

The Theory of Photoelectric Absorption for X-Rays and γ -Rays

HARVEY HALL, *New York University, University Heights, New York, New York**

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* Now at College of the City of New York.

1. Definitions

THROUGHOUT the nonrelativistic sections energies will be measured in Rydberg units. That is, in units of

$$\begin{aligned} 2\pi^2me^4/h^3 &= 2.1535 \times 10^{-11} \text{ ergs} \\ &= 13.53 \text{ e-volts.} \end{aligned}$$

The Rydberg unit of frequency is

$$2\pi^2me^4/h^3 = 3.2900 \times 10^{15} \text{ sec.}^{-1}.$$

The unit of length will be the first Bohr radius for hydrogen.

$$\begin{aligned} a_0 &= h^2/4\pi^2me^2 = 0.5281 \times 10^{-8} \text{ cm,} \\ a &= a_0/Z, \quad Z = \text{atomic number.} \end{aligned}$$

The symbol α_0 will be used consistently for the fine structure constant.

$$\begin{aligned} \alpha_0 &= 2\pi e^2/hc = 1/137.3 = 7.283 \times 10^{-3}, \\ \alpha &= \alpha_0 \cdot Z. \end{aligned}$$

In the relativistic sections the unit of energy will be taken as

$$\begin{aligned} mc^2 &= 8.121 \times 10^{-7} \text{ ergs} \\ &= 0.5104 \text{ Mev.} \end{aligned}$$

The unit of length will be

$$a_0\alpha_0 = h/2\pi mc = 3.847 \times 10^{-11} \text{ cm.}$$

2. Introduction

The theory of photoelectric absorption by deeply bound atomic electrons, in the light of recent work, may now be considered complete for all wave-lengths between medium x-rays and the hardest γ -rays. That it is possible to apply the existing theory successfully to this problem, without resort to purely numerical methods, depends mainly on one essential feature. The absorption increases very rapidly with the tightness of binding of the electron, and because of this the absorption due to outer shells is negligible, or nearly so, whenever the frequency is greater than the critical K or L frequency. This circumstance makes unnecessary a detailed knowledge of the atomic field in which the loosely bound M , N , \dots electrons move. Their part in the absorption may be crudely estimated on the basis of an adequately screened central field $(Z-s)e/r$, and although the number of outer electrons is large their total contribution to the absorption is rather small.

For the K and L shells, especially for the former, the field is almost wholly due to the nuclear term $-Ze^2/r$, which is much larger than the interelectronic interactions $e^2/r_{1,2}$ in the case of medium and heavy elements.

A test of the assumption indicated here is not altogether lacking, in that one may introduce an arbitrary screening constant in the potential energy to represent the repulsive effect of the outer electrons on the innermost shell. It turns out that the magnitude of the absorption is very insensitive to the size of this constant. Furthermore, when this constant is determined by means of a consistent theory, excellent agreement is found between the observed and calculated absorption limits.

This latter statement concerning the critical frequencies is true only when the K electrons are treated relativistically, but this necessity should be expected when one remembers that a K electron of lead, for example, is bound with an energy of about 100 kv, which strongly suggests the importance of relativistic effects.

To emphasize the agreement between the theoretical and experimental absorption limits, curves have been prepared (Figs. 2-5), in which the K discontinuity occurs at the observed critical wave-length.

The single application of the theory to the study of nuclear disintegration by γ -rays (the deuteron) is included because it is a problem whose statement and meaning are unambiguous. It provides an example almost completely analogous to hydrogen in the atomic field. Unfortunately at present the general features of nuclear structure do not permit extensions to be made with the same degree of meaning as in atomic theory, and consequently no attempt is made here to apply the theory to more complex nuclei.

With the exception of the calculation on the deuteron, where different units from the rest of the paper are used, all of the mathematics has been relegated to separate sections from the body of results. In fact, because of the lengthy nature of all relativistic calculations, only the barest sketch of the theory is given at all.

The writer takes pleasure in expressing his gratitude to Dr. M. H. Johnson, Jr., for a critical reading of the manuscript, and for many helpful

suggestions. He is also indebted to Dr. Cornelius Brenecke for preparing some of the curves, to Mr. Benjamin Roth for help in checking some of the numerical work, to Mr. O. H. Clark for some suggestions, and to Mr. Perry Pepper for help in preparing the manuscript.

3. General expression for the absorption coefficient

Let the energy of binding of an electron in an atomic system be E_0 . Then, when light of quantum energy $h\nu$ falls on this system, a quantum may be absorbed, if $h\nu > E_0$. The (photo) electron should then have the kinetic energy,¹

$$E = h\nu - E_0. \quad (1)$$

Let the incident light be monochromatic, and let the Poynting vector of this incident radiation have the magnitude $S_0 = h\nu N$. The ratio $S_0/h\nu = N$ will be the number of quanta falling on each cm^2 per sec. Then, the probability that the atom will absorb one quantum per sec., according to the light quantum field theory, is²

$$|a_E(0, 0, \dots, N_s - 1, 0)|^2 \cdot \frac{1}{t} = S_0 \frac{2\pi}{h^2 \nu^2 c} |J_{E, n, \nu}|^2. \quad (2)$$

The matrix element here is written

$$J_{E, n, \nu} = \sqrt{2} \int \sin(\boldsymbol{\kappa} \cdot \mathbf{r} + \beta) (\mathbf{A} \cdot \mathbf{j}_{E, n}) d\tau \quad (\text{A})$$

or

$$J_{E, n, \nu} = \int \exp(i(\boldsymbol{\kappa} \cdot \mathbf{r})) (\mathbf{A} \cdot \mathbf{j}_{E, n}) d\tau, \quad (\text{B})$$

where $\boldsymbol{\kappa}$ is the propagation vector of magnitude $2\pi\nu/c$. \mathbf{A} is a unit vector parallel to the polarization vector of the light. If the first form (A) (as

¹ The conservation laws for energy and momentum in quantum mechanics are identical with classical theory. When the atom has infinite mass, momentum is automatically conserved, and Eq. (1) holds for the energy because the nucleus can take up any necessary amount of momentum without increasing its energy. When the atomic, or, say, nuclear mass is finite ($=M$), the nucleus takes up some momentum and Eq. (1) must be corrected by a term of the order of $(1/2M)(m\nu - h\nu/c)^2$, which is small.

Far from the ionization limit the residual momentum taken up by the nucleus is roughly proportional to $h\nu/c$ on the basis of the Schrödinger theory. But in the relativistic problem where $\nu \sim c$, the residual momentum approaches a constant value (about mc).

² See, for instance, E. Fermi, *Rev. Mod. Phys.* **4**, 87 (1932); J. R. Oppenheimer, *Phys. Rev.* **35**, 461 (1930); also the articles by Wentzel and Bethe, *Handbuch der Physik* **24/1**.

in Fermi's article) is used, the phase β must be averaged over. This is to take account of the fact (when the radiation field is analyzed into standing waves) that the electron may be anywhere between a crest and a node. In the second form the phase β does not appear because in the derivation the electric vector was written so as to have constant absolute value for every wave in a given direction. The two forms (A) and (B) lead to the same absorption probabilities; the difference between them being only formal in this connection. The vector $\mathbf{j}_{E, n}$ is the current density between the states characterized by n and E . In the nonrelativistic theory it is written

$$\mathbf{j}_{E, n} = (\hbar e / 2im) (\psi_E^* \text{grad } \psi_n - \psi_n \text{grad } \psi_E^*).$$

When terms in $(v/c)^2$ are important, and the Dirac equation must be used, we write³

$$\mathbf{j}_{E, n} = ce\psi_E^* \boldsymbol{\alpha} \psi_n.$$

The components of the vector $\boldsymbol{\alpha}$, $\alpha_1, \alpha_2, \alpha_3$ (which are analogous to the three components of velocity v_x, v_y, v_z) are matrices each of four rows and four columns. They are conventionally defined in section 18.

In the above expressions the wave function ψ_E , corresponding to the energy E , is normalized⁴ to $d(E/h)$. That is, the number of electrons in the frequency range $d(E/h)$ leaving the system to infinity per unit time, is equal to $d(E/h)$.

We multiply the right member of Eq. (2) by the number of atoms N_0 per cm^2 , and divide by N . The resulting ("linear") absorption coefficient

$$\tau = N_0 (2\pi/h\nu c) |J_{E, n, \nu}|^2 \quad (4)$$

is the probability per cm of path a light quantum will be absorbed. If ρ is the density of matter, in c.g.s. units, τ/ρ is called the *mass-absorption coefficient*. Finally τ/N_0 is called the *atomic absorption coefficient*, or the *cross section* for absorption (CSA).

