligible		116.1	39.241	121.9	.32191	
			108.7	.4	negligible		109.3	20.117	112.7	.17850	
			108.1	.4	negligible		108.7	16.298	109.0	.14952	
								8.76	.5985	14.637	
8 7 6 5 4 3 2 1.5104* 1.0 5 4 132* 0.05414* 0	.07928 .05336 .03379 .01972 .01025 .00449 .00147 $6.92 \times 10^{-4}$ $2.52 \times 10^{-4}$ $.507 \times 10^{-4}$ $.418 \times 10^{-4}$ $.549 \times 10^{-5}$ 0	.07880 .07912 .07952 .08004 .08074 .08176 .08348 .08538 .08736 .08746 .08746 0	0	.4221	.0168	↑ negligible ↓	.5970	28.33	.5828	48.610	} 199.16
				.4192	.0168		.5685	28.317	.5572	50.820	
				.4156	.0167		.5458	24.097	.5356	44.991	
				.4087	.0166		.5254	16.499	.5156	31.938	
				.3999	.0165		.5077	8.320	.4999	16.643	
				.3894	.0162		.4921	2.649	.4914	5.503	
				.3696	.0159		.4707	.3063	.4630	.5616	
				.3534	.0156		.4553	.08240	.1034	.7969	
				0	.0151		.1030	.01042	.1026	.1016	
				0	.0144		.1022	$1.55 \times 10^{-4}$	.1020	$1.520 \times 10^{-3}$	
	0	.0142	.1019	$1.35 \times 10^{-4}$	.03769	$1.540 \times 10^{-3}$					
	0	0	0	.00023	.08769	$4.34 \times 10^{-8}$	.08746	$4.962 \times 10^{-7}$	} .90		
	0	.08746	0	0	.08746						
										$A \Lambda_0 = 200.$	

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TABLE E

## CONTRIBUTION TO THE CONTINUOUS OPACITY NEAR THE K EDGE: IONIC TREATMENT

Ion Types K L M N	Electron in Ion Occupation	$I_n/kT$ or $u$	Contribution to $B_{bf}$	$D(u)$	$\frac{\Delta_S}{D(u)}$
		9.0		109.3	.05076
1 x x x	.04494	8.7630	2.7514	108.56	.08138
2 0 0 0	.7151	8.4145	40.367	105.80	
2 0 0 1	.2471	8.3713	13.807	65.43	.01772
2 0 1 0	.1990	8.3358	13.318	51.63	.01691
2 0 0 2	.0414				.02761
2 0 1 1	.06878	8.2950	3.773	38.31	.02499
2 0 2 0	.02617	8.2619	1.424	34.53	.00900
2 1 0 0	.2649	8.2505	14.379	33.11	.05850
2 1 0 1	.09156	8.2088	4.919	18.73	.06523
2 1 1 0	.07375	8.1747	3.929	13.809	.2335
2 2 0 0	.04295	8.0881	2.240	9.875	.3534
Remainder	.13836	7.9873	7.038	7.635	
					$\Sigma: .9390$

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#### 4. Contribution of Lines

From our results on the continuous opacity, we see that the only important spectral region is that between the L ionization limit  $u = 1.510$  or  $h\nu = 111.0$  Rho and the lowest lying edge of the K ionization limit  $u = 7.987$ ,  $h\nu = 587.0$  Rho. The only lines in this region will be those in which a 1s electron is raised to an excited state, and we may restrict our considerations to this rather simple portion of the spectrum.

##### a. Position of the Lines

At first we examine the gross structure of the line spectrum by considering only the spherically symmetric part of the electrostatic interactions. Later we shall see that the splittings of the lines are unimportant. In order to get the positions of the lines in the correct relative positions to the absorption edges, it is easiest to compute the lines by the difference in ionization potentials of the electron involved in the transition. In an ion with  $x_j$  electrons in the  $j$ th level, the ionization potential of an electron in the  $k$ th level is approximately

$$(8.4) \quad I_k = -\mathcal{E}_k^0(Z) - \sum_{j \neq k} x_j F^0(j, k) - (x_k - 1) F^0(k, k) \\ - \frac{Z^2 e^2}{2a_Z} \left\{ 5 - \left( \frac{r}{a_Z} \right)^2 \right\}^k - 3/5 \sum \frac{N_Z}{Z} \frac{Z^2 e^2}{2a_Z} .$$

The frequency of the line resulting from the one electron transition  $k \rightarrow l$  is

$$(8.5) \quad I_k - I_l = -\mathcal{E}_k^0 + \mathcal{E}_l^0 - Z^2 \frac{e^2}{2a_0} \left( \frac{a_0}{a_Z} \right)^3 \left\{ \left( \frac{r}{a_0} \right)^{2l} - \left( \frac{r}{a_0} \right)^{2k} \right\} \\ + \left\{ (x_k - x_l - 1) F^0(l, k) - (x_k - 1) F^0(k, k) + x_l F^0(l, l) \right\} \\ - \sum_{\substack{j \neq k \\ j \neq l}} x_j \left[ F^0(j, k) - F^0(j, l) \right]$$

The first two terms are the frequency of the one electron line in the isolated ion; the next term is the lowering of the frequency caused by the electrostatic shielding of the

free electrons. This latter term is a constant for all ions with the same nuclear charge. The next set of terms in (8.5) give the interaction with electrons in the same shell as the initial and final shells of the transition electron. The final set gives the electrostatic screening of the remaining bound electrons. This last contribution is additive for the electrons of any ion undergoing a particular transition. In Table F are recorded the first two sets of terms of (8.5), that is the frequency of a one electron line in the free electron atmosphere.

Table F

Transition	Frequency of Line in Isolated Ion $h\nu/Rhc = -\frac{\epsilon_k^0 + \epsilon_l^0}{Rhc}$	Screening of Frees $Z' \left( \frac{a_0}{az'} \right)^3 \left\{ \left( \frac{r}{a_0} \right)^2 - \left( \frac{r}{a_0} \right)^2 \right\}$	Frequency of Line in free electron atmosphere $h\nu/Rhc$
1s → 2p $\frac{1}{2}$	511.25	.048	511.20
1s → 2p $\frac{3}{2}$	512.81	.048	512.76
1s → 3p $\frac{1}{2}$	606.39	.317	606.07
1s → 3p $\frac{3}{2}$	606.85	.317	606.53
1s → 4p $\frac{1}{2}$	639.63	.941	638.69
1s → 4p $\frac{3}{2}$	639.82	.941	638.88

If we neglect the small differences in screening of ns, np, nd etc. electrons we can readily express the contributions of the last two sets of terms to the line frequency. The following Table G gives the energy in units of 2Z Rhc which must be subtracted from the values in Table F for each bound electron in the ion in addition to the transition electron.

Table G Contribution of Additional Bound Electron (Units of 2Z Rho)

Transition	Shell of Additional Bound Electron			
	n = 1	n = 2	n = 3	n = 4
1s → 2p	.3822	.0578	.0090	.0029
1s → 3p	.5162	.1416	.0347	.0086
1s → 4p	.5633	.1758	.0559	.0177

As mentioned above the contributions of the additional bound electrons in the ion are additive.

With the use of Tables F and G, we prepare a list, Table H, of the stronger  $1s \rightarrow np\frac{1}{2}$  lines and their frequencies. The  $1s \rightarrow np\frac{3}{2}$  line will be split from their  $1s \rightarrow np\frac{1}{2}$  counterpart by just the splitting of Table F. We can see that for each transition the lines form into 2 groups, one formed from ions with a single K electron, the other from ions with 2K electrons. The  $p\frac{1}{2}$ ,  $p\frac{3}{2}$  splitting, and also the electrostatic splitting will not change the group to which a line belongs, but will simply increase the number of lines in each group. The differences within each group are so small that we may well expect them to be smaller than the wingspread of the lines. In that event it is no longer necessary to consider all the details of each line. We therefore stop to consider the dispersion of the lines.

b. The Doppler Breadth.

The energy half breadth for Doppler broadening is given by (5.29). The calculation for iron at  $kT = 1000$  volts gives to lines of frequency  $\sim 7kT$  (the K electron lines) a half breadth of .0836 Rydberg units, or  $\nu = \frac{h\nu}{kT} = 1.138 \times 10^{-3}$ .

c. The Natural Breadth:

In opacity calculations, the natural breadth phenomenon differs in two important respects from the ordinary case encountered in optical spectra. First the radiation density is so high that absorption and induced emission processes as well as spontaneous emission contribute to the breadth of the levels. Second the atoms are so highly ionized that

TABLE HSpectrum of K Electron Lines (Rhc units)

Ion Type K L M N	K Electron in Ion Occupation	1s $2p_{\frac{1}{2}}$	1s $3p_{\frac{1}{2}}$	1s $4p_{\frac{1}{2}}$
1 0 0 0	.01683	511.20	606.07	638.69
1 0 0 1	.00605	511.05	605.62	637.77
1 0 1 0	.00468	510.73	604.27	635.78
1 1 0 0	.00624	508.19	598.70	629.55
Remainder	.01114	505.18		
2 0 0 0	.7151	491.33	579.23	609.40
2 0 0 1	.2471	491.17	578.78	608.48
2 0 1 0	.1990	490.86	577.42	606.49
2 1 0 0	.2649	488.32	571.87	600.26
2 0 0 2	.0414	491.02	578.33	607.56
2 0 2 0	.02617	490.39	575.62	603.58
2 2 0 0	.04295	485.31	564.50	591.12
2 0 1 1	.06878	490.71	576.98	599.34
2 1 0 1	.09156	488.17	571.42	597.35
2 1 1 0	.07375	487.86	570.06	581.97
Remainder 2300	.1384	482.31	557.14	



many transitions contribute to the breadth.

In general the energy half breadth at half maximum is  $\alpha\gamma/2$ , and this breadth is the sum of the breadths of the initial and final states of the transition. The half breadth of a level  $i$  is

$$(8.6) \quad \bar{\Gamma}_i = \frac{\alpha \gamma_i}{2kT} = \frac{\alpha^3}{2} \frac{kT}{\text{Rho}} \sum_j \frac{u_{ij}^2 f_{ij}}{e^{u_{ij} - 1}}$$

where  $u_{ij} = \frac{h\nu_{ij}}{kT}$  and  $h\nu_{ij}$  is the energy of the transition  $i$  to  $j$ . We note that  $u_{ij}$  and  $f_{ij}$  are both negative for downward transitions. The sum  $\sum_j$  includes all possible transition which shift the frequency of the line in question by more than its breadth.

While (8.6) is very convenient for transitions between discrete states, we can put it into simpler form for transitions to and from the continuum. For transitions from a bound to a free state

$$(8.7) \quad \sum_j \frac{u_{ij}^2 f_{ij}}{e^{u_{ij} - 1}} \text{ goes over into } \int_{u_i}^{\infty} \frac{u^2 \frac{df}{du} du}{e^{u-1}}$$

where  $u_i$  is the ionization potential in units of  $kT$  of the  $i$ th level. Introducing the result of (2.22) into (8.7) we get

$$\sum_j \text{continuum} = \frac{2^4}{3\sqrt{3}\pi} \frac{1}{n_i} u_i^2 \int_{u_i}^{\infty} \frac{g_i(u) du}{u(e^{u-1})}$$

The maximum value of the integrand occurs at  $u = u_i$  and we may replace the slowly varying function  $g_i(u)$  by  $g_i(u_i)$ . Then the integral may be expressed in terms of the exponential integral  $-E_i(-x)$  tabulated, for example, in Jahnke und Emde, pp. 6 ff. The contribution of the bound-free transitions to the breadth is thus

$$(8.8) \quad \bar{\Gamma}_{bf} = \sum_{\text{all bound electrons}} \frac{\alpha^3}{2} \frac{kT}{\text{Rho}} \frac{2^4}{3\sqrt{3}\pi} \frac{1}{n_i} (u_i)^2 g_i(u_i) \sum_{\lambda=1}^{\infty} -E_i(-\lambda u_i)$$

In addition to the bound free transitions, the process of free electron capture contributes to the breadth of a level. In this case we must multiply the contribution from a free to a bound state transition by the probability that the free state is occupied,  $p \approx e^{-\alpha x - \epsilon \epsilon_f} = e^{-\alpha x - u + u_k}$ , and sum over all free states. We get exactly the same

integral as in (8.7) so the resulting contribution of these processes is

$$(8.9) \quad \Gamma_{i \rightarrow b} = \sum_{\substack{\text{all empty} \\ \text{bound states } k \\ \text{(not levels)}}} \frac{d^3}{2} \frac{kT}{Rhc} e^{-\frac{h\nu}{kT} + u_k} \left\{ \frac{2^4}{3\sqrt{3}} \pi \frac{1}{n_k} u_k^2 \epsilon_k(u_k) \sum_{\lambda=1}^{\infty} -E_i(-\lambda u_k) \right\}.$$