The theoretical range of validity of the formula for τ is very great and may be understood as follows: The condition $|a^2| = Pt (= (S_0 \tau / h\nu N_0) t) \ll 1$, must be satisfied in order for the perturbation

³ P. A. M. Dirac, *Proc. Roy. Soc. A* **117**, 610 (1928); **A118**, 351 (1928).

⁴ J. R. Oppenheimer, *Phys. Rev.* **31**, 66 (1928); Mott and Massey, *Theory of Atomic Collisions* (Oxford Press, 1933), p. 256.

calculation leading to Eq. (2) to have a meaning. On the other hand, since the calculation was for a periodic disturbance (light wave), we must have $\nu l \gg 1$. That is ($P \ll 1/t \ll \nu$, which requires that $(S_0/h\nu)(\tau/N_0) \ll \nu$). For ordinary radiation densities this latter condition is always well satisfied.

4. General formula for angular distribution of the photoelectrons

The formulas for this part of the calculations were originally derived on the basis of the Schrödinger perturbation theory,⁵ very much in the same way as the formulas of dispersion theory. Although various authors have written about the spatial distribution⁶ of photoelectrons, these papers are chiefly of historical interest. For a treatment of this problem the reader is referred to Sommerfeld, Sommerfeld and Schur, and H. Bethe⁷ for the nonrelativistic treatment; to J. Waller, and F. Sauter,⁸ for the relativistic discussion.

Sommerfeld's formula, which will be given shortly, was derived on the basis of the Schrödinger equation, and hence must be reconsidered when relativistic effects are important. The generalization of his method to account for these effects was carried through by J. Waller, K. Nikolsky, T. Muto⁸ and others.

The angular distribution can be obtained from the wave function of the perturbed problem (atom perturbed by incident light wave) at a large distance from the atom, and is found to be formally the same, regardless of which form of theory is used. It is obtainable from the formula

$$\Psi = (ecA_0/2\nu) \sum J_{E, n} \psi_{\alpha_s}^E, \quad (5)$$

where A_0 is the amplitude of the electric vector, and the summation is extended over all final states ψ^E corresponding to the energy E . ψ^E is the

⁵ See *Collected Papers on Wave Mechanics* (London, 1928).
⁶ G. Wentzel, *Zeits. f. Physik* **40**, 574 (1926); **41**, 828 (1927); G. Beck, *ibid.* **41**, 443 (1927); A. Carelli, *ibid.* **56**, 694 (1929); S. E. Sczeniewski, *Phys. Rev.* **35**, 347 (1930); J. Frenkel, *Phys. Rev.* **37**, 1276 (1931); H. Hall and J. R. Oppenheimer, *Phys. Rev.* **35**, 71 (1931).

⁷ A. Sommerfeld, *Wave Mechanics* (Methuen, 1930), 177. See also, H. Bethe, *Ann. d. Physik* **4**, 443 (1930); and Sommerfeld and Schur, *Ann. d. Physik* **4**, 409 (1930); Schur, *Ann. d. Physik* **4**, 433 (1930); H. Bethe, *Handbuch der Physik*, Vol. 24/1.

⁸ J. Waller, *Zeits. f. Physik* **61**, 837 (1930); T. Muto, *Scientific Papers of the Inst. of Phys. and Chem. Research*, Tokyo; K. Nikolsky, *Zeits. f. Physik* **56**, 709 (1929); F. Sauter, *Ann. d. Physik* **9**, 217 (1931).

normalized solution of the unperturbed problem, and $\psi_{\alpha_s}^E$ is the outgoing part of its asymptotic value far from the atom. When $(v/c)^2 \ll 1$, $\psi_{\alpha_s}^E$ is found by solving the Schrödinger equation, and, as it has the asymptotic form e^{ikr}/r , it is evident that the current in the radial direction is equal to $\Psi\Psi^*ev$. In the relativistic problem, for large energies this is not the case, and here a result of Gordon's is useful.⁹ It gives, as the conduction current in the direction x_k ,

$$s_k = -\frac{e}{2mc} \left\{ \frac{\hbar}{i} \left(\psi^* \alpha_4 \frac{\partial \psi}{\partial x_k} - \psi \alpha_4^* \frac{\partial \psi^*}{\partial x_k} \right) + \frac{2e}{c} \varphi_k \psi^* \alpha_4 \psi \right\}$$

where α_4 is the coefficient of $mc\psi$ in the Dirac equation, and ζ_k is the vector potential. The vector potential will be zero in our considerations.

RESULTS OF NONRELATIVISTIC THEORY OF THE PHOTO-EFFECT

5. Absorption coefficient of the K shell for long wave-lengths

If both K electrons of an atom are supposed to be unaffected by all other (L , M ... shells) electrons, and by each other, while each is supposed to be in the same field, Ze/r of the nucleus, the evaluation of the absorption coefficient from Eq. (4) may be carried through without difficulty. The retardation factor $\exp(i\mathbf{k}\cdot\mathbf{r})$, for reasons of consistency with the nonrelativistic approximation, must be set equal to unity when the wave function is limited to atomic distances of the order of the first Bohr radius; and this leads to the selection rule $l=0 \rightarrow 1$ in the orbital angular momentum. One finds for the mass-absorption coefficient of the K shell

$$(\tau/\rho)_K = \frac{N_0 h a_0 2^3 \pi}{\rho mc 3} \times \frac{\exp\{-4(v_0/v) \tan^{-1}(v/v_0)\}}{Z^2(1+v^2/v_0^2)^4(1-e^{-2\pi v_0/v})}, \quad (6)$$

$$\text{where} \quad 1 + v^2/v_0^2 = v/v_1. \quad (7)$$

Eq. (7) expresses the conservation of energy in the absorption process. The ideal absorption limit v_1 occurring here is given by the equation

$$v_1 = Z^2 \cdot (2\pi^2 m e^4) / h^3 = Z^2 R y.$$

⁹ W. Gordon, *Zeits. f. Physik* **50**, 630 (1928).

In c.g.s. units, taking $\lambda_1 = c/\nu_1$,

$$\lambda_1 = \frac{h}{mc} \frac{2}{\alpha_0^2 Z^2} = \frac{912.3}{Z^2} \cdot 10^{-8} \text{ cm.}$$

Finally, $v_0 = 2\pi e^2 Z/h = \alpha c =$ orbital velocity of bound electron.

For the case near the absorption limit, where $v/v_0 \ll 1$, Eq. (6) may be expanded in powers of $(v/v_0)^2$. Neglecting terms of magnitude $\frac{1}{2}(v/v_0)^4$ compared to unity¹⁰ in this expansion one finds

$$\begin{aligned} (\tau/\rho)_K &\cong \frac{N_0 h a_0 2^9 \pi}{\rho mc 3e_1^4 Z^2} \frac{1}{Z^2} \left(\frac{\nu_1}{\nu}\right)^{8/3} \\ &\cong \frac{7.6 \times 10^6}{AZ^2} \left(\frac{\nu_1}{\nu}\right)^{8/3}, \text{ (in c.g.s. units).} \end{aligned}$$

In the first equation above, e_1 is the base of the Napierian logarithms ($e_1 = 2.71828 \dots$), and in the second equation A is the atomic weight.

It so happens that the function $\exp(4 - (4/x) \times \tan^{-1} x)$ is rather well represented by the expression $(1 + (4/3)x^2)$, even for x^2 as large as 2. Consequently a much better representation for τ_K , which gives results correct to within one percent as long as $\nu \leq 3\nu_K$, may be written

$$\frac{\tau_K}{\rho} = \frac{7.6 \times 10^6}{AZ^2} \left(\frac{\nu_1}{\nu}\right)^{4/3} \left[1 + \frac{4}{3} \left(\frac{\nu}{\nu_1} - 1\right)\right]. \quad (8)$$

This same expression represents Eq. (6) correctly to within 3 percent for all $\nu < 6\nu_1$.

When $v/v_0 \gg 1$, we find, after neglecting $\pi v_0/v$ compared to unity,

$$\frac{\tau_K}{\rho} = \frac{N_0 h a_0 2^8}{\rho mc 3} \left(\frac{\nu_1}{\nu}\right)^{3.5} = \frac{6.34 \times 10^7}{A} \left(\frac{\nu_1}{\nu}\right)^{3.5}$$

The condition $\pi v_0/v \ll 1$, for the validity of this formula, may be satisfied only for the lightest elements, in the nonrelativistic range of velocities v .

The maximum value of the cross section for absorption τ_K/N_0 for any given element, occurs

¹⁰ The theoretical dependence of τ_K on frequency in the neighborhood of ν_1 is correctly given by this formula. That is, by $\tau_K \sim \nu^{-3/2}$, and not by $\tau_K \sim \nu^{-4}$ as one so often finds in the literature; M. Stobbe, *Ann. d. Physik* 7, 696, Eq. (43') (1930); F. Sauter, *Ann. d. Physik* 11, 497, Eq. (43a) (1931); Compton and Allison, *X-Rays in Theory and Experiment* (Van Nostrand, 1935), p. 560, Eq. (7.61). Corresponding errors are also frequent regarding the L shells.

at the ionization limit $\nu = \nu_1$, and is there given by

$$\frac{\tau_K}{N_0} = \frac{h a_0 2^9 \pi}{mc 3e_1^4 Z^2} \frac{1}{6} \text{ area of } K \text{ shell.}$$

For the CSA, $\tau_K/N_0 \cong 1.26 \times 10^{-17} (\nu_1/\nu)^{8/3}/Z^2$, near the series limit.

In applying these formulas to physical atoms the meaning of each approximation may be qualitatively considered.

(a) First, to express the validity of the Schrödinger equation, we have the condition $(v/c)^2 \ll 1$. This condition applies to the velocity v of the photoelectron as well as to v_0 , the mean velocity of the bound electron in its orbit. The condition $(v/c)^2 \ll 1$ for the final state, it is clear, can merely limit the frequency of the incident beam. This limiting frequency will be given, from Eq. (7), by the condition

$$(v/c)^2 = (\nu/\nu_K - 1)\alpha^2 \ll 1$$

and will be different for different elements (Z). If the Schrödinger equation is assumed to hold for all ν up to $(v/c)^2 = 1/20$, say, we find

$$\nu_{\text{limiting}} \sim (mc^2/h)(1/40 + \alpha^2/2).$$

In the bound state, the orbital velocity may be crudely determined by balancing the nuclear force of attraction against the centrifugal force, assuming the electron to be moving in a circle of radius $r = a_0/Z$. This gives

$$v_0 = (Z^2 e^2 / m a_0)^{1/2} = 2\pi Z e^2 / h.$$

Hence in this instance the theory would seem to be better applied to light elements than heavy, since v_0 as determined above may be as large as 0.6 c , or larger, when applied to the heaviest elements. We shall see later on that all relativistic effects, from the normal state, final state, and from the retardation, combine in such a way as to leave the CSA (cross section for absorption) unaffected to a good approximation, as long as $\nu < \nu_{\text{limiting}}$. At that time we shall, however, make the notion of ν_{limiting} somewhat more precise. It is solely on the basis of this future work that the results of this section have any meaning when applied to the heavy elements.

(b) Concerning the neglect of electrostatic interactions

$$e^2/r_{KK'}, \quad e^2/r_{KL}, \quad e^2/r_{KM},$$

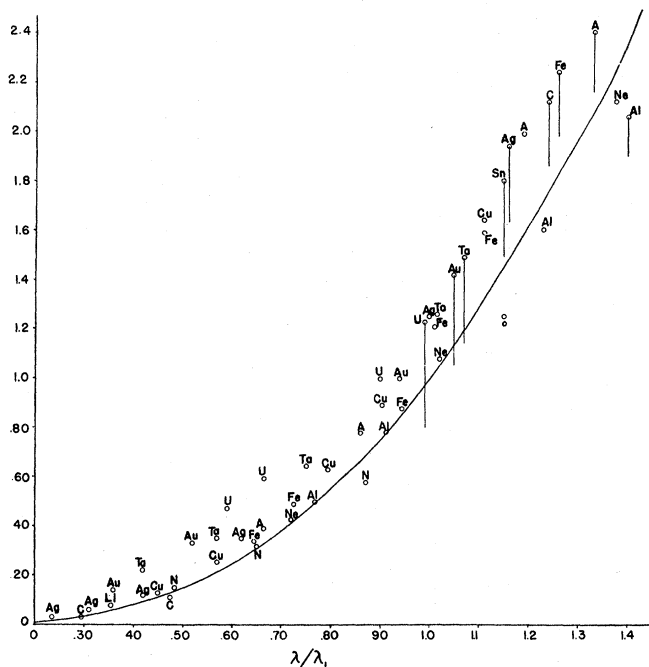


FIG. 1. Theoretical curve (Eq. (8) for $\lambda/\lambda_1 > 1$ as well as for $\lambda/\lambda_1 < 1$) of the mass-absorption coefficient τ_K/ρ , for all elements, in units of $7.6 \times 10^6/A(Z-0.3)^2$. $\lambda_1 = 912/(Z-0.3)^2 A$. Experimental points represent the total absorption $\mu/\rho = \tau/\rho + \sigma/\rho$, according to S. J. M. Allen. The vertical lines represent the difference between the maximum and minimum total absorption observed at the K absorption limit, also according to S. J. M. Allen.

etc., the validity is best for heavy atoms. Some of these terms are always comparable with the electron-nuclear term, $-Ze^2/r$ unless $Z \gg 1$. When this latter condition is fulfilled it will be possible to ascribe a meaning to the model, although even here the outer shells effectively "screen" (i.e., repel) the K electrons and thereby diminish the ionization energy. The two K electrons do not have a very strong effect on each other.

When we attempt (see Fig. 1) to compare Eq. (8) with experiment, a difficulty arises at once, since the observed ionization frequencies are smaller than $\nu_1 = Z^2 Ry$ for the reason mentioned above, and therefore do not satisfy the conservation law Eq. (7) in which the effect of screening was neglected. The theory does not therefore apply for observed frequencies less than ν_1 , which is the minimum frequency allowed by the con-

servation law, although Eq. (8) agrees rather well with experiment when extrapolated into this region.* Outside of this region, where it does apply the agreement is rather good, especially for large atomic numbers. This may be seen directly from the experimental data (Fig. 1), or from Gray's empirical formula,¹¹

$$\tau_{\text{atom}} = 1.92(1 + 0.008Z) \times \left(1 - \frac{\lambda}{4\lambda_K} - \frac{\lambda}{50\lambda_K^2}\right) Z^4 \lambda^3 \times 10^{-26} \text{ cm}^2$$

* In Fig. 1 the observed K absorption limit for all elements except uranium is seen to come from wavelengths greater than the ideal limit λ_1 . The justification for extrapolating Eq. (8) into this region is contained in the sequel, where the presence of $Z-0.3$ in place of Z will also be explained.

¹¹ J. A. Gray, Proc. Roy. Soc. Canada 21, 179 (1927).

which gives the *atomic* CSA. The *K* shell CSA may be taken to be about 4/5 of σ_{atom} . In the formula λ_K is the observed critical wave-length, in angstrom units, and λ is the wave-length in angstrom units.

That $\nu_1 = Z^2 Ry$ is greater than ν_K (obs) is easily understood, since $Z^2 Ry$ measures the energy necessary to remove a *K* electron to infinity from an atom stripped of all other electrons, while ν_K (obs) measures the corresponding energy for an actual atom. However it is a little surprising in this connection that the difference $Z^2 Ry - \nu_K$ (obs) falls off for $Z > 56$. This latter circumstance will be explained later, on the basis of the correct relativistic binding energy, which is greater than $Z^2 Ry$.

6. Screening

We shall now consider the effects of a screening function in the potential energy, with the aim of applying this theory of the *K* shell to medium heavy and heavy elements, which really do possess other (*L*, *M*, ...) electrons. If the potential energy is written as

$$-Ze^2/r + V(r),$$

such a $V(r)$ could be determined numerically, as in the Hartree self-consistent field. It must have certain reasonable limiting properties. For $r \rightarrow 0$, only the nuclear field can be of relative importance, and therefore, for small r , $V(r) \rightarrow V_0 + V_1(r)$ where V_0 is a constant, characteristic of the atom, and $V_1(r) \rightarrow 0$, for $r \rightarrow 0$. On the other hand, if the electron is considered to be removed from the atom, at large distances it will be in a field $-e^2/r$. Hence, at large distances from the atom, we must have $V(r) = (Z-1)e^2/r$.