The contributions (8.8) and (8.9) are generally small compared to that of the bound-bound transitions. In Table I are recorded the natural breadth contributions of the various transitions for the case of iron  $Z = 26$ ,  $kT = 1000$  volts and normal density. The natural breadths of the stronger K electron lines is given in table J. The natural breadth is much smaller than the Doppler breadth and the collision breadth (see next section) and may therefore be neglected.

d. The Collision Breadth:

The problem of collision broadening has been analyzed by R. Sternheimer.<sup>1</sup> We quote his results without proof. The energy half breadth at half maximum is analogous to the natural breadth  $\pi \delta/2$ . The breadth is the sum of the initial and final breadths of the states involved in the transition. In turn the breadth of a state is the sum of contributions from all the transitions which the ion can undergo which shift the line more than the breadth. A transition of an electron from an initial state to a final state  $j$ , both discrete states, gives the contribution to the energy half breadth on an ionic level

$$(8.10) \quad \frac{2}{3} \sqrt{2\pi} \frac{n_f}{V} \frac{1}{Z^2} \sqrt{\frac{mc^2}{kT}} \left( \frac{h}{mc} \right)^3 \frac{1}{2\lambda_1 + 1} \left| R_{n_i, l_{ij}, n_j, l_j} \right|^2 I_{ij}$$

where

$$(8.11) \quad I_{ij} = e^{-u_{ij}} \ln \frac{4|\beta \bar{E}'_{ij}|}{u_{ij}} - E_i(-u_{ij}) \quad \text{if } |u_{ij}| > \frac{u_{ij}^2}{4|\beta \bar{E}'_{ij}|} > \frac{\lambda a'}{kT}$$

$$I_{ij} = -E_i \left( -\frac{u_{ij}^2}{4|\beta \bar{E}'_{ij}|} \right) \quad \text{if } \frac{u_{ij}^2}{4|\beta \bar{E}'_{ij}|} > |u_{ij}| > \frac{\lambda a'}{kT}$$

$$I_{ij} = \ln \frac{4|\beta \bar{E}'_{ij}|}{\left( \frac{\lambda a'}{kT} \right)^2} - .577216 \quad \text{if } |u_{ij}| < \frac{\lambda a'}{kT}$$

1. Unpublished Report.

and,  $\bar{n} a'$  the plasma energy is given by

$$(8.12) \quad \bar{n} a' = \sqrt{\frac{n_f}{V} \frac{\bullet^2}{\gamma m}} = \sqrt{\frac{4}{\pi} \frac{n_f}{N} \frac{N a_0^3}{V}} \text{ Rho}$$

while  $|R_{ni} l_i, m_j l_j|^2$  is recorded in Tables by Bethe<sup>2</sup>. We must sum (8.10) over all final states  $j$  available for the transition and all initial state  $i$  occupied by electrons in the ion. We then get for the partial energy half breadth of the level due to discrete transitions

$$(8.13) \quad \frac{\bar{n} \delta \ell}{2 \text{ Rho}} = \frac{8}{3} \sqrt{\pi} \frac{n_f}{N} \frac{N a_0^3}{V} \left(\frac{\text{Rho}}{kT}\right)^{\frac{1}{2}} \frac{1}{2} \sum_i \sum_j \frac{\ell_{\max}}{2\ell_i+1} |R_{i,j}|^2 I_{ij} \cdot$$

Transitions to and from the free states should also be included as contributing to the breadth. For the former we may use the results of Bethe<sup>3</sup> quoted by Mott and Mossey.<sup>4</sup> He gives the cross-section for ionization which leads to a collision breadth contribution of

$$(8.14) \quad \frac{\bar{n} \delta \ell}{2 \text{ Rho}} = 4\pi^{3/2} \frac{n_f}{N} \frac{N a_0^3}{V} \left(\frac{\text{Rho}}{kT}\right)^{\frac{1}{2}} \frac{n^2 c_{ng}}{2 m_e} \times$$

$$\times \left\{ \text{erfc} \left| \frac{\bar{E}_{ng}}{kT} \right| \ln \frac{80 kT}{|\bar{E}_{ng}|} + \chi \left( \frac{\bar{E}_{ng}}{kT} \right) \right\};$$

where

$$(8.15) \quad \text{erfc } x = 1 - \text{erf } x = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-y^2} dy,$$

$$\chi(x) = \frac{1}{\sqrt{\pi}} \int_x^{\infty} y^{-\frac{1}{2}} e^{-y} \ln y dy,$$

and  $c_{ng}$  is given in the following table.

Table of  $c_{ng}$

State	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
$c_{ng}$	0.28	0.21	0.13	0.17	0.14	0.07	0.15	0.13	0.09	0.04

2. Handbuch der Physik: Second Edition, Vol. 24, 1; p. 442
3. Annalen der Physik, 5 (1930) pp. 325 H.
4. Theory of Atomic Collisions, Oxford 1933, p. 182.

Table I: Contributions to Energy Half Breadth of Electronic Transition

Electron	Transition	Natural Breadth $10^6 \frac{\lambda}{2 Rho}$	Collision Breadth $10^6 \frac{\lambda}{Rho}$	Electron	Transition	Natural Breadth $10^6 \frac{\lambda}{2 Rho}$	Collision Breadth $10^6 \frac{\lambda}{Rho}$	
1s	1s - 2p	21.01	1.360	3d	3d - 2p	990.7	883.1	
	1s - 3p	1.5624	.05395		3d - 3p	0	181500.	
	1s - 4p	.4074	.01163		3d - 4p	4.084	467.	
	Total 1s - np	22.98	1.427		3d - 4f	377.7	43110.	
	1s - free	2.960	0		Total 3d - n	1372.	256000.	
Grand Total	25.94	1.427	3d - free	121.97	108400.			
2s	2s - 2p	0	.1382	4s	4s - 2p	1064.	.005938	
	2s - 3p	288.0	.002519		4s - 3p	1060.	707.7	
	2s - 4p	69.62	.000233		4s - 4p	0	1910600.	
	Total 2s - np	357.6	.1410		Total 4s - np	2124.	1911300.	
	2s - free	204.7	8546.0		4s - free	22.83	859300.	
Grand Total	562.3	8546.1	Grand Total	2147.	2770600.			
2p	2p - 1s	6940.0	.01108	4p	4p - 1s	1488.	14.16	
	2p - 2s	0	.45900		4p - 2s	1104.	0.0	
	2p - 3s	8.999	79.00		4p - 3s	1067.	1171.	
	2p - 3d	460.3	4049.0		4p - 3d	1053.	133.7	
	2p - 4s	2.058	6.9		4p - 4s	0	635800.	
	2p - 4d	82.52	270.3		4p - 4d	0	1018000.	
	Total 2p - n	7494.	50310.		Total 4p - n	4712.	1655100.	
	2p - free	207.2	9555.		4p - free	22.83	744700.	
Grand Total	7701.2	59865.	Grand Total	4735.	2399800.			
3s	3s - 2p	96.87	1004.	4d	4d - 2p	1168.	0	
	3s - 3p	0	731600.		4d - 3p	1089.	1345.	
	3s - 4p	180.5	21140.		4d - 4p	0	610800.	
	Total 3s - np	277.4	753700.		4d - 4f	0	534300.	
	3s - free	125.1	263200.		Total 4d - n	2257.	1146000.	
Grand Total	402.5	1016900.	4d - free	22.83	515600.			
3p	3p - 1s	1851.	47.20	4f	4f - 2p	1128.	5292.	
	3p - 2s	344.4	511.8		4f - 3d	1128.	0	
	3p - 3s	0	242900.		4f - 4d	0	0	
	3p - 3d	0	330200.		Total 4f - nd	1128.	5292.	
	3p - 4s	12.01	1590.		4f - free	22.83	229130.	
	3p - 4d	230.2	26500.		Grand Total	1151.	234420.	
	Total 3p - n	2458.	601300.		Free	Free - 1	251.0	
	3p - free	123.3	216770.			Free - 2s	19.76	
Grand Total	2561.	818070.	Free - 2p	56.37				
			Free - 3	34.18				
			Free - 4	7.989				
			Total Free - Bound	369.7				

The integral (8.15) has been evaluated through the good offices of Mr. Bengt Carlson, whose results are contained in Table IX.

Transitions involving the capture of an electron will be relatively unimportant, and transitions from one free state to another will not appreciably alter the frequency of the absorption line and hence must not be considered as contributing to the collision width.

In Table I, the contributions of the various transitions to the collision breadth is given. The largest contributions come from those transitions requiring very little energy change. The contribution of ionizing transitions also is appreciable except for the most tightly bound electrons. Values of the breadths for the strong K lines of iron are recorded in Table J along with the natural breadths.

#### e. Stark Broadening

To adequately discuss the Stark Effect broadening of the lines we shall have to refine slightly the treatment given in IV 6 to include effects of shielding by the free electrons. As before (c.f. 4.59) the number of ions with effective charge  $Z'$  at a distance  $r_{12}$  from a particular ion with effective charge  $Z''$  is

$$(8.15) \quad N_{Z'}(r_{12}) dr = \frac{N_{Z'}}{V} \left\{ e^{-\mathcal{E}(r_{12})/kT} \right\} 4\pi r_{12}^2 dr_{12}$$

The mutual potential energy  $\mathcal{E}(r_{12})$  is not given, however, by the simple form (4.58), but instead by

$$(8.16) \quad \mathcal{E}(r_{12}) = Z'Z'' \frac{e^2}{a_0} \left\{ \frac{a_0}{r_{12}} - \frac{3}{2} \frac{a_0}{a_{Z''}} + \frac{r_{12}^2}{2a_0^2} \left( \frac{a_0}{a_{Z''}} \right)^3 \right\}, r_{12} \leq a_{Z''}$$

$$\mathcal{E}(r_{12}) \sim 0, r_{12} > a_{Z''}$$

The electric field due to the invading ion is

$$(8.17) \quad \vec{\mathcal{E}} = \frac{Z'e}{a_0^2} \left\{ \frac{a_0^2}{r_{12}^2} - \frac{r_{12}}{a_0} \left( \frac{a_0}{a_{Z''}} \right)^3 \right\}$$

directed radially. This field is not uniform as is the case in the laboratory Stark effect,

However we may expand the field in spherical harmonics. Keeping only the leading term, we get the usual uniform field case. The terms we neglect in the development are of the same order as effects not considered at all in this crude treatment, for example the resultant field due to all neighboring ions and free electrons acting as an assemblage of dipoles, and indeed these neglected terms are of about the order of the term considered.

The electric field  $\vec{E}$  will split and shift the levels of the ion affected, causing a displacement of the absorption line of magnitude.

$$(8.18) \quad \Delta = (C_n + C_n') |\vec{E}| + (C'_n + C''_n) |\vec{E}|^2 + \dots$$

where the first term gives the linear Stark effect shift, the second term the quadratic, etc. The quantity  $C_n |\vec{E}|$  is the change in energy of the state  $n$  caused by the linear Stark effect of the field  $|\vec{E}|$ ; for example, in a one electron ion

$$(8.19) \quad C_n |\vec{E}| = -\frac{3}{2} \frac{a_0}{Z^n} n k e |\vec{E}| \quad k = 0, \pm 1, \pm 2 \dots$$

For the higher levels of an ion where the Stark effect is most important, the linear Stark effect may be present. In this case the number of ions which suffer a shift between

$\Delta$  and  $\Delta + d\Delta$  in a particular line can be approximated by

$$(8.20) \quad \frac{N_Z^n}{N_2^n} (D) d(\Delta) = \frac{N}{V} 2\pi a_0^3 \left\{ \frac{(C_{nn'})^{3/2}}{D^{5/2}} - 3 \frac{(C_{nn'})^{3/2}}{D} \left(\frac{a_0}{a_Z^n}\right)^3 + \dots \right\} d(\Delta) \\ \times \exp \left\{ -2Z'Z^n \frac{Rho}{kT} \left[ \left(\frac{D}{C_{nn'}}\right)^{1/2} - 3/2 \left(\frac{a_0}{a_Z^n}\right) + \frac{(C_{nn'})}{D} \left(\frac{a_0}{a_Z^n}\right)^3 \dots \right] \right\}$$

where

$$(8.21) \quad C_{nn'} = (C_n + C_n') Z' \frac{e}{a_0^2}$$

This asymptotic development is valid for large  $\Delta$ , the region in which we are particularly interested.