The essential thing about such a screening function in a first approximation is the constant V_0 , which one may presumably determine from some consistent theory. The Fermi-Thomas model,¹² which is based on statistical ideas, provides us with such a plausible theory. If we define $\varphi(r)$ by the equation

$$V(r) = ((Z-1)e^2/r)[1 - \varphi(r)],$$

where $V(\infty) = V_0$,

¹² L. H. Thomas, Proc. Camb. Phil. Soc. 23, 542 (1927); E. Fermi, Zeits. f. Physik 48, 73 (1928).

the differential equation for φ may be written

$$d^2\varphi/dx^2 = \varphi^3/x^4, \quad (9)$$

where $x = r/\mu$, and $\mu = a_0(9\pi^2/128Z)^{1/3}$

according to the Fermi-Thomas treatment. An asymptotic solution for φ , valid for r large was found by Sommerfeld.¹³ It shows that φ decreases like r^{-6} at great distances from the atom. We shall need only the value of φ for r small, for the present at least, and this is given by the expansion¹⁴

$$\varphi = 1 - 1.589x + (4/3)x^3 - \dots$$

Thus, we get

$$V_0 = 1.589 \frac{e^2(Z-1)}{\mu} = 1.79 \frac{e^2}{a_0} (Z-1) Z^{1/3}$$

or $V_0 \sim 3.6Z^{4/3}$, in Rydberg units.

Now, whereas Eq. (1), with $V_0 = 0$, took the form $E = h\nu - Z^2 Ry$, we now find it should be written $E = h\nu - Z^2 Ry + V_0$ since V_0 is merely an additive constant to the energy in the Schrödinger equation. Hence, the theoretical ionizing frequency, becomes¹⁵

$$\nu_1' = Z^2 - V_0 \cong Z^2 - 3.6Z^{4/3} Ry,$$

which is smaller than the corresponding expression with $V_0 = 0$, and in fact is smaller than the ionizing frequencies observed, by an amount between fifteen ($Z = 50$) and thirty percent ($Z = 19$). One may now calculate the absorption at ν_K (obs) however, since, as we have said above, ν_1' is smaller than ν_K (obs).

The constant term V_0 in the potential energy modifies the Coulomb potential by a fractional amount $\sim 3.6Z^{4/3}/2Z^2$ in the neighborhood of the first Bohr orbit. The correlation between this change, and the change produced by it in ν_1 provides a basis for estimating the effect on the theoretical frequency of ionization of other perturbations in the potential. For example, a consideration of relativistic effects on the Fermi-Thomas potential¹⁶ shows that the atomic potential is decreased through these effects by only 0.3 percent well inside the first Bohr orbit, where they are

¹³ A. Sommerfeld, Zeits. f. Physik 78, 283 (1932).

¹⁴ E. O. Wollan, Rev. Mod. Phys. 4, 205 (1932).

¹⁵ Of course, if the system were quantized correctly with the potential energy given by the Fermi-Thomas potential, one would find a ν_1' somewhat different from this. The change would be in the same direction however, and, as we shall see later, the results would not alter appreciably the conclusions of this discussion.

¹⁶ M. S. Vallarta and N. Rosen, Phys. Rev. 41, 708 (1932).

largest. Terms of this magnitude would consequently be expected to have a negligible effect on the ionization frequency.

It is desirable however, if possible, to improve the ionization frequency predicted by a screening model. Further study shows indeed that part of the discrepancy lies, as one might expect, in neglecting the contraction occurring in the outer shells when one K electron is removed to infinity. Kennard and Roess¹⁷ have adapted the Fermi-Thomas potential to take account of this contraction. From the potential function given by them (Eq. (9)), one finds the screening constant

$$V_0 = 3.6Z^{4/3} - 3.3Z - 4Z^{\frac{1}{2}}, \quad (10)$$

in Rydberg units. The ionization frequencies

$$\nu_1'' = Z^2 - (3.6Z^{4/3} - 3.3Z - 4Z^{\frac{1}{2}}) \quad (10')$$

provided by this V_0 fit better than those given by ν_1' . They are still lower than the experimental ones, nevertheless, by from five ($Z=30$) to thirteen ($Z=82$) percent. But, as we shall see in Section 10, this latter discrepancy is almost completely accounted for by the relativistic binding energy.

The problem of finding the absorption coefficient corresponding to a potential energy

$$V = -Ze^2/r + V_0, \quad r < r_0; \quad V = -e^2/r, \quad r > r_0,$$

where $r_0 = (Z-1)e^2/V_0$, is rather easy, inasmuch as evaluating the matrix element presents no difficulties at all. But for frequencies greater than ν_1'' given above, and less than $\nu_1 = Z^2$, which are just the frequencies of interest, the wave function for the photoelectron corresponds to a virtual energy, $E - V_0 < 0$. At points within the atom it consequently has somewhat the behavior of a wave function corresponding to a discrete state, whose principal quantum number is not an integer. The normalization of this wave function is therefore something of a problem. It is carried through to a pretty fair approximation in Section 16. The final result, using that normalization, and neglecting terms in $(v/v_0)^4$ is merely to justify the use of our previous formula for τ_K for all frequencies greater than ν_1'' . This does *not* mean that $\nu_1 = Z^2$ is to be replaced by $\nu_1'' = Z^2 - V_0$ in Eq. (8). That equation as it stands is to be used. The results, compared with experiment for

¹⁷ E. H. Kennard and L. C. Roess, Phys. Rev. **38**, 1267 (1931).

two elements, are given in Table V.¹⁸ In the case of Pb, Eq. (8) does not apply as far out as $\lambda = \frac{1}{2}\lambda_K$ because here $(v/c)^2$ is comparable with unity. The good agreement which obtains in spite of this is accounted for by the relativistic model.

7. Absorption coefficient of the L shell

The L shell is customarily thought of as being made up of three sub-shells L_I , L_{II} and L_{III} . This designation had its origin in x-ray studies and has little meaning in a theoretical discussion where relativity and screening effects are ignored, because in that case all eight electrons have the same binding energy $\frac{1}{4}Z^2Ry$. Even so, there is a formal separation between the L_I (two $2s$ electrons) and the $L_{II}+L_{III}$ (six $2p$ electrons) shells which may be preserved with advantage for purposes of comparing the results with certain experiments.

If we now attempt to treat the L shell by assuming each L electron to move in a screened Coulomb field, $(Z-s)e/r$, of the nucleus, we are at once faced with the necessity of assigning a reasonable value to the screening constant s . This model has not as precise a meaning as the corresponding thing for the K shell, because of the large number of electrons in the L shell. It may be expected to provide a fairly good description however, because the electron-nuclear force is still quite large compared to the other forces involved. To determine the screening constant s , Slater¹⁹ has given rules which were arrived at from an examination of experimental ionization energies. According to Slater's rules for any $2s$ or $2p$ electron, we have $s_2 = 2(0.85) + 7(0.35) = 4.15$. For the K electrons, in agreement with the screening observed in helium, he offers a screening constant $s_1 = 0.3$. There is no direct reference to screening by the outer shells (M, N, \dots) in Slater's formulation.

Of course there is no *a priori* reason to expect *accurate* results from the use of Slater's constants

¹⁸ A similar table occurs in the literature where the experimental points do not agree with those given here. See Roess, Phys. Rev. **37**, 532 (1931). Roess presumably constructed these data from his Figs. 1 and 2, or rather from Allen's equivalents. Whereas Allen in his article, Phys. Rev. **27**, 266 (1926), Table (IB) gives no points for Sn for $\lambda > 0.320\text{\AA}$ it is probable, in the light of Allen's recent values as shown in Table V, that the experimental values of τ_K/ρ near $\lambda = 0.424\text{\AA}$ are lower than those Roess gives.

¹⁹ J. C. Slater, Phys. Rev. **36**, 57 (1930).

when we compare the L absorption with experiment, particularly in the event these results are at all sensitive to the choice of s_2 . For if the integral giving the transition probability has its chief contribution for values of r somewhat less than the radius of the L shell, a smaller screening constant should be used, while in the event of the main contribution coming from farther out, a larger value should perhaps be used. We shall include an arbitrary "inner" screening, s_2 , in the sequel, and give some attention to the effect on the absorption of reasonable changes in it. We could further account qualitatively for the "outer" screening, which is essentially concerned with the discrepancy between the theoretical ionizing energy $\frac{1}{4}(Z-s_2)^2$ and the observed value, by expanding the Fermi-Thomas or some other atomic potential in the neighborhood of the L shell, and obtaining a constant term V_1 , analogous to the V_0 previously discussed for the K shell. Since a term of this kind has no effect on the magnitude of τ/ρ , in a first approximation as we have seen, we shall omit any explicit reference to V_1 .