We cannot use this expression directly to define a half intensity half breadth, for it diverges for no shift  $\Delta = 0$ . However, we can compare the number of ions having a shift  $\Delta_2$

with the number having a shift  $\Delta_2$  provided both shifts are fairly large. This gives, with neglect of the correction terms

$$(8.22) \quad \frac{N_{Z^n}(\Delta_2)}{N_{Z^n}(\Delta_1)} = \left(\frac{\Delta_1}{\Delta_2}\right)^{5/2} \exp - \frac{2Z'Z^n}{(kT/Rho)} \left[ \left(\frac{\Delta_2}{C_{nn'}}\right)^{1/2} - \left(\frac{\Delta_1}{C_{nn'}}\right)^{1/2} \right]$$

Now a great number of ions will be at a distance  $a_{Z^n}$ . To the same approximation as (8.22) these will cause a shift

$$(8.23) \quad \Delta_1 = (C_n + C_{n'}) \frac{\bar{Z}'e}{a_{Z^n}} = C_{nn'} \left(\frac{a_0}{a_{Z^n}}\right)^2$$

We can define somewhat arbitrarily a half breadth  $\Delta_2$ , by requiring that the ratio (8.22) be  $\frac{1}{2}$  when  $\Delta_1$  is given by (8.23). This gives

$$(8.24) \quad \frac{\Delta_2}{C_{nn'}} = \frac{(kT/Rho)^2}{4 Z'Z^n} \left\{ \ln 2 + \frac{2 \bar{Z}'Z^n}{(kT/Rho)} \frac{a_0}{a_{Z^n}} + \frac{5}{2} \ln \frac{\Delta_1}{\Delta_2} \right\}^2$$

For the case of iron at  $kT = 1000$  volts,  $\rho = 7.85$  gm/cm<sup>3</sup>. This gives  $\Delta_2/C_{nn'} = .162$  or

by means of (8.21) and (8.19)

$$(8.25) \quad \Delta_2 = .486 (nk + n'k') Rho$$

which corresponds to a field of intensity

$$(8.26) \quad |\mathcal{E}| = .162 \frac{Z'e}{a_0}$$

We will get the maximum shift and split from the unperturbed line when  $k = (n-1)$ .

$k' = (n-1)$ . For  $K$  electron lines this gives a half breadth in Rydberg units as follows

Final state	$\Delta_2/Rho$
$n = 2$	.972
$n = 3$	2.92
$n = 4$	5.83

To test whether our approximation of the linear Stark shift is correct, we examine the splittings of the upper states of our ions. For example, we have the following deviations from the zero order energy.

Table J  
Energy Half Breadths of Strong K Electron Lines (Rhc Units)

Transition	Doppler Breadth	Natural Breadth	2 x Collision Breadth	Stark Breadth
1s→2p	.084	.00833	.0599	.5
(1s) <sup>2</sup> →(1s)(2p)	.084	.00466	.0599	.5
(1s) <sup>2</sup> (2s)→(1s)(2s)(2p)	.084	.0576	.1710	.5
(1s) <sup>2</sup> (2p)→(1s)(2p) <sup>2</sup>	.084	.00937	.1796	.5
(1s) <sup>2</sup> →(1s) (3p)	.084	.0021	.818	2.9
(1s) <sup>2</sup> →(1s)(4p)	.084	.0044	2.40	5.8

Contribution of Additional Electrons  
to Collision Breadth

Shell of Additional Electron	2 x Contribution to Half Breadth Rhc
2	.0941
3	1.176
4	2.49



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State	Energies in $\frac{\text{Rhc}}{Z^2}$ Units		
	$n = 2$	$n = 3$	$n = 4$
(1s) (ns) $1_g$	.2318	.1053	.060
(1s) (ns) $3_g$	.1879	.0937	.0552
(1s) (np) $1_p$	.2599	.1108	.0624
(1s) (np) $3_p$	.2257	.1068	.0607

For the  $n = 4$  state the largest splitting that affects the calculation is .286 Rhc and for  $n = 3$  it is .681 Rhc so we are quite safe in using a linear Stark effect for these lines. For  $n = 2$ , however, the split is 1.97 Rhc compared to a linear Stark effect shift of .972 Rhc, so we must use the formula for the quadratic Stark effect. This will give a result of approximately 0.5 Rhc.

#### f. Treatment and effect of the Lines.

A glance at Tables D and E shows that only those lines with energies below 590 Rhc can affect the transmission appreciably. Referring to Table H we find that three groups of lines -  $1s \rightarrow 2p$  with 1 K electron,  $1s \rightarrow 2p$  and  $1s \rightarrow 3p$  with 2K electrons have appreciable strength below this limit.

From the table of line breadths, Table J, we see that the lines will be sufficiently broad so that different components of a line caused by electrostatic and spin interactions will overlap. Furthermore most of the lines from the different ions will overlap. Because of this extensive overlapping the smearing out formula will apply. In its most refined form, this approximation is given by (5.74) which correctly treats the contribution of the lines outside of their groups. We have, therefore, for the line contribution

$$(8.27) \quad \Delta A_{\ell} = \int_0^{\infty} \frac{W(u)}{D(u)} \frac{Z^2 E_{nk}}{1 + Z^2 E_{nk}} du,$$

where

$$(8.28) \quad \sum_k E_{nk} = \sum_k \frac{N^k f_k q_k}{2\Delta_k S} g_k(u).$$

Here  $N^k$  is the electron in ion occupation number, Table C,  $f_k$  the one electron  $f$  number,  $q_k$  the probability that the final state of the transition is unoccupied and  $2\Delta_k$  the extent (in units of  $h\nu/kT$ ) of the group of lines. The function  $g_k$  can be obtained from the nomographs, Fig. IIIa, and b, with

$$(8.29) \quad x = \frac{|u_k^* - u|}{\Gamma_k} \quad y = \frac{\Delta_k}{\Gamma_k}.$$

For values of  $x \gg y$ , it is a valid approximation to use

$$(8.30) \quad g(x,y) = \frac{2}{\pi} \frac{y}{x^2 - y^2 + 1}.$$

The data for the three groups of lines is collected in the following table.

Table K:

Group	Group 1 1s → 2p 1K Electron	Group 2 1s → 2p 2K electrons	Group 3 1s → 3p 2K Electrons
$u_k^*$ in Rhc	508.2	486.8	568.2
$N^k$	.04494	1.9091	1.9091
$f_k$	.4162	.4162	.07910
$q_k$	.9564	.9564	.9847
$2\Delta_k$ in Rhc	6.02	9.02	22.09
$\Gamma_k$ in Rhc	.62	.62	1.65

For the breadths of the lines we have used a strength weighted average collision plus natural breadth for the ions present. Doppler breadth is small enough to neglect. The Stark broadening, though larger than the collision broadening has an exponential dispersion shape, and will not be important much outside the group limits. Within the group limits, it is the Stark breadth which effectively smears out the line strength. The formulae we have used are appropriate for a smeared out group of lines with the collision shape dispersion outside the group limits. We may factor out the slowly varying function  $\frac{W(u)}{D(u)}$ . Then the integration (8.27) is done numerically in the neighborhood of the

center of the group. The region far from the group center can be done analytically, for then

$$\frac{\sum E_{nk}}{1 + \sum E_{nk}} \sim \sum E_{nk} \sim \frac{\sum N_k^k f_k^q k}{2 \Delta_k S} \frac{2}{\pi} \frac{\sqrt{k \Delta k}}{|u_k^* - u|}$$

and

(8.31)

$$\int_{u_1}^{\infty} \frac{\sum E_{nk}}{1 + \sum E_{nk}} du \sim \frac{\sum N_k^k f_k^q k}{2 \Delta_k S} \frac{2}{\pi} \frac{\sqrt{k \Delta k}}{|u_k^* - u_1|}$$

The contribution (8.31), we term the long range tail effect.

The final result for the opacity of iron may now be given.

Table L

$A \wedge_0$	= 186	$K_c$	= 6.24 cm <sup>2</sup> /gm.
$A \wedge$	= 129	$K$	= 20.2 cm <sup>2</sup> /gm.
$A \wedge$	= 57.6	$\frac{K}{K_c}$	= 3.24
$\wedge$	= 6.31 x 10 <sup>-3</sup> cm.		

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Appendix I: Thermodynamic Properties

This appendix continues the statistical mechanical treatment of Chapter IV, 4. Whereas the latter section merely derived the occupation numbers for the system, we now proceed to calculate, the thermodynamic functions and the pressure. From the last we get the equation of state.

The electronic partition function of the system is

$$(AI.1) \quad Q = \sum_J \Omega_J e^{-\beta E_J}$$

where  $E_J$  is given by (4.12) and  $\Omega_J$  by (4.14). We can rewrite this by virtue of (4.13) as

$$(AI.2) \quad Q = e^{nd'} \sum_J P_J = e^{nd''} \sum_J P_J$$

Carrying out the summation to first order in  $V_{ij}$ , the interactions, we get

$$(AI.3) \quad \ln Q = nd'' - \sum_i c_i \ln g_i \\ + \frac{\beta}{2} \sum_i V_{ii} c_i \beta_i (\bar{m}_i - c_i \beta_i - g_i) + \frac{\beta}{2} \sum_i \sum_{j \neq i} V_{ij} c_i \beta_i (\bar{m}_j - c_j \beta_j)$$

We introduce the same values for the arbitrary parameters  $\bar{m}_j$  as we did in the treatment of occupation numbers (4.21). These were selected to make the first order term in the occupation numbers (4.18) vanish. Such a choice then gave occupation numbers identical in form to an independent electron treatment and agreeing with it to first order terms. This choice has no particular advantage besides consistency for the present calculation. Then, since the Helmholtz free energy is  $A = -kT \ln Q$

$$(AI.4) \quad A = -kT nd'' + kT \sum_i c_i \ln g_i - \frac{1}{2} \sum_i V_{ii} M_i^2 (1 - 1/c_i) \\ - \frac{1}{2} \sum_i \sum_{j \neq i} V_{ij} M_i M_j$$

From this equation we find the chemical potential

$$\mu = \left. \frac{\partial A}{\partial n} \right)_{V,T} = -kT d''$$

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By differentiation we can now get the other thermodynamic functions. It is easier in the case of the energy, however, to return to our general treatment. The energy is

$$(A1.4) \quad E = \sum_J E_J P_J$$

The energy  $E_J$  from (4.12) can be written as

$$(A1.5) \quad E_J = \sum_i M_{Ji} (E_i^0 + E'_{Ji})$$

where

$$(A1.6) \quad E_i^0 = \epsilon_i + \frac{1}{2} \sum_{j \neq i} \bar{m}_j V_{ij} + \frac{1}{2} (\bar{m}_i - 1) V_{ii}$$

$$(A1.7) \quad E'_{Ji} = \frac{1}{2} \sum_{j \neq i} (M_{Jj} - \bar{m}_j) V_{ij} + \frac{1}{2} (M_{Ji} - m_i) V_{ii}$$

Then in (A1.4) the summation order may be inverted, giving

$$(A1.8) \quad E = \sum_i E_i^0 \sum_J M_{Ji} P_J + \sum_i \sum_J M_{Ji} E'_{Ji} P_J$$

We recognize in the first term the quantity  $m_i = \sum_J M_{Ji} P_J$  of (4.16).

The second term contains parts all of which occurred in the evaluation of the partition function. The result of the operations on (A1.8) is

$$(A1.9) \quad E = \sum_i E_i^0 c_i p_i \left\{ 1 + \frac{\theta}{2} g_i \left[ V_{ii} [(\bar{m}_i - 1) - 2(c_i - 1)p_i] + \sum_{j \neq i} V_{ij} \bar{m}_j - \sum_{j \neq i} V_{ji} c_j p_j \right] \right\} \\ + \sum_i \left\{ \frac{1}{2} V_{ii} c_i p_i (c_i p_i - \bar{m}_i + g_i) + \sum_{j \neq i} \frac{1}{2} V_{ij} c_i p_i (c_j p_j - \bar{m}_j) \right\}$$

Again introducing the values of  $\bar{m}_j$  from (4.21) and  $E_i^0$  from (A1.6) this reduces to

$$(A1.10) \quad E = \sum_i m_i \bar{\epsilon}_i \\ \bar{\epsilon}_i = \epsilon_i + m_i \left(1 - \frac{1}{c_i}\right) \frac{V_{ii}}{2} + \sum_{j \neq i} m_j \frac{V_{ij}}{2}$$

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We see that for purposes of calculating the total energy of the system we can assume that each electron has the energy  $\bar{\epsilon}_i$  and that the energy of the system is just the sum of these energies of the individual electrons. We should contrast this energy with  $\bar{\epsilon}_i$  of (4.22). The latter gives the ionization energy of the  $i$ th electron, and the sum of the ionization energies is not the total energy of the system.

The entropy may now be found from (AI.4) and (AI.10) by the equation

$S = (E - A) / T$ . We obtain

$$(AI.11) \quad S = k N d - k \sum_i c_i \ln g_i + \frac{1}{T} \sum_i M_i \bar{\epsilon}_i,$$

where

$$(AI.12) \quad \bar{\epsilon}_i = \epsilon_i + M_i \left(1 - \frac{1}{c_i}\right) V_{ii} + \sum_{j \neq i} M_j V_{ij}$$

is the ionization energy (4.22).

We now return to (AI.10) and introduce the same type of approximations which lead to (4.34). First we break up the energy

$$(AI.13) \quad E = \sum_i M_i \bar{\epsilon}_i = \sum_Z N_Z \sum_i \frac{M_{iZ}}{N_Z} \bar{\epsilon}_{iZ}$$

into sums of energy of average type ions. We now compute  $\bar{\epsilon}_{iZ}$ .

For a bound electron, we have the following contributions.

- 1) Kinetic energy plus full interaction with the nucleus =  $\epsilon_{iZ}^0$ ,
- 2) 1/2 interaction with all other bounds =  

$$- \frac{1}{2} \frac{d \epsilon_{iZ}^0}{dz} \left\{ \sum_{j \neq i} \frac{M_{jZ}}{N_Z} \sigma_{i,j} + \frac{M_{iZ}}{N_Z} \left(1 - \frac{1}{c_{iZ}}\right) \sigma_{i,i} \right\},$$
- 3) 1/2 interaction with frees =  $\frac{1}{2} \frac{z' e^2}{2 a_{z'}} \left\{ 3 - \left(\frac{z}{a_{z'}}\right)^2 \right\}$

For a free electron, we get

- 1) Kinetic energy =  $\epsilon_f$
- 2) Full interaction with nucleus =  $-3 \sum_Z \frac{N_Z}{M_f} \frac{z' z e^2}{2 a_{z'}}$

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$$3) \text{ 1/2 interaction with bounds (considered at the nucleus)} = \frac{3}{2} \sum_z \frac{N_z}{N_f} z'(z-z') \frac{e^2}{2a_{z'}},$$

$$4) \text{ 1/2 interaction with other frees} = \frac{6}{5} \sum_z \frac{N_z}{N_f} \frac{z'^2 e^2}{2a_{z'}}.$$

Now the number of bound electrons attached to the average type ion of nucleus  $Z$  is  $M_{bz}/N_z = (Z-Z')$ . Using these relations, we gather all the terms contributing to (AI.13). It is a good approximation to consider the bound electrons at the nucleus in computing the interaction with the frees - hence  $\bar{r}_i^2$  is put equal to zero. We have finally

$$(AI.14) \quad E = \sum_z N_z \left\{ \sum_i \frac{M_{iz}}{N_z} \epsilon_i^0(\bar{z}_i) + \frac{e^2}{2a_{z'}} \left\{ \frac{3}{2} z'(z-z') - 3zz' + \frac{3}{2} z'(z-z') + \frac{6}{5} z'^2 \right\} \right\} + \int_0^\infty \epsilon_f M(\epsilon_f) d\epsilon_f,$$

where

(AI.15)

$$\bar{z}_i = Z - \frac{1}{2} \sum_{j \neq i} \frac{M_{jz}}{N_z} \sigma_{ij} - \frac{1}{2} \frac{M_{iz}}{N_z} \left(1 - \frac{1}{\epsilon_{iz}}\right) \sigma_{ii}.$$

We can rewrite (AI.14) in a way soon to prove significant.

$$(AI.16) \quad E = E_b + P.E. + (K.E.)_f,$$

where

$$(AI.17) \quad E_b = \sum_z N_z \sum_i \frac{M_{iz}}{N_z} \epsilon_i^0(\bar{z}_i)$$

is the energy of the bound electrons excluding interactions with the frees

$$(AI.17) \quad P.E. = - \frac{9}{5} \sum_z N_z \frac{z'^2 e^2}{2a_{z'}}$$

is a potential energy term, and

$$(AI.18) \quad (K.E.)_f = \int_0^{\infty} \epsilon_f M(\epsilon_f) d\epsilon_f \\ = \frac{3}{2} N_f kT \left\{ 1 + \frac{5}{4} \frac{kT}{mc^2} - \frac{5}{4} \left( \frac{kT}{mc^2} \right)^2 \dots \right\} \left\{ 1 + \frac{e^{-\alpha^2}}{2^{5/2}} \left( 1 - \frac{15}{16} \frac{kT}{mc^2} \dots \right) \dots \right\}$$

is the kinetic energy of the free electrons corrected for degeneracy and relativity.

The pressure may be found from the Helmholtz free energy  $A$ , since  $P = - \left( \frac{\partial A}{\partial V} \right)_T$ . This complicated computation can be avoided to the approximation we are working here, since all the forces are due to the coulomb interactions. (We have neglected exchange energies). Then we may use the virial theorem to find the pressure.

In non relativistic theory this gives

$$(AI.19) \quad PV = \frac{2}{3} K.E. + \frac{1}{3} \text{Potential Energy} .$$

In relativistic theory as well as non-relativistic, the bound electrons include the proper balance of kinetic and potential energy to make the contribution to the pressure zero. The kinetic of the free electrons, however, does not contribute the full  $2/3$  K.E. to the pressure because of the relativity correction. This is known to give exactly  $PV = N_f kT$  for the non-degenerate case, and we merely keep the additional degeneracy corrections. So, finally we get

$$(AI.20) \quad PV = N_f kT \left\{ 1 + \frac{e^{-\alpha^2}}{2^{5/2}} \left( 1 - \frac{15}{16} \frac{kT}{mc^2} \right) \dots \right\} - \frac{3}{5} \sum_i N_i \frac{z_i^2 e^2}{2 a_i}$$

Thus far we have not considered the nuclear motion. This contribution has been worked out in Chapter IV, section 6. We get the following additive contributions to the energy and the pressure in the two limiting cases considered:



	Free Nuclei	Harmonic Vibrations
Kinetic Energy	$(3/2)NkT$	$(3/2)NkT$
Potential Energy	0	$(3/2)NkT$
Total Energy	$(3/2)NkT$	3 NkT
(FV) Nuclei	NkT	$(3/2)NkT$

The nuclear contribution to the energy and the pressure is so small (since  $N \ll M_f$ ) that we need not bother refining our treatment of them further. We can use a rough criterion that when  $\bar{r}_c/a_{z'}$  of (4.54) is less than  $1/3$  we consider the nuclei to exert pure harmonic vibrations, while if  $\bar{r}_c/a_{z'} > 1/3$  we shall consider the nuclei as free. Referring to Fig. 2, we see that  $\bar{r}_c/a_{z'} = 1/3$  when  $S = \frac{z'e}{\sqrt{2kT}a_{z'}} = 3.4$ . For smaller values of  $S$  we should use the free nuclei approximation, while for larger values of  $S$  we should use the approximation of harmonic vibrations.

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Appendix II

The assumption that the free electrons are uniformly distributed was made throughout Chapter IV. We can correct this by the use of the classical statistical approach. Within each ionic polyhedron, assume we have an electrostatic potential  $\phi$ . Then the density of electrons in phase space will be

$$(AII.1) \quad n(\vec{r}, \vec{p}) = \frac{2}{h^3} \exp\left\{-\alpha - \frac{p^2}{2mKT} - \frac{e\phi}{kT}\right\} \sim \frac{2}{h^3} \left\{ \exp\left(-\alpha - \frac{p^2}{2mKT}\right) \right\} \left\{ 1 + \frac{e\phi}{kT} \right\}.$$

The density in configuration space  $n(\vec{r})$  is found by integrating over the momentum. This gives a charge density  $\rho = -en(\vec{r})$ , and the potential  $\phi$  must satisfy Poisson's equation with this density. Since we have used the expansion  $\exp\left(-\frac{e\phi}{kT}\right) = 1 + \frac{e\phi}{kT}$  we keep terms in our result only to this order. The potential which replaces (4.31) is

$$(AII.2) \quad \phi = \frac{z'e}{\kappa} \left[ \frac{\sinh x (1 - \kappa/a_2) - x \cosh x (1 - \kappa/a_2)}{\sinh x - x \cosh x} \right] - \frac{kT}{e},$$

where  $x$  is a root of the transcendental equation

$$(AII.3) \quad \cosh x - \frac{\sinh x}{x} = \lambda,$$

and  
(AII.4)  $\lambda = z'e^2 / (a_2 kT).$

Expanding in powers of

$$(AII.5) \quad x^2 = 3\lambda - 0.9\lambda^2 + .44358\lambda^3 + \dots,$$

$$\frac{1}{x^2} = \frac{1}{3\lambda} [1 + 0.3\lambda - .05786\lambda^2 + \dots].$$

The quantity which replaces  $\frac{3}{5} \frac{z'e^2}{2a_2}$  in (4.32) is  $\frac{3z'e^2}{a_2 x^2} - kT$  and on putting in our expansion for  $1/x^2$  we get

$$(AII.6) \quad \bar{\epsilon}_f = \epsilon_f - \frac{1}{V} \sum_z N_z \frac{4\pi}{3} a_z^3 \frac{z'e^2}{2a_z} \left( \frac{3}{5} - .1157\lambda \right).$$

The radii  $a_z$  must be chosen so that (4.24) is satisfied. However, it is no longer appropriate to use (4.25), for the electron distribution is not uniform.

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Instead we must be sure that the free energy of the electrons is the same throughout the system. This is so if the quantity,

$$(AII.7) \quad Q = \frac{kT}{4\pi e^2 a_{z'}^2} x^2 \sim \frac{3 z' e^2}{4\pi a_{z'}^3} [1 - .3\lambda + .44358 \lambda^2],$$

is independent of  $Z$ . The  $a_{z'}$ , then are chosen to satisfy (4.24) and (4.25).

In most cases the effect of non-uniform free electron distribution may be disregarded. The criterion for this is

$$(AII.8) \quad \lambda = \frac{z' e^2}{a_{z'} kT} < 1.$$

Referring to Chapter IV, section 6, we find that the criterion for the nuclei to be considered as performing harmonic vibrations in a lattice is  $s = \frac{z'e}{\sqrt{2kT a_{z'}}} > 3.4$ . Combining this with (AII.8) we find the condition for uniformity in the distribution of free electrons, simultaneously with a lattice structure for the nuclei is

$$AII.9) \quad \frac{23}{z'} < \frac{z' e^2}{kT a_{z'}} < 1.$$

This can never be true for the very light nuclei, but is fulfilled by the heaviest nuclei. This is another reason for the qualitative difference between the opacity of high  $Z$  and low  $Z$  elements.

Appendix III: Formulae and Tables of Gaunt Factors

This Appendix summarizes the formulae and numerical results for the bound-free Gaunt factors applicable to a non-relativistic electron in a Coulomb field. Only the leading dipole contribution is considered, so that these Gaunt factors are the appropriate analogue of the electron numbers recorded in Table I. Most of the results and computations are the work of Dr. Boris Jacobsohn.