We shall now summarize the results of the theory for the L shell.²⁰ For the two $2s$ electrons of the L_I shell we find

$$\tau_{L_I} = \frac{2^{14}\pi ha_0}{3 mc} N_0 \frac{(\nu_2/\nu)^4}{(Z-s_2)^2} \left(1 + 3\frac{\nu_2}{\nu}\right) \times \frac{\exp(-8(v_1/\nu) \tan^{-1}(v/v_1))}{1 - \exp(-4\pi v_1/\nu)} \quad (11)$$

and for the six $2p$ electrons of the $L_{II}+L_{III}$ shell we find

$$\tau_{L_{II}} + \tau_{L_{III}} = \frac{2^{14}\pi ha_0}{3 mc} N_0 \frac{(\nu_2/\nu)^5}{(Z-s_2)^2} \left(3 + 8\frac{\nu_2}{\nu}\right) \times \frac{\exp(-8(v_1/\nu) \tan^{-1}(v/v_1))}{1 - \exp(-4\pi v_1/\nu)} \quad (12)$$

²⁰ The formula of M. Stobbe, Ann. d. Physik 7, 661 (1930), for τ_{L_I} agrees with ours, but his formula for $\tau_{L_{II}} + \tau_{L_{III}}$ should be reduced by a factor $\frac{1}{2}$. See Stobbe's Eqs. (45), (45'), etc. Since Bethe's Eqs. (47.19), (47.20), *Handbuch der Physik*, Vol. 24/1, p. 480, were taken from Stobbe, most of his computations for the L shell would appear to be wrong. It is surprising therefore, in Bethe's table on p. 481, that the agreement with Skinner for the ratio $\tau_{L_{II}} + \tau_{L_{III}} : \tau_{L_I}$ is so good. An examination of other data, however, makes it appear probable that Skinner's values are too high. The agreement which Bethe finds with experiment for the K discontinuity, δ_k , is due to an error in computation. I am indebted to Professor Bethe for the benefit of a discussion, during which he mentioned that Stobbe had found an error in his own paper.

TABLE I. Ratio of the photo-effect in the $L_{II}+L_{III}$ shell to that in the L_I shell. $\nu(\text{Mo } K\alpha_1) = 1288Ry$; $\nu(\text{Mo } K\alpha_2) = 1280Ry$; $\nu(\text{Mo } K\beta_1) = 1445Ry$; $\nu(\text{Mo } K\beta_2) = 1472Ry$; $\nu(\text{Cu } K\alpha_1) = 593Ry$.

Reference	Element	$\nu(Ry)$	$\nu_2(Ry)$	ν_2/ν	Ratio $\tau_{L_{II}} + \tau_{L_{III}} : \tau_{L_I}$	
					Calc.	Obs.
21a	82Au	1288	1520	1.18	3.2	3.3
"	"	1445	"	1.05	2.9	4.3
"	74W	1288	1225	0.950	2.6	4.0
"	"	1280	"	.957	2.6	3.3
"	58Ce	1288	730	.566	1.6	2 +
"	56Ba	1288	680	.528	1.5	2.0
"	"	1445	"	.470	1.3	2.0
"	47Ag	1288	462	.359	1.0	1.8
"	"	1455	"	.320	0.91	0.71
"	42Mo	1288	362	.281	.80	.75
"	40Zn	1288	325	.252	.72	.67
"	"	1472	325	.220	.63	.40
"	35Bi	1288	241	.187	.54	.30
"	29Cu	1288	156	.121	.35	.2-
"	"	593	"	.263	.75	.75
21b	56Ba	593	680	1.15	3.1	7.0
"	53I	"	600	1.01	2.8	4.5
"	50Sn	"	530	0.894	2.5	4.0
"	47Ag	"	460	.775	2.2	3.0
"	42Mo	"	360	.607	1.7	3.0
"	38Sn	"	290	.490	1.4	2.0
"	29Cu	"	156	.263	0.75	0.75

In these formulas ν_2 and v_1 are defined as follows:

$$\nu_2 = \frac{1}{4}(Z-s_2)^2 Ry,$$

$v_1 = \frac{1}{2} \cdot (2\pi e^2/h)(Z-s_2) =$ orbital velocity of electron in initial state. These quantities are connected by the conservation law

$$1 + (v/v_1)^2 = \nu/\nu_2,$$

which can be used to express τ_L as a function of ν .

From Eqs. (11), (12) and Eq. (6), neglecting s compared to Z and ν_2 and ν_1 compared to ν we may write for large frequencies

$$\tau_K \cong 8\tau_{L_I} \cong (8/3)(\nu/\nu_2)(\tau_{L_{II}} + \tau_{L_{III}}).$$

Eqs. (11), (12) furnish the relation

$$\frac{\tau_{L_{II}} + \tau_{L_{III}}}{\tau_{L_I}} = \frac{\nu_2}{\nu} \frac{3 + 8\nu_2/\nu}{1 + 3\nu_2/\nu},$$

which may be compared with experiments on magnetic spectra of photoelectrons, which are ejected from elements by the $K\alpha$ and $K\beta$ radiations of various substances.²¹ In Table I we give

²¹ (a) H. R. Robinson and A. M. Cassie, Proc. Roy. Soc. A113, 282 (1926); (b) H. W. B. Skinner, Proc. Camb. Phil. Soc. 22, 379 (1924); (c) F. K. Richtmyer, Phys. Rev. 23, 292 (1924). See also A. H. Compton and S. K. Allison for further references, *X-Rays in Theory and Experiment* (Van Nostrand, 1935).

the results. Robinson and Cassie used the frequencies Mo $K\alpha_1=1288$, Mo $K\alpha_2=1280$, Mo $K\beta_1=1445$ and Mo $K\beta_2=1472$ all in Rydberg units. Where these frequencies occur in the table, the corresponding emission line above is indicated. Skinner used the frequency Cu $K\alpha_1=593Ry$. The agreement is not of the best, but, considering the experimental difficulties involved in estimating intensities, it is satisfactory. Where the authors give a range for the intensities, such as 4-5 for $\tau_{L_{II}}+\tau_{L_{III}}$ say, and 6 for τ_{L_I} , we take the mean, and in this case for example would write 0.75 for the ratio.

We now proceed to discuss the absorption coefficients separately. For frequencies close to the L limit we may expand the cross section as before.

$$\frac{\exp(-8(v_1/v) \tan^{-1}(v/v_1))}{1 - \exp(-4\pi v_1/v)} = e^{-8\left(\frac{v}{v_2}\right)^{8/3}} \left\{ 1 - \frac{4}{15} \left(\frac{v}{v_1}\right)^4 + \dots \right\}.$$

Then, neglecting terms $\sim \frac{1}{6}(v/v_1)^4$ and smaller, we find the following formulas (in c.g.s. units);

$$\begin{aligned} \tau_{L_I} &= 2.93 \times 10^{-17} N_0 (v_2/v)^{2.08} / (Z-s_2)^2, \\ \tau_{L_{II}} + \tau_{L_{III}} &= 8.06 \times 10^{-17} N_0 (v_2/v)^{3.06} / (Z-s_2)^2 \end{aligned} \quad (13)$$

and for the total contribution from the L shell

$$\begin{aligned} \tau_L = \tau_{L_I} + \tau_{L_{II}} + \tau_{L_{III}} &= 11.0 \\ &\times 10^{-17} N_0 (v_2/v)^{2.80} / (Z-s_2)^2. \end{aligned}$$

This gives for the CSA at the absorption limit

$$\tau_L/N_0 \sim (1/13) \times \text{area of } L \text{ shell}$$

or a maximum value of about 9 times the maximum value of τ_K/N_0 . Finally, for numerical

computation near the L limit, we may also write

$$\tau_L/\rho = 66.6 \times 10^8 (v_2/v)^{2.8} / A (Z-s_2)^2.$$

From Eqs. (11), (12) one may also obtain a simple formula when $v/v_2 \gg 1$, which is the first term of an expansion in powers of $2\pi v_1/v$. For these large frequencies one finds

$$\begin{aligned} \tau_{L_I} &\sim (v_2/v)^{3.6}, \\ \tau_{L_{II}} + \tau_{L_{III}} &\sim (v_2/v)^{4.6}. \end{aligned}$$

However, we must bear in mind the restriction to nonrelativistic velocities $(v/c)^2 \ll 1$, which is here equivalent to the condition $(v/v_2-1)\alpha^2/4 \ll 1$. This condition, together with the condition that the expansion be valid gives

$$(\pi\alpha)^2 \ll (v/v_2-1)(\alpha^2/4) \ll 1.$$

We see therefore that the expansions for v large can be valid only for the very lightest elements. They are useful mainly in suggesting the more rapid decrease with increasing frequency of $\tau_{L_{II}} + \tau_{L_{III}}$ over τ_{L_I} .