The Gaunt factor is defined by (2.22).

$$(AIII.1) \quad \epsilon_{bf} = \frac{3\sqrt{3}\pi}{2^4} m \left( \frac{h\nu}{I_n} \right)^2 \nu \frac{df_{bf}}{d\nu}.$$

The ionization potential  $I_n$  is, however,

$$(AIII.2) \quad I_n = \frac{Z^2}{n^2} Rhc.$$

We can also express the energy of the free electron after ionization by a quantum number  $k$ , defined so that

$$(AIII.3) \quad \epsilon_f = \frac{Z^2 Rhc}{k^2}.$$

We then have for the frequency

$$(AIII.4) \quad h\nu = I_n + \epsilon_f,$$

whence

$$(AIII.5) \quad \nu \frac{df}{d\nu} = \nu \frac{dk}{d\nu} \frac{df}{dk} = \frac{k^3}{2} \left[ \frac{1}{n^2} + \frac{1}{k^2} \right] \frac{df}{dk},$$

so that the Gaunt factor reduces to

$$(AIII.6) \quad \epsilon_{nk} = \frac{3\sqrt{3}\pi}{2^5} \frac{k^3}{n} \left[ 1 + \frac{n^2}{k^2} \right]^3 (-1) \frac{df}{dk}.$$

The  $f$  numbers for bound-bound transitions have been computed by many previous workers. Since it is possible to find the bound-free  $\frac{df}{dk}$  rather simply from the appropriate bound-bound  $f$  number, we have included a list of formulae, Table I, for the latter. The procedure to be used in going from  $f_{n'l' \rightarrow n_l}$  to  $\frac{df}{dk} n'l' \rightarrow kl$  is to substitute  $ik$  for  $n$  in  $f_{n'l' \rightarrow n_l}$  and multiply the result by  $i/(1-e^{-2\pi k})$ . To

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illustrate in the simplest case, if

$$(AIII.7) \quad f_{ls \rightarrow np} = \frac{2^8}{3} \frac{n^5}{(n^2-1)^4} \left( \frac{n-1}{n+1} \right)^{2n},$$

then we get

$$\frac{df_{ls \rightarrow kp}}{dk} = \frac{i}{1 - e^{-2\pi k}} \frac{2^8}{3} \frac{(ik)^5}{(k^2+1)^4} \left( \frac{ik-1}{ik+1} \right)^{2ik},$$

or

$$(AIII.8) \quad \frac{df_{ls \rightarrow kp}}{dk} = -\frac{2^8}{3} \frac{k^5}{(k^2+1)^4} \frac{\exp(-4k \operatorname{ctn}^{-1}k)}{1 - \exp(-2\pi k)}.$$

Substitution in AIII.6 gives the appropriate bound-free Gaunt factor. The resulting formulae for this and other cases are summarized in Table VII. Numerical values are recorded in Table VIII. For  $n = 1, 2, 3, 4$ , these values were calculated from the formulae of Table VII. For  $n \geq 5$  it is possible to obtain the asymptotic expression presented in Table VII for the Gaunt factor, and the values are based upon this expression except for that at  $k = 1$  which was calculated exactly. The asymptotic formula is good to .08% at  $k = 1$ , and is even better for larger  $k$ . Values of the Gaunt factor for  $n = 5, 6, 7, 8, 9, 10$  were found by graphical interpolation. In most instances a plot of  $\epsilon_n \rightarrow k$  vs.  $1/n^2$  for fixed  $k$  gave a smooth curve which did not deviate markedly from a straight line, permitting accurate interpolation. Fig. I presents graphically the values for the Gaunt factor averaged over a complete shell.

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1 Menzel & Pekeris op. cit.

Table I

Formulae for Dipole Oscillator Strengths  
For Coulomb Field (Non-Relativistic)

<u>Transition</u>	<u>Electron Number</u>
$1s \rightarrow np$	$f = \frac{2^8}{3} \frac{n^5}{(n^2-1)^4} \frac{(n-1)^{2n}}{(n+1)^{2n}}$
$2s \rightarrow np$	$f = \frac{2^{15}}{8} n^5 \frac{(n^2-1)}{(n^2-4)^5} \left(\frac{n-2}{n+2}\right)^{2n}$
$2p \rightarrow ns$	$f = \frac{2^{15}}{3^3} \frac{n^7}{(n^2-4)^5} \left(\frac{n-2}{n+2}\right)^{2n}$
$2p \rightarrow nd$	$f = \frac{2^{18}}{3^3} \frac{n^7(n^2-1)}{(n^4-4)^6} \left(\frac{n-2}{n+2}\right)^{2n}$
$3s \rightarrow np$	$f = 2^8 3^4 n^5 (n^2-1) \frac{(7n^2-27)^2}{(n^2-9)^7} \frac{(n-3)^{2n}}{(n+3)^{2n}}$
$3p \rightarrow ns$	$f = 2^{11} 3^3 n^7 \frac{(n^2-3)^3}{(n^2-9)^7} \left(\frac{n-3}{n+3}\right)^{2n}$
$3p \rightarrow nd$	$f = 2^{12} 3^5 n^7 \frac{(n^2-1)(n^2-4)}{(n^2-9)^7} \left(\frac{n-3}{n+3}\right)^{2n}$
$3d \rightarrow np$	$f = \frac{2^{12} 3^4}{5^2} \frac{n^9 (n^2-1)}{(n^2-9)^7} \left(\frac{n-3}{n+3}\right)^{2n}$
$3d \rightarrow nf$	$f = \frac{2^{13} 3^7}{5^2} \frac{n^9(n^2-4)(n^2-1)}{(n^2-9)^8} \left(\frac{n-3}{n+3}\right)^{2n}$

TABLE I a

## DIPOLE OSCILLATOR STRENGTHS (NON-RELATIVISTIC)

## FOR COULOMB FIELD

n	$f_{1s \rightarrow np}$	$f_{2s \rightarrow np}$	$f_{2p \rightarrow ns}$	$f_{2p \rightarrow nd}$	$f_{3s \rightarrow np}$	$f_{3p \rightarrow ns}$	$f_{3p \rightarrow nd}$	$f_{3d \rightarrow np}$	$f_{3d \rightarrow nf}$
1	0	---	-.13873	---	---	-.026367	---	---	---
2	.41620	0	0	---	-.040769	-.14495	---	-.41693	---
3	.079102	.43488	.013590	.69580	0	0	0	0	---
4	.028991	.10277	.003044	.12181	.48472	.032250	.618285	.010957	1.01432
5	.012938	.04193	.001213	.04437	.12102	$7.428 \times 10^{-8}$	.139235	.002210	.15649
6	.007799	.02163	$6.180 \times 10^{-4}$	.02163	.051394	3.032	.056136	$8.420 \times 10^{-4}$	.05389
7	.004814	.01274	3.613	.01233	.027369	1.579	.029009	4.213	.02559
8	.003183	.00818	2.309	.007757	.016549	.941	.017210	2.448	.01442
9	.002216	.00558	1.570	.005221	.010863	.612	.011153	1.564	.00903
10	.001605	.00399	$1.119 \times 10^{-4}$	.003693	.007554	$.218 \times 10^{-8}$	.003972	$.552 \times 10^{-4}$	.00314
n>10	$1.6 n^{-5}$	$3.7 n^{-3}$	$0.1 n^{-3}$	$3.3 n^{-3}$	$6.2 n^{-3}$	$.3 n^{-3}$	$6.1 n^{-3}$	$.07 n^{-3}$	$4.4 n^{-3}$
Discrete Spectrum	.5641	.638	-.119	.923	.707	-.121	.904	-.402	1.502
Continuum	.4359	.362	.008	.293	.293	.010	.207	.002	.098
Total	1.0000	1.000	-.0111	1.111	1.000	-.111	1.111	-.400	1.400

TABLE II

NON-RELATIVISTIC SCREENING CONSTANTS

$$\sigma_{ij} = \frac{F_0(i,j)}{\frac{d\epsilon_1}{dz}}$$

$\begin{matrix} i \\ j \end{matrix}$	1s	2s	2p	3s	3p	3d			
1s	.6250	.8395	.9712	.8954	.9795	.9992			
2s	.2099	.6016	.6484	.7570	.8101	.9322			
2p	.2428	.6484	.7266	.7808	.8455	.9570			
3s	.0995	.3365	.3470	.5977	.6191	.6582			
3p	.1088	.3600	.3758	.6191	.6464	.6924			
3d	.1110	.4143	.4253	.6582	.6924	.7744			

$\begin{matrix} i \\ j \end{matrix}$	1	2	3	4	5	6	7	8	9	10
1	.6250	.9383	.9811	.987	.994	.997	.999	1.000	1.000	1.000
2	.2346	.6895	.8932	.94	.97	.984	.990	.993	.995	1.00
3	.1090	.3970	.7018	.85	.92	.955	.97	.98	.99	1.00
4	.06169	.2350	.4781	.705	.83	.90	.95	.97	.98	.99
5	.03976	.1552	.3312	.531	.72	.83	.90	.95	.97	.98
6	.02769	.1093	.2388	.400	.854	.735	.83	.90	.95	.97
7	.02039	.08082	.1782	.3102	.459	.610	.745	.83	.90	.95
8	.01563	.06250	.1378	.2425	.371	.506	.635	.750	.83	.90
9	.01234	.04938	.1106	.1936	.299	.431	.544	.656	.760	.83
10	.01000	.04000	.0900	.1584	.245	.353	.466	.576	.67	.765

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TABLE III

## RELATIVISTIC ENERGY LEVELS FOR ELECTRON IN COULOMB FIELD

Values tabulated are -  $\frac{E^{\circ}_{n,j}(z)}{Rhc}$

z	$n=1$ $j=1/2$	$n=2$ $j=1/2$	$n=2$ $j=3/2$	$n=3$ $j=1/2$	$n=3$ $j=3/2$	$n=3$ $j=5/2$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$	$n=9$	$n=10$
10	100.13	25.042	25.0083	11.1259	11.1160	11.1127	6.2521	4.0009	2.7782	2.0411	1.5626	1.2347	1.0001
11	121.20	30.3111	30.2622	13.4662	13.4516	13.4468	7.5655	4.8413	3.3617	2.4698	1.8908	1.4940	1.2101
12	144.28	36.087	36.0173	16.0308	16.0102	16.0034	9.0043	5.7619	4.0009	2.9393	2.2503	1.7780	1.4401
13	169.38	42.3694	42.2738	18.8202	18.7918	18.7825	10.5684	6.7626	4.6957	3.4497	2.6411	2.0867	1.6901
14	196.51	49.161	49.0320	21.8349	21.7967	21.7841	12.2580	7.8434	5.4462	4.0009	3.0631	2.4201	1.9602
15	225.68	56.4619	56.2922	25.0753	25.0250	25.0083	14.0730	9.0045	6.2523	4.5931	3.5164	2.7782	2.2503
16	256.88	64.274	64.0546	28.5420	28.4768	28.4552	16.0136	10.2459	7.1141	5.2261	4.0010	3.1611	2.5604
17	290.12	72.6002	72.3196	32.2355	32.1523	32.1248	18.0798	11.5675	8.0316	5.9000	4.5169	3.5687	2.8905
18	325.41	81.441	81.0875	36.1565	36.0518	36.0172	20.2718	12.9694	9.0047	6.6148	5.0640	4.0010	3.2406
19	362.75	90.7975	90.3589	40.3056	40.1755	40.1325	22.5896	14.4517	10.0336	7.3705	5.6425	4.4580	3.6108
20	402.15	100.67	100.134	44.6834	44.5235	44.4707	25.0333	16.0143	11.1183	8.1672	6.2523	4.9398	4.0010
21	443.62	111.069	110.413	49.2908	49.0961	49.0320	27.6030	17.6574	12.2587	9.0048	6.8934	5.4463	4.4112
22	487.16	121.99	121.196	54.1284	53.8936	53.8163	30.2987	19.3810	13.4549	9.8833	7.5659	5.9775	4.8414
23	532.78	133.431	132.484	59.1971	58.9162	58.8238	33.1207	21.1851	14.7069	10.8028	8.2697	6.5335	5.2917
24	580.48	145.40	144.277	64.4978	64.1642	64.0546	36.0690	23.0697	16.0148	11.7632	9.0048	7.1142	5.7620
25	630.28	157.903	156.576	70.0313	69.6378	69.5087	39.1437	25.0350	17.3786	12.7646	9.7713	7.7197	6.2524
26	682.19	170.94	169.382	75.7985	75.3374	75.1863	42.3450	27.0809	18.7982	13.8071	10.5692	8.3499	6.7628
27	736.21	184.506	182.694	81.8005	81.2633	81.0875	45.6730	29.2076	20.2738	14.8906	11.3984	9.0049	7.2933
28	792.36	198.61	196.514	88.0382	87.4158	87.2123	49.1278	31.4150	21.8052	16.0150	12.2590	9.6847	7.8438
29	850.64	213.261	210.842	94.5127	93.7953	93.5608	52.7096	33.7033	23.3927	17.1806	13.1510	10.3893	8.4144
30	911.05	228.46	225.678	101.225	100.402	100.133	56.4185	36.0725	25.0362	18.3872	14.0743	11.1186	9.0050

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TABLE III (Continued)