A further application of some interest is the calculation of the so-called K absorption jump.²² This quantity, δ_K , is effectively a measure of the ratio of the K shell absorption to the absorption from all other shells. It is defined as

$$\delta_K = \left(\frac{\tau_K + \tau_L + \tau_M + \dots}{\tau_L + \tau_M + \dots} \right)_{\nu=\nu_K}$$

If all kinds of screening are neglected, and the theoretical value $\nu_1 = Z^2 Ry$ is used for ν_K , one finds from the formulas previously given

$$\delta_K = 1 + (8/3) \exp((8/\sqrt{3}) \tan^{-1} \sqrt{3-4}) = 7.15$$

the same for all elements. If, however, we set $s_2 = 4.15$ and $s_1 = 0.3$, and calculate δ_K for ν equal to ν_K , the *observed* value of the critical frequency, then δ_K changes with Z . To compute δ_K we derive the formula†

$$\frac{\tau_K}{\tau_L} = 8 \left(\frac{Z-s_1}{Z-s_2} \right)^6 \frac{[1 + (4/3)(v/v_1-1)] \exp\{8(v/v_2-1)^{-1/2} \tan^{-1}(v/v_2-1)^{1/2} - 4\}}{1 + 6(v_2/v) + 8(v_2/v)^2} \quad (14)$$

²² See Compton and Allison, reference 21, p. 528; E. Jönsson, Diss. Upsala (1928), Table 115; Richtmyer, Phys. Rev. 30, 755 (1927).

† When calculations are made with Eq. (14) for light elements (Z less than about 35), the factor $[1 + (4/3) \times (v/v_1-1)]$ must be reduced because of screening (according to Section 16). For Fe the reduction is about 4 percent.

Expanding this about $\nu=4\nu_2$ we find

$$\delta_K \approx 1 + 6.15 \left(\frac{Z-s_1}{Z-s_2} \right)^{10/9} \left[1 + 0.066 \left(\frac{\nu_K}{\nu_2} - 4 \right) \right].$$

Applying this to Fe26, Ag47, W74, with the experimental values 525, 1888, 5120Ry, respectively, for ν_K , we find for δ_K the values

$$11.2 \text{ for Fe, } 9.31 \text{ for Ag, } 8.49 \text{ for W.}$$

Bethe calculates* the M shell absorption to be 23 percent of the L absorption for Fe, and 35 percent for W. Correcting our values for this, according to the definition of δ_K , gives the values

$$9.2 \text{ for Fe, } 7.4 \text{ for Ag, } 6.5 \text{ for W,}$$

TABLE II. General functions for computing the L absorption coefficients for all elements. $(\tau/\rho)_{L_I} = (7.6 \times 10^8/A(Z-s_2)^2) f_{L_I}$ (Definition of f_{L_I} with Eq. (11)). Similarly for $f_{L_{II+L_{III}}}$. $f_{L_I} = 2^8 e^{-4} (1+3\lambda/\lambda_2) f$ (Definition of f) $f_{L_{II+L_{III}}} = 2^8 e^{-4} \lambda/\lambda_2 \times (3+8\lambda/\lambda_2) f$. Writing $f_L = f_{L_I} + f_{L_{II+L_{III}}}$, $(\tau/\rho)_L = (7.6 \times 10^8/A(Z-s_2)^2) \cdot f_L$. For completeness, $\lambda_2 = 912.3 \times 4/(Z-s_2)^2$ A.U.

λ_2/λ	f	f_{L_I}	$f_{L_{II+L_{III}}}$	f_L
2.0	0.3479	0.50985	0.71379	1.22364
2.1	.3198	.45531	.60801	1.06332
2.2	.2952	.40901	.52197	0.93098
2.3	.2727	.36834	.45029	.81863
2.4	.2516	.33187	.38921	.72108
2.5	.2341	.30190	.34039	.64229
2.6	.2176	.27471	.29808	.57279
2.7	.2023	.25037	.26197	.51234
2.8	.1896	.23021	.23245	.46266
2.9	.1762	.21020	.20517	.41537
3.0	.1649	.19339	.18263	.37602
3.1	.1549	.17869	.16350	.34219
3.2	.1460	.16586	.14716	.31302
3.3	.1372	.15355	.13218	.28573
3.4	.1291	.14242	.11911	.26153
3.5	.1216	.13241	.10766	.24007
3.6	.1150	.12362	.097838	.22146
3.7	.1088	.11552	.089038	.20456
3.8	.1029	.10791	.081049	.18896
3.9	.09737	.10099	.073908	.17490
4.0	.09239	.094781	.067701	.16248
4.1	.08776	.089089	.062133	.15122
4.2	.08328	.083699	.057021	.14072
4.3	.07938	.079006	.052613	.13162
4.4	.07541	.074354	.048414	.12277
4.5	.07190	.070246	.044753	.11500
4.6	.06859	.066431	.041439	.10787
4.7	.06533	.062751	.038331	.10108
4.8	.06216	.059216	.035425	.09464
4.9	.05974	.056460	.033125	.08959
5.0	.05690	.053370	.030688	.08406
5.5	.046008	.041682	.021845	.06353

* *Handbuch der Physik*, 24, p. 480. In this reference Bethe gives these estimates as 16 and 25 percent, respectively. However, since the value he took for ν_L was too large by the factor 17/12 = 1.4, his estimates for τ_M must presumably be raised by the corresponding amount.

which are in fair agreement with Jönssen's, who gives

$$8.5-9.2 \text{ for Fe, } 6.7-7.8 \text{ for Ag, } 5.7-6.4 \text{ for W.}$$

The experimental values are rather sensitive to the scattering correction however, and Jönssen's results, for example, could easily be brought into agreement with the theoretical ones by attributing slightly more absorption than he did to the scattering. Similarly, the theoretical results are somewhat in doubt from the nature of the model employed, and could perhaps reasonably be made a trifle lower. The agreement must be considered as satisfactory in any case, except perhaps for the lightest elements,** which are not discussed in this connection.

TABLE III. Mass-absorption coefficient of the L shell for tin, $S_{II}(50)$, $\lambda_2 = 1.7358A$.

λ_2/λ	$\lambda(A)$	$(\tau/\rho)_{L_I}$	$(\tau/\rho)_{L_{II+L_{III}}}$	$(\tau/\rho)_L$
1.55	1.1199	27.615	49.636	77.251
1.65	1.0521	24.063	40.623	64.686
1.75	0.9918	21.051	33.546	54.597
1.85	.9382	18.490	27.921	46.411
1.90	.9136	17.445	25.670	43.115
1.95	.8901	16.483	23.560	40.043
2.0	.8679	15.494	21.689	37.180
2.1	.8266	13.835	18.474	32.310
2.2	.7889	12.428	15.861	28.289
2.3	.7547	11.191	13.683	24.874
2.4	.7233	10.085	11.826	21.911
2.5	.6943	9.173	10.343	19.517
2.6	.6676	8.347	9.058	17.405
2.7	.6429	7.609	7.961	15.566
2.8	.6199	6.995	7.065	14.059
2.9	.5985	6.387	6.235	12.622
3.0	.5785	5.877	5.548	11.425
3.1	.5600	5.430	4.968	10.398
3.2	.5424	5.041	4.473	9.511
3.3	.5259	4.667	4.017	8.681
3.4	.5105	4.327	3.619	7.946
3.5	.4959	4.023	3.273	7.296
3.6	.4822	3.756	2.972	6.730
3.7	.4692	3.510	2.704	6.217
3.8	.4569	3.279	2.461	5.743
3.9	.4451	3.042	2.245	5.314
4.0	.4339	2.881	2.057	4.938
4.1	.4234	2.707	1.887	4.594
4.2	.4133	2.543	1.732	4.275
4.3	.4037	2.400	1.598	3.998
4.4	.3945	2.261	1.470	3.731
4.5	.3857	2.133	1.361	3.494
4.6	.3774	2.018	1.258	3.276
4.7	.3694	1.908	1.164	3.072
4.8	.3616	1.799	1.076	2.875
4.9	.3543	1.717	1.006	2.723
5.0	.3472	1.623	0.933	2.556
5.5	.3156	1.267	.622	1.929

** The writer is indebted to Professor S. J. M. Allen who has obligingly supplied him with the data for oxygen contained in Fig. (1) as well as with new results for lead, and considerable other data on tin and silver which are presented herein.

TABLE IV. Mass-absorption coefficient of the L shell for lead, Pb (82), $\lambda_2=0.6027\text{\AA}$.

λ_2/λ	$\lambda(\text{\AA})$	$(\tau/\rho)_{L_I}$	$(\tau/\rho)_{L_{II}L_{III}}$	$(\tau/\rho)_L$
1.55	0.3889	5.505	9.895	15.400
1.65	.3653	4.797	8.098	12.895
1.75	.3444	4.197	6.687	10.884
1.85	.3258	3.686	5.566	9.252
1.90	.3172	3.478	5.117	8.595
1.95	.3091	3.286	4.697	7.983
2.0	.3013	3.088	4.324	7.412
2.1	.2870	2.758	3.683	6.441
2.2	.2739	2.478	3.162	5.639
2.3	.2620	2.231	2.728	4.959
2.4	.2511	2.010	2.358	4.368
2.5	.2411	1.829	2.062	3.891
2.6	.2318	1.664	1.806	3.470
2.7	.2232	1.517	1.587	3.103
2.8	.2152	1.394	1.408	2.803
2.9	.2078	1.273	1.243	2.516
3.0	.2009	1.171	1.106	2.278
3.1	.1944	1.082	0.990	2.073
3.2	.1883	1.005	.891	1.896
3.3	.1826	0.930	.801	1.731
3.4	.1772	.863	.722	1.584
3.5	.1722	.802	.652	1.454
3.6	.1674	.749	.593	1.341
3.7	.1629	.700	.539	1.239
3.8	.1586	.654	.491	1.145
3.9	.1545	.612	.448	1.060
4.0	.1507	.574	.410	0.984
4.1	.1470	.540	.376	.916
4.2	.1435	.507	.345	.853
4.3	.1402	.479	.319	.798
4.4	.1370	.450	.293	.743
4.5	.1339	.426	.271	.697
4.6	.1310	.402	.251	.653
4.7	.1282	.380	.232	.612
4.8	.1255	.359	.215	.574
4.9	.1230	.342	.200	.542
5.0	.1205	.323	.186	.509
5.5	.1096	.252	.132	.384

TABLE V. Comparison of the mass-absorption coefficients with experiment, for wave-lengths shorter than the critical wave-length of the K shell. The empirical data were sent to the author by S. J. M. Allen. The values (σ/ρ) est in the sixth column are estimated values of the scattering, according to Allen. The values for lead indicated by the bracket are recent ones obtained by J. Read (Proc. Roy. Soc. A152, 402 (1935)). His estimates of σ/ρ were taken from the Klein-Nishina formula, and consequently they neglect coherent scattering. Since the mean atomic radius for lead is of the same order (0.06\AA) as the wave-length one would expect σ/ρ to be larger than Read's values in this region (and probably smaller than Allen's). See below Fig. 3 for the effect of the M shell.

$\lambda(\text{\AA})$	λ_1/λ	$(\tau/\rho)_K$ Eq. (8)	$(\tau/\rho)_L$ Eq. (11, 12)	(σ/ρ) Obs.	(σ/ρ) Est.	(τ/ρ) Est.	$(\tau/\rho)_{K+L}$ Calc.
Sn (50), $\lambda_1=0.3693\text{\AA}$; $A=119$; $\lambda_K=0.424\text{\AA}$							
0.424	0.8710	37.21	4.62	46.6	1.05	45.6	41.83
.417	.8856	35.97	4.43	44.7	1.0	43.7	40.40
.400	.9232	31.96	3.89	39.8	0.99	38.8	35.65
.380	.9718	27.90	3.34	34.3	.98	33.3	31.24
.370	.9981	25.99	3.09	32.2	.97	31.2	29.08
.331	1.1158	19.26	2.24	23.8	.94	22.9	21.50
.300	1.2310	14.73	1.62	18.10	.90	17.20	16.35
.260	1.4204	10.17	1.10	12.40	.86	11.54	11.27
.220	1.679	6.199	0.67	8.00	.82	7.18	6.87
.200	1.8465	4.735	.50	6.12	.78	5.34	5.235
Pb (82), $\lambda_1=0.1367\text{\AA}$; $A=207$; $\lambda_K=0.1407$							
0.1407	0.9716	5.94	0.81	7.75	0.91	6.84	6.75
.130	1.0516	4.806	.64	6.45	1.00	5.45	5.45
.113	1.2097	3.286	.43	4.70	1.04	3.66	3.72
.098	1.3949	2.217	.28	3.50	1.06	2.44	2.50
.080	1.7088	1.255	.15	2.46	1.10	1.36	1.41
.072	1.8986	0.9300	.11	2.04	1.05	0.99	1.04
.064	2.1359	.6644	.078	1.63	0.92	.71	0.74
.050	2.7340	.3260	.037	1.00	.67	.33	.37
.051	2.6804	.3452	.039	0.642	.089	.553	.38
.048	2.8479	.2896	.033	.554	.086	.468	.32
.045	3.0378	.2401	.027	.475	.083	.392	.27
.042	3.2548	.1963	.021	.407	.082	.325	.22

The formula for δ_K may also be open to question when applied to heavy elements, for the reason that relativity effects may then be important. Although such effects are shown later to leave τ_K unaffected at the K limit, an electron leaving the L shell with an energy corresponding to ν_K has the velocity $v \sim 3^1/2 \alpha c/2$, which may be as high as one-half the velocity of light for heavy elements. Since the correction to τ_L due to this effect may be $\sim (v/c)^2$, Eq. (14) must be considered uncertain to some extent until the effect of relativity on τ_L has been studied. In this connection, a somewhat more detailed treatment of the problem at ν_L would result. For example, 2p electrons, as is well known according to the Dirac equation, divide into two groups of three $2p_{1/2}(L_{II})$ and three $2p_{3/2}(L_{III})$ electrons. Electrons of the L_{II} group are more strongly bound than the L_{III} electrons, by an amount $Z^2(\alpha^2/16)(1 + \frac{5}{8}\alpha^2 + \dots)$, in Rydberg units. This separation, which is fractionally $\sim \alpha^2/4$ of ν_L , agrees with that observed if Z is replaced by $Z-s$, where the value of s is practically constant for all elements (≈ 3.5), and is not far from Slater's value for 2s, 2p electrons (4.15). The rather smaller $L_I L_{II}$ splitting is accounted for in a different way from the $L_{II} L_{III}$ splitting. Its magnitude may be obtained, in the theory already given, by writing $s \approx 4$ for p electrons, $s=3$ for s electrons.

8. Direction of emitted photoelectrons²³

(a) The K shell

When all relativistic effects are neglected, i.e., momentum of the light quantum, change of photoelectronic mass with velocity, and effects due to deep binding (large Z) of the electron initially, Eq. (5) gives for the K shell²⁴

$$\Psi_{1,0} \Psi_{1,0}^* \sim \sin^2 \theta \cos^2 \varphi = \cos^2 \Theta, \quad (15)$$

²³ The experimental literature on angle distribution includes: F. W. Bubb, Phys. Rev. 23, 137 (1924); F. Kirchner, Ann. d. Physik 83, 521 (1927); P. Auger, J. d. physique 8, 85 (1927). These workers were mainly concerned with studies near the series limit, where the distribution is given by $\sin^2 \theta \cos^2 \varphi$. Work on the advance of the maximum was carried on by: W. Bothe, Zeits. f. Physik 26, 59 (1924) (Geiger counter); Williams, Nuttal and Barlow, Proc. Roy. Soc. A121, 611 (1928); P. Auger, Comptes rendus 186, 758 (1928); 187, 141 (1928); 188, 447 (1929), (Wilson Cloud Chamber); Auger and Meyer, Comptes rendus 192, 672 (1931); Lutz, Ann. d. Physik 9, 853 (1931); see Compton and Allison, reference 10, p. 564 for other references.

²⁴ See A. Sommerfeld, reference 13, p. 182.