## RELATIVISTIC ENERGY LEVELS FOR ELECTRON IN COULOMB FIELD

Values tabulated are -  $\frac{\epsilon_{n,j}^0(z)}{\text{Rho}}$ 

Z	n=1 j=1/2	n=2 j=1/2	n=2 j=3/2	n=3 j=1/2	n=3 j=3/2	n=3 j=5/2	n=4 j=1/2	n=4 j=3/2	n=4 j=5/2	n=4 j=7/2	n=5	n=6	n=7	n=8	n=9	n=10
60	3791.1	960.08	911.07	421.15	406.56	402.15	234.57	228.46	226.59	225.69	145.2	100.6	73.8	56.4	44.6	36
61	3925.8	994.64	942.01	436.12	420.46	415.75	242.82	236.26	234.27	233.29	150.0	104.0	76.3	58.3	46.1	37
62	4063.4	1030.0	973.53	451.40	434.60	429.57	251.24	244.20	242.07	241.02	155.1	107.4	78.8	60.3	47.6	38
63	4203.9	1066.1	1005.6	466.99	448.99	443.62	259.82	252.28	250.00	248.88	160.2	111.0	81.4	62.2	49.1	39
64	4347.5	1103.1	1038.3	482.89	463.63	457.91	268.57	260.50	258.06	256.86	165.3	114.5	84.0	64.3	50.7	41
65	4493.9	1140.8	1071.5	499.12	478.52	472.42	277.49	268.85	266.25	264.98	170.6	118.2	86.7	66.3	52.3	42
66	4643.0	1179.2	1105.2	515.66	493.66	487.16	286.57	277.34	274.57	273.23	175.9	121.8	89.4	68.3	54.0	43
67	4795.1	1218.5	1139.5	532.54	509.05	502.14	295.83	285.97	283.03	281.61	181.4	125.6	92.1	70.4	55.6	44
68	4950.3	1258.6	1174.3	549.76	524.59	517.34	305.26	294.74	291.62	290.11	186.9	129.4	94.9	72.6	57.3	46
69	5108.4	1299.6	1209.7	567.31	540.57	532.79	314.86	303.66	300.35	298.73	192.4	133.3	97.7	74.7	59.0	47
70	5269.6	1341.4	1245.6	585.21	556.71	548.45	324.65	312.71	309.21	307.49	198.2	137.2	100.6	76.9	60.7	49
71	5434.0	1384.0	1282.1	603.45	573.11	564.34	334.62	321.91	318.20	316.38	203.9	141.1	103.5	79.1	62.5	50
72	5601.6	1427.5	1319.2	622.03	589.76	580.44	344.77	331.24	327.31	325.40	209.8	145.2	106.5	81.4	64.2	52
73	5772.3	1471.9	1356.8	640.97	606.67	596.83	355.09	340.72	336.54	334.55	215.7	149.3	109.5	83.7	66.1	53
74	5946.5	1517.3	1394.9	660.29	623.83	613.45	365.61	350.35	345.91	343.82	221.7	153.4	112.6	86.0	67.9	54
75	6124.1	1563.6	1433.6	679.98	641.26	630.29	376.33	360.12	355.43	353.22	227.8	157.7	115.6	88.4	69.7	56
76	6305.1	1610.8	1472.9	700.05	658.94	647.35	387.24	370.04	365.11	362.76	234.0	161.9	118.7	90.7	71.6	58
77	6489.6	1659.0	1512.7	720.49	676.88	664.65	398.34	380.10	374.91	372.42	240.3	166.3	121.9	93.2	73.5	59
78	6677.6	1708.2	1553.1	741.31	695.09	682.19	409.55	390.30	384.84	382.20	246.7	170.5	125.1	95.5	75.5	61
79	6869.0	1758.5	1594.1	762.51	713.57	699.97	421.15	400.64	394.89	392.11	253.1	175.1	128.3	98.1	77.4	62
80	7064.3	1809.7	1635.6	784.18	732.27	718.00	432.86	411.15	405.07	402.14	259.7	179.6	131.6	100.6	79.4	64
81	7263.1	1862.0	1677.7	806.18	751.28	736.23	444.75	421.80	415.41	412.31	266.3	184.2	135.0	103.2	81.4	66
82	7465.8	1915.4	1720.4	828.62	770.55	754.70	456.87	432.60	425.98	422.51	273.0	188.8	138.3	105.7	83.4	67
83	7672.5	1969.9	1763.6	851.52	790.08	773.40	469.21	443.55	436.47	433.06	279.8	193.5	141.8	108.3	85.5	69
84	7883.1	2025.5	1807.4	874.86	809.87	792.33	481.77	454.65	447.18	443.64	286.7	198.2	145.2	111.0	87.6	70
85	8097.8	2082.3	1851.8	898.61	829.94	811.53	494.55	465.90	458.05	454.33	293.7	203.0	148.8	113.7	89.7	72
86	8316.6	2140.2	1896.9	922.79	850.29	830.98	507.54	477.30	469.07	465.13	300.7	207.9	152.3	116.4	91.8	74
87	8539.7	2199.3	1942.4	947.46	870.87	850.63	520.76	488.79	480.19	476.06	307.9	212.8	155.9	119.1	94.0	76
88	8767.0	2259.7	1988.6	972.63	891.76	870.54	534.21	500.44	491.46	487.18	315.2	217.8	159.5	121.9	96.2	77
89	8998.7	2321.5	2035.3	998.21	912.94	890.67	547.92	512.31	502.84	498.37	322.5	222.6	163.2	124.7	98.4	79
90	9235.0	2384.4	2082.7	1024.4	934.32	911.03	561.85	524.33	514.41	509.68	329.9	227.9	166.9	127.5	100.6	81
91	9476.1	2448.9	2130.6	1051.0	956.07	931.65	576.05	536.50	526.09	521.17	337.4	233.1	170.7	130.4	102.9	83
92	9722.2	2514.7	2179.2	1078.2	978.08	952.53	590.51	548.82	538.00	532.78	345.0	238.3	174.5	133.3	105.2	85

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TABLE IV

AVERAGE SQUARE RADIUS OF ELECTRON ORBITS

Values of  $\overline{\left(\frac{r}{a_0}\right)^2}^{2n\ell}$  and  $\overline{\left(\frac{r}{a_0}\right)^2}^{2n}$

$$\overline{\left(\frac{r}{a_0}\right)^2}^{2n\ell} = \frac{n^4}{z^2} \left\{ 1 + \frac{3}{2} \left[ 1 - \frac{\ell(\ell+1) - 1/3}{n^2} \right] \right\}$$

$$\overline{\left(\frac{r}{a_0}\right)^2}^{2n} = \frac{2n^4}{z^2} \left\{ 1 + \frac{1}{2n^2} \right\}$$

Orbital	$\overline{\left(\frac{r}{a_0}\right)^2} z^2$	Averaged over all Angular Momenta	
		Principal Quantum Number n	$\overline{\left(\frac{r}{a_0}\right)^2} z^2$
1s	3.0000	1	3.00
2s	42.000	2	36.00
2p	30.000	3	171.00
3s	207.00	4	528.00
3p	180.00	5	1275.0
3d	126.00	6	2628.0
		7	4851.0
		8	8255.9
		9	13203.
		10	20100.

TABLE V

THE FREQUENCY FACTOR  $F(a, u)/F(a, \infty)$

FOR LINES OF EQUAL STRENGTH

$$F(a, u) = \frac{2}{\pi a} \int_0^u \left\{ 1 - \frac{a}{1+z^2} \right\} dz$$

u	$t = \frac{1}{1+u^2}$	a	0	0.1	0.2	0.3	0.4	0.5	1.0	1.5	2.0
		$F(a, \infty)$	1.0000	.9761	.9528	.9307	.9096	.8896	.80182	.73138	.67399
8	0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
4.3589	.05	.8564	.8530	.8496	.8461	.8427	.8393	.8325	.8061	.7905	
3	.10	.7952	.7902	.7855	.7808	.7761	.7714	.7485	.7265	.7056	
2.3805	.15	.7474	.7411	.7354	.7298	.7235	.7187	.6918	.6662	.6421	
2	.20	.7048	.6984	.6921	.6859	.6796	.6735	.6438	.6157	.5895	
1.7321	.25	.6667	.6597	.6529	.6462	.6395	.6329	.6011	.5714	.5439	
1.5275	.30	.6310	.6237	.6165	.6094	.6024	.5955	.5622	.5314	.5032	
1.3628	.35	.5970	.5894	.5819	.5746	.5673	.5602	.5260	.4946	.4661	
1.2247	.40	.5641	.5563	.5487	.5412	.5337	.5265	.4918	.4602	.4317	
1.1055	.45	.5319	.5240	.5163	.5087	.5012	.4938	.4591	.4276	.3995	
1.0000	.50	.5000	.4921	.4844	.4767	.4693	.4619	.4274	.3965	.3670	
.9045	.55	.4681	.4603	.4526	.4450	.4376	.4304	.3965	.3663	.3397	
.8165	.60	.4359	.4282	.4207	.4133	.4060	.3989	.3659	.3368	.3113	
.7071	.65	.3918	.3956	.3882	.3810	.3740	.3672	.3354	.3076	.2834	
.6547	.70	.3690	.3619	.3548	.3480	.3413	.3347	.3046	.2783	.2558	
.5774	.75	.3333	.3266	.3200	.3135	.3072	.3011	.2729	.2486	.2278	
.5	.80	.2952	.2890	.2828	.2769	.2711	.2655	.2398	.2178	.1990	
.4201	.85	.2532	.2477	.2422	.2369	.2318	.2268	.2041	.1848	.1685	
.3333	.90	.2048	.2003	.1957	.1913	.1870	.1829	.1640	.1481	.1347	
.2294	.95	.1436	.1400	.1368	.1336	.1305	.1275	.1148	.1026	.0932	
0	1.00	0	0	0	0	0	0	0	0	0	

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TABLE V (Continued)

u	$t = \frac{1}{1+u^2}$	4.	5.	6.	8.	10.	15.	20.	25.	30.
	$F(a, \infty)$	.5241	.4770	.4402	.3860	.3478	.2864	.2491	.2234	.2043
$\infty$	0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
31.6070	.001	---	.9592	---	---	---	.9311	.9206	.9114	.9032
9.9499	.01	---	.8685	---	---	---	.7836	.7530	.7265	.7032
4.3589	.05	.7349	---	.6893	.6511	.6187	---	---	---	---
3	.10	.6331	.6040	.5761	.5303	.4929	.4232	.3742	.3378	.3145
2.3805	.15	.5605	---	.4987	.4509	.4132	---	---	---	---
2	.20	.5027	.4696	.4395	.3921	.3560	.2942	.2550	.2278	.2077
1.7321	.25	.4547	---	.3918	.3462	.3122	---	---	---	---
1.5275	.30	.4133	.3804	.3521	.3087	.2772	.2260	.1952	.1741	.1587
1.3628	.35	.3770	---	.3181	.2773	.2482	---	---	---	---
1.2247	.40	.3445	.3137	.2883	.2503	.2236	.1815	.1565	.1396	.1272
1.1055	.45	.3149	---	.2619	.2266	.2021	---	---	---	---
1	.50	.2877	.2606	.2379	.2053	.1829	.1482	.1278	.1140	.1039
.9045	.55	.2622	---	.2159	.1859	.1655	---	---	---	---
.8165	.60	.2382	.2146	.1953	.1679	.1495	.1210	.1043	.0931	.0848
.7071	.65	.2151	---	.1759	.1510	.1343	---	---	---	---
.6547	.70	.1927	.1747	.1571	.1347	.1199	.0970	.0837	.0746	.0680
.5774	.75	.1705	---	.1387	.1188	.1067	---	---	---	---
.5	.80	.1481	.1335	.1208	.1030	.0916	.0741	.0639	.0570	.0519
.4201	.85	.1247	---	.1010	.0866	.0769	---	---	---	---
.3333	.90	.0992	.0890	.0802	.0688	.0611	.0494	.0426	.0380	.0346
.2294	.95	.0683	---	.0551	.0473	.0420	---	---	---	---
0	1.00	0	0	0	0	0	0	0	0	0

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TABLE VI

## THE WEIGHTING FUNCTION

$$W(u) = \frac{15}{4\pi^4} u^7 e^{2u} (e^u - 1)^{-3}$$

## AND THE STROMGREN FUNCTION

$$S(u) = \int_0^u W(x) dx$$

u	W(u)	S(u)	u	W(u)	S(u)
0.0	0	0	3.5	8.2003	6.2881
.1	4.0390x10 <sup>-6</sup>	8.015x10 <sup>-8</sup>	3.6	8.9572	7.1469
.2	6.7737x10 <sup>-5</sup>	2.669x10 <sup>-6</sup>	3.7	9.7404	8.0619
.3	3.5814x10 <sup>-4</sup>	2.103x10 <sup>-5</sup>	3.8	10.546	9.0957
.4	1.1801x10 <sup>-3</sup>	9.185x10 <sup>-5</sup>	3.9	11.371	10.1902
.5	2.9948x10 <sup>-3</sup>	2.902x10 <sup>-4</sup>	4.0	12.211	11.3676
.6	6.4396x10 <sup>-3</sup>	7.454x10 <sup>-4</sup>	4.1	13.064	12.6309
.7	.012339	1.660x10 <sup>-3</sup>	4.2	13.926	13.9808
.8	.021726	3.351x10 <sup>-3</sup>	4.3	14.793	15.4174
.9	.035822	6.170x10 <sup>-3</sup>	4.4	15.660	16.9409
1.0	.056077	1.071x10 <sup>-2</sup>	4.5	16.525	18.5793
1.1	.084103	1.765x10 <sup>-2</sup>	4.6	17.384	20.2476
1.2	.12175	2.787x10 <sup>-2</sup>	4.7	18.232	22.0290
1.3	.17101	4.214x10 <sup>-2</sup>	4.8	19.067	23.8940
1.4	.23401	6.257x10 <sup>-2</sup>	4.9	19.884	25.8403
1.5	.31303	8.981x10 <sup>-2</sup>	5.0	20.681	27.8664
1.6	.41042	.1258	5.1	21.453	29.9725
1.7	.52859	.1724	5.2	22.199	32.1510
1.8	.67064	.2313	5.3	22.915	34.4014
1.9	.83681	.3066	5.4	23.599	36.7225
2.0	1.0316	.3994	5.5	24.249	39.1128
2.1	1.2564	.5129	5.6	24.861	41.5698
2.2	1.5134	.6502	5.7	25.436	44.0895
2.3	1.7970	.8144	5.8	25.970	46.6656
2.4	2.1307	1.009	5.9	26.463	49.2917
2.5	2.4940	1.238	6.0	26.913	51.9633
2.6	2.8948	1.505	6.1	27.319	54.6755
2.7	3.3344	1.815	6.2	27.682	57.4249
2.8	3.8128	2.173	6.3	28.000	60.2082
2.9	4.3302	2.582	6.4	28.278	63.0213
3.0	4.8857	3.048	6.5	28.502	65.8637
3.1	5.4791	3.568	6.6	28.686	68.7225
3.2	6.1087	4.1483	6.7	28.826	71.5978
3.3	6.7735	4.7923	6.8	28.923	74.4853
3.4	7.4715	5.5041	6.9	28.977	77.3810

TABLE VI (Continued)

u	W(u)	S(u)	u	W(u)	S(u)
7.0	28.991	80.2800	10.2	17.027	157.1759
7.1	28.961	83.1773	10.4	16.163	160.3624
7.2	28.895	86.0698	10.6	15.053	163.3490
7.3	28.789	88.9546	10.8	13.815	166.1404
7.4	28.646	91.8283			
7.5	28.470	94.6856	11.0	12.530	168.7424
7.6	28.258	97.5219	11.5	10.787	174.4525
7.7	28.016	100.3346	12.0	8.4757	179.1535
7.8	27.742	103.1223	12.5	7.0717	182.9749
7.9	27.439	105.8825	13.0	5.4602	186.0382
8.0	27.110	108.6119	13.5	4.4377	188.4766
8.1	26.757	111.3053	14.0	3.3745	190.3846
8.2	26.379	113.9608	15.0	2.0121	193.0267
8.3	25.981	116.5797	16.0	1.1629	194.5800
8.4	25.562	119.1587	18.0	.35896	195.9583
8.5	25.126	121.6939	20.0	.10157	196.3685
8.6	24.673	124.1825	22.0	.028787	196.4813
8.7	24.206	126.6251	24.0	.0066659	196.5103
8.8	23.726	129.0210	26.0	.0015798	196.5174
8.9	23.234	131.3691	30.0	.000071419	196.5194
9.0	22.732	133.6682	$\infty$	0	196.5194
9.1	22.222	135.9163			
9.2	21.706	138.1127			
9.3	21.183	140.2571			
9.4	20.658	142.3489			
9.5	20.127	144.3881			
9.6	19.596	146.3742			
9.7	19.066	148.3066			
9.8	18.535	150.1856			
9.9	18.007	152.0119			
10.0	17.480	153.7856			

Table VII Formulae for Bound Free Gaunt Factors

$$\text{Define } F_n(k) = \frac{\exp(-4k \tan^{-1} n/k)}{1 - \exp(-2\pi k)}$$

---


$$\epsilon_{1s \rightarrow kp} = 8\pi\sqrt{3} \frac{k^2}{k^2 + 1} F_1(k)$$

---


$$\epsilon_{2s \rightarrow kp} = 2^9 \pi \sqrt{3} \frac{(1 + 1/k^2)}{(1 + 4/k^2)^2} F_2(k)$$

$$\epsilon_{2p \rightarrow ks} = \frac{2^7 \pi \sqrt{3}}{3^2} \frac{1}{(1 + 4/k^2)^2} F_2(k)$$

$$\epsilon_{2p \rightarrow kd} = \frac{2^{12} \pi \sqrt{3}}{3^2} \frac{(1 + 1/k^2)}{(1 + 4/k^2)^3} F_2(k)$$

$$\epsilon_{2p \rightarrow k} = \frac{2^7 \pi \sqrt{3}}{3^2} \frac{(35 + k^2)}{(1 + 4/k^2)^3} F_2(k)$$

$$\epsilon_{\bar{2} \rightarrow k} = \frac{2^5 \pi \sqrt{3} (15 + \frac{2}{k^2} + \frac{1}{k^4})}{(1 + \frac{4}{k^2})^3} F_2(k)$$

---


$$\epsilon_{3s \rightarrow kp} = \frac{2^3 3^4 \sqrt{3} \pi (1 + \frac{1}{k^2})(7 + \frac{27}{k^2})}{k^2 (1 + 9/k^2)^4} F_3(k)$$

$$\epsilon_{3p \rightarrow k} = \frac{2^6 3^3 \sqrt{3} \pi (19 + \frac{96}{k^2} + \frac{81}{k^4})}{(1 + 9/k^2)^4} F_3(k)$$

$$\epsilon_{3d \rightarrow k} = \frac{2^7 3^4 \sqrt{3} \pi (1 + 1/k^2)(11 + \frac{45}{k^2})}{5 (1 + 9/k^2)^5} F_3(k)$$



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TABLE VII (Continued)

$$\varepsilon_3 \rightarrow k = \frac{2^3 3^2 \sqrt{3} \pi \left[ 13 + \frac{78}{k^2} + \frac{81}{k^4} \right] \left[ 29 + \frac{126}{k^2} + \frac{81}{k^4} \right]}{\left( 1 + \frac{9}{k^2} \right)^5} F_3(k)$$


---

$$\varepsilon_4 \rightarrow k = \frac{2^7 \sqrt{3} \pi}{3^2 \left( 1 + \frac{16}{k^2} \right)^7} \left[ 539 + \frac{6800}{k^2} + \frac{2073}{k^4} + \frac{12288}{k^6} \right]$$

$$\times \left[ 197 + \frac{3152}{k^2} + \frac{13056}{k^4} + \frac{12288}{k^6} \right] F_4(k)$$


---

$$\lim_{n \rightarrow \infty} \varepsilon_n \rightarrow k = \left\{ 1 + \frac{.1728261}{k^{2/3}} - \frac{.0495957}{k^{4/3}} \right.$$

$$\left. - \frac{.0171429}{k^2} + \frac{.0020450}{k^{8/3}} \right\}$$

Table VIII Values for Bound Free Gaunt Factors

$1/k^2$	$k$	$\epsilon_{ls} \rightarrow kp$
0	$\infty$	.79730
.001	31.623	.79770
.01	10	.79989
.05	4.4721	.81001
.1	3.1623	.82167
.2	2.2361	.84331
.5000	1.414	.89240
1.000	1.000	.94236
2.0	.70711	.98447
5.0	.44721	.98592

Table VIII Values for Bound Free Gaunt Factors (Continued)

$1/k^2$	k	$\epsilon_{2s} \rightarrow kp$	$\epsilon_{2p} \rightarrow ks$	$\epsilon_{2p} \rightarrow kd$	$\epsilon_{2p} \rightarrow k$	$\epsilon_{2'} \rightarrow k$
0	$\infty$	.93460	.025961	.83075	.85671	.87619
.0625	4.	1.13689	.029723	.80845	.83818	.91286
.12755	2.8	1.32462	.032632	.77965	.81229	.94037
.25	2.00	1.62592	.036129	.72258	.75871	.97549
.37180	1.64	1.87276	.037922	.67064	.70856	.99860
.52510	1.38	2.12688	.038738	.60977	.64852	1.01811
.74316	1.16	2.41104	.038420	.53946	.57790	1.03618
1.000	1.000	2.66420	.037003	.47363	.51064	1.04903
1.5625	.8	3.03132	.032860	.37165	.40452	1.06122
2.25	.66667	3.28819	.028104	.29228	.32039	1.06234

$1/k^2$	k	$\epsilon_{3s} \rightarrow kp$	$\epsilon_{3p} \rightarrow k$	$\epsilon_{3d} \rightarrow k$	$\epsilon_3 \rightarrow k$
0	$\infty$	1.06160	1.09768	.76259	.90751
.02777	6.	1.31070	1.23028	.68433	.93591
.056689	4.2	1.55462	1.33175	.61340	.95743
.11111	3.0	1.9759	1.4544	.5059	.9854
.23338	2.07	2.77863	1.55574	.34854	1.02095
.3333	1.732	3.32160	1.55697	.26988	1.03799
.4444	1.5	3.83427	1.52290	.21072	1.05073
.6944	1.2	4.73641	1.40219	.13321	1.06767
1.000	1.000	5.52416	1.24884	.085635	1.07765

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Table VIII Values for Bound Free Gaunt Factors (Concluded)

$1/k^2$	k	$\epsilon_{4 \rightarrow k}$	$\epsilon_{5 \rightarrow k}$ *	$\epsilon_{6 \rightarrow k}$ *	$\epsilon_{7 \rightarrow k}$ *	$\epsilon_{8 \rightarrow k}$ *	$\epsilon_{9 \rightarrow k}$ *	$\epsilon_{10 \rightarrow k}$ *	$\epsilon_{\infty \rightarrow k}$
0	$\infty$	.92474	.9360	.9438	.9498	.9545	.9578	.9605	1.0000
.001111	30	.92672*	.9386	.9470	.9535	.9582	.9625	.9656	1.01735
.01	10	.941*	.9590	.9722	.982	.9895	.995	1.00	1.0349
.027778	6	.9618*	.980	.994	1.0035	1.0115	1.0175	1.022	1.04733
.06250	4	.98992	1.0088	1.0210	1.0290	1.0353	1.0395	1.0427	1.05976
.1111	3	1.0132*	1.0290	1.0401	1.0470	1.0518	1.0557	1.0579	1.0699
.25000	2.00	1.04743	1.0597	1.0668	1.0712	1.0744	1.0767	1.0781	1.0853
.5000	1.414	1.0723*	1.0807	1.0857	1.0888	1.0909	1.0923	1.0935	1.0982
1.0000	1.000	1.08874	1.0945	1.0983	1.1009	1.1026	1.1036	1.1044	1.1088

\* Indicates interpolated values.

TABLE IX

The function  $\chi(x) = \frac{1}{\sqrt{x}} \int_x^\infty y^{-\frac{1}{2}} e^{-y} \ln y \, dy$

x	$\chi(x)$
0	-1.9636
.01	-1.2202
.05	- .7183
.1	- .4627
.2	- .2149
.3	- .0907
.4	- .0190
.5	+ .0241
.6	.0507
.8	.0754
1.0	.0807
1.1	.0799
1.2	.0776
1.3	.0744
1.4	.0707
1.5	.0666
1.6	.0624
1.7	.0582
1.8	.0541
1.9	.0501
2.0	.0462
2.1	.0426
2.2	.0392
2.3	.0359
2.4	.0329

x	$\chi(x)$
2.5	.0302
2.6	.0276
2.7	.0252
2.8	.0230
2.9	.0210
3.0	.0191
3.2	.0158
3.4	.0131
3.6	.0108
3.8	.0089
4.0	.0073
4.2	.0060
4.4	.0049
4.6	.0040
4.8	.0033
5.0	.0027
5.5	.0016
6.0	.0009
6.5	.0005
7.0	.0002
7.5	.0001
8.0	

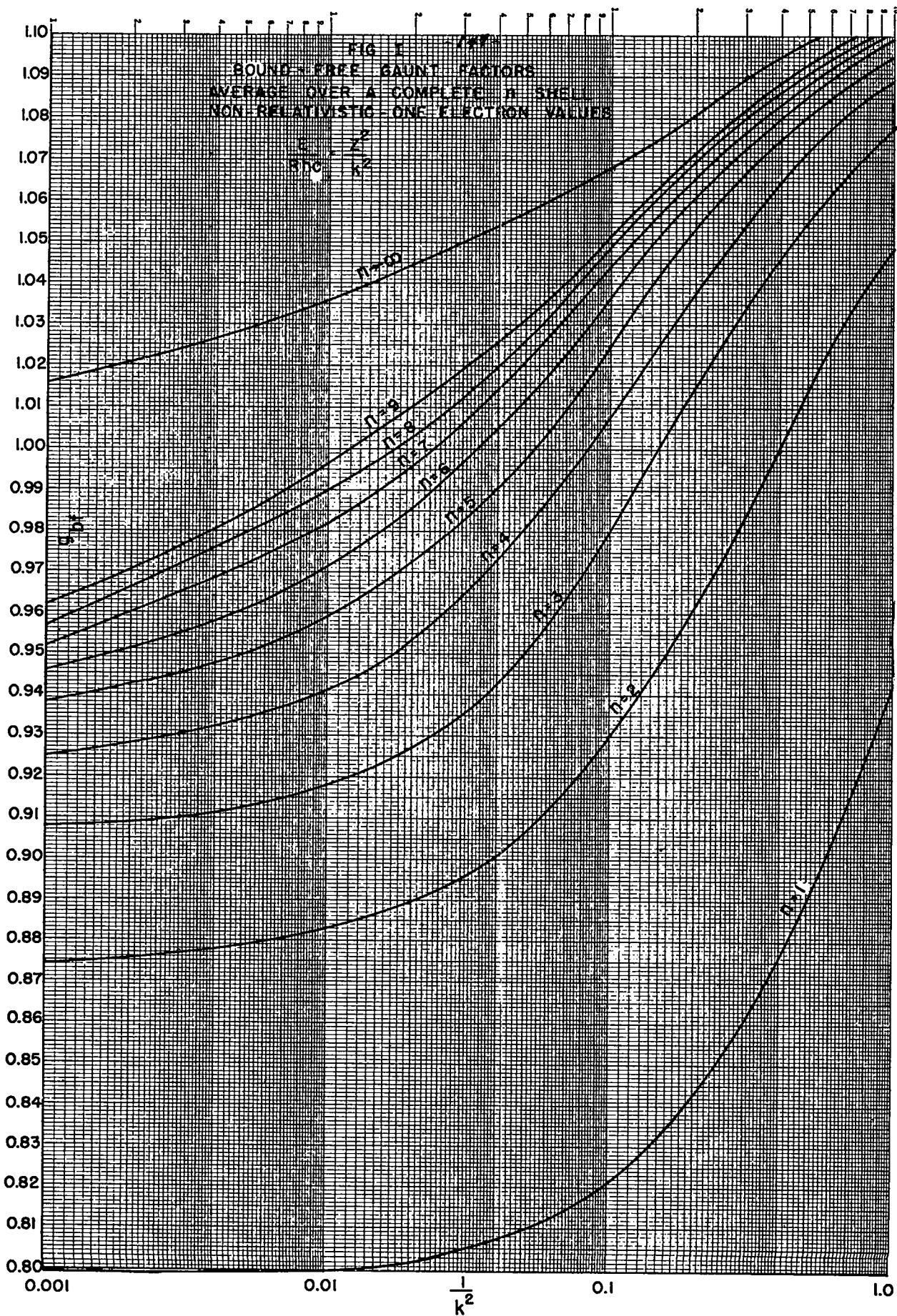
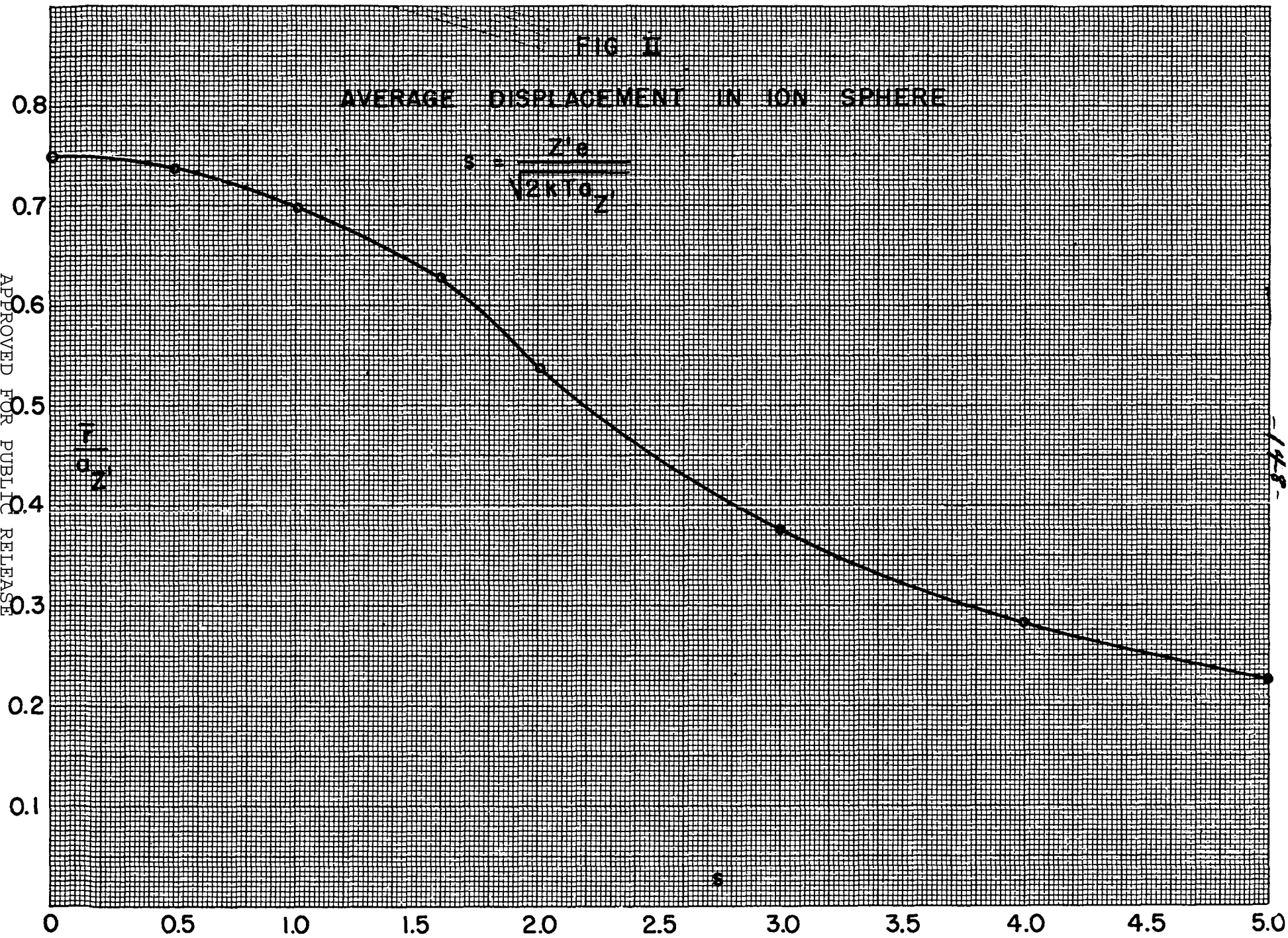


FIG. 1

AVERAGE DISPLACEMENT IN ION SPHERE

$$s = \frac{Z'e}{\sqrt{2kT\epsilon_0 Z}}$$



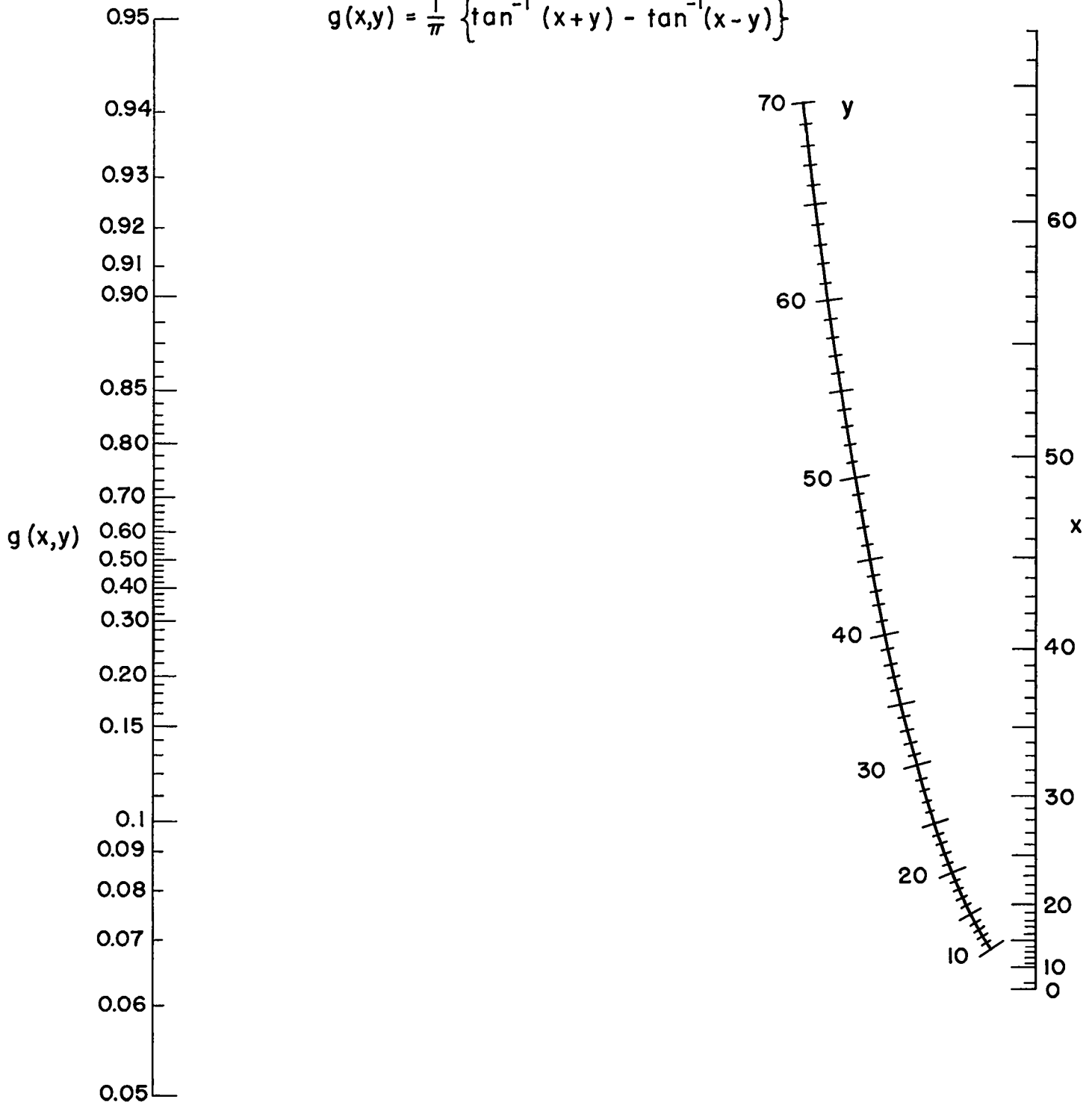
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FIG IIIa

NOMOGRAPH OF

$$g(x,y) = \frac{1}{\pi} \{ \tan^{-1}(x+y) - \tan^{-1}(x-y) \}$$





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FIG III b

NOMOGRAPH OF

$$g(x,y) = \frac{1}{\pi} \left\{ \tan^{-1}(x+y) - \tan^{-1}(x-y) \right\}$$