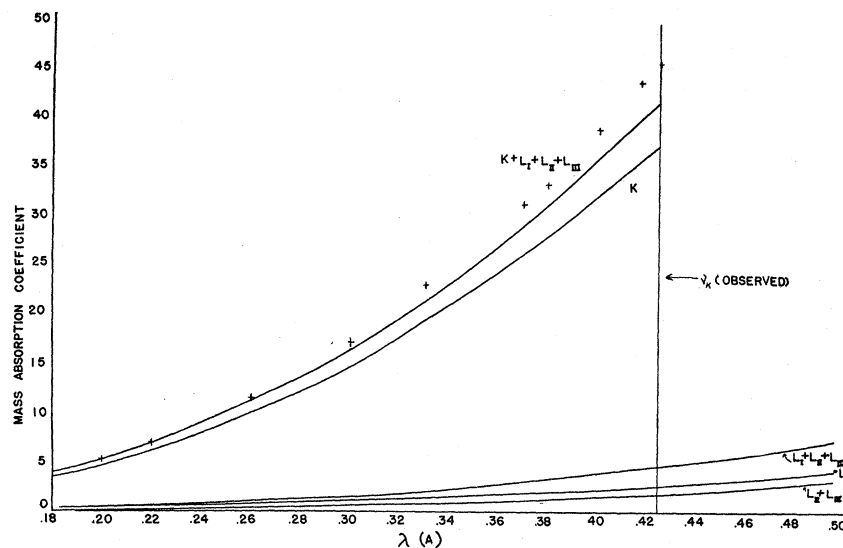


FIG. 2. Theoretical curves of the K and L mass-absorption coefficients τ/ρ for tin, in the region $\lambda < \lambda_K$. The experimental points were supplied by S. J. M. Allen. They represent a weighted mean of the results of several observers, which has been corrected for scattering. The points on this graph correspond to Table V. The wavelength is in Å.U.

where θ is the angle between the velocity v of the photoelectron and the electric vector of the incident light. The angle θ is the angle between v and the propagation vector of the light. For an unpolarized beam the distribution is proportional to $\sin^2 \theta$. If the momentum $h\nu/c$ of the light quantum is taken into account in first order, but all other relativistic effects are ignored, the Schrödinger theory may be used to find the distribution in angle, which is given by

$$\Psi_{1,0}\Psi_{1,0}^* \sim \sin^2 \theta \cos^2 \varphi (1 + 4\beta \cos \theta), \quad (15')$$

where $\beta = v/c$. It is mathematically consistent to compute this effect with nonrelativistic wave functions, because all other relativistic effects enter only through integer powers of $(v/c)^2$.

This result follows from a straightforward application of the theory, as shown by Sommerfeld and Schur.⁷ The term $4\beta \cos \theta$, which favors emission in the forward direction, is of course connected with the radiation pressure. A calculation of the asymmetry in distribution here contained, by elementary considerations, does not

lead to the above term, according to Sommerfeld, except in a qualitative sense.²⁵

The agreement between experiment and theory, in connection with the results of this section, is generally rather good.

(b) The L and higher shells

The angular distribution, $\sin^2 \theta$, just given for the K shell, which holds when all v/c effects are neglected, also applies to any s electron, regardless of which shell it may occupy. This is true because an electron initially in an s state ($l=0$) has zero angular momentum along the z axis ($m=0$), and can consequently undergo only transitions in which m changes to ± 1 .

For a p electron however, this is not the case. Transitions may in this instance occur to states characterized by $m=0$, which circumstance gives rise to an isotropic term in the angular distribution. This term has been found to occur. In fact Bethe has found that the angular distribution for

²⁵ See also H. R. Hulme, Proc. Roy. Soc. A133, 391 (1931).

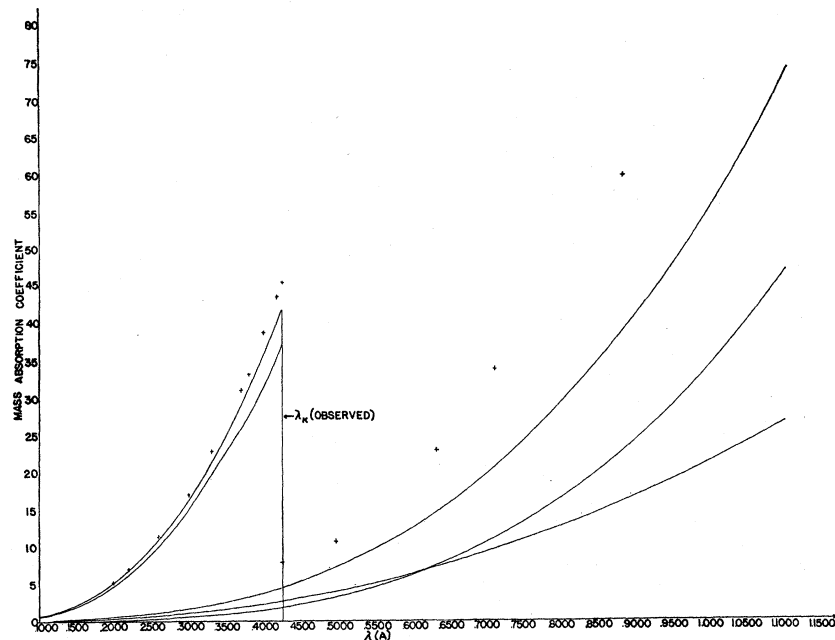


FIG. 3. Theoretical curves of the *K* and *L* mass-absorption coefficients for tin τ_L/ρ , according to Table III, on a different scale from Fig. 2. The experimental points for $\lambda < \lambda_k$ have been corrected for scattering, according to S. J. M. Allen, by an amount $\sigma/\rho \sim 1$. The points for $\lambda > \lambda_k$ contain the scattering, which is fractionally small, however, in this region.

Note added in proof: For computing absorption by the 18 electrons of the *M* shell the formula

$$\tau_M = N_0 \frac{h a_0}{mc} \frac{2^9 \pi}{3} \cdot 3^3 \frac{(\nu_3/\nu)^4}{(Z-s_3)^2} \left(1 + 8 \frac{\nu_3}{\nu}\right) \cdot \left\{ 27 + 136 \frac{\nu_3}{\nu} + 208 \left(\frac{\nu_3}{\nu}\right)^2 + 96 \left(\frac{\nu_3}{\nu}\right)^3 \right\} \frac{\exp[-4n_3 \tan^{-1} 3/n_3]}{1 - e^{-2\pi n_3}}$$

was derived. Here $n_3 = 3(\nu/\nu_3 - 1)^{-1/2}$, where $\nu_3 = (Z-s_3)^2/9Ry$. This term, added to τ_L , accounts rather well for the absorption observed in the region $\lambda > \lambda_k$.

any (n, l) shell may be written as $\alpha + \beta \sin^2 \theta \cos^2 \varphi$, where α and β are given in terms of radial integrals corresponding to the transitions $(n, l \rightarrow E, l \pm 1)$. In the above treatment β is positive. The direction of maximum emission is consequently in the direction of the electric vector.

Schur²⁶ has carried out the calculations for the $2p$ shell. He gives

$$\Psi_{2, 1} \Psi_{2, 1}^* \sim \nu + 2(Z-s)^2 \sin^2 \theta \cos^2 \varphi.$$

²⁶ Schur, reference 7. See the article by Bethe, reference 7, p. 484.

For the entire *L* shell he also gives the result

$$\Psi_L \Psi_L^* \sim \sin^2 \theta \cos^2 \varphi + \frac{(Z-s)^2}{4\nu + 3(Z-s)^2} \left(1 + 2 \frac{(Z-s)^2}{\nu} \sin^2 \theta \cos^2 \varphi\right),$$

where ν is to be expressed in Rydberg units.

RESULTS OF RELATIVISTIC THEORY

9. First-order relativity corrections to τ_K

Relativistic effects may enter the discussion of absorption processes in several ways. Physically

they are usually referred to as change of mass with velocity, electron spin, and radiation pressure or retardation which enters through $h\nu/c$.

We consider an electron, described by the Dirac equation, to be in a central field Ze/r . The most deeply bound state turns out to have the energy $E_0 = mc^2(1 - \alpha^2)^{1/2}$, where $\alpha = Z/137$ is the fine structure constant times the atomic number, as previously defined. The physical interpretation of α , for this bound state, may be arrived at from a consideration of the average potential and kinetic energies. One finds for these quantities

$$V^* = -mc^2\alpha^2/(1 - \alpha^2)^{1/2},$$

$$T^* = mc^2\alpha^2/(1 - \alpha^2)^{1/2}[1 + (1 - \alpha^2)^{1/2}],$$

and hence $-V^*/T^* = 1 + (1 - \alpha^2)^{1/2}$ instead of the value two, which obtains in nonrelativistic mechanics. From the expression above, one sees α plays the role of v_0/c for the bound state, where v_0 is equal to the orbital velocity. This corresponds exactly with the meaning ascribed to α in Section 5.

If we let p designate the momentum, in units of mc , for states of continuous energy E , to which transitions occur, then $E = mc^2(1 + p^2)^{1/2}$, and Eq. (1) gives for the relation between $h\nu$, E_0 and E , the equation

$$h\nu + mc^2(1 - \alpha^2)^{1/2} = mc^2(1 + p^2)^{1/2}. \quad (16)$$

This reduces at once to the equation

$$v/v_1 = [1 + (v/v_0)^2],$$

or Eq. (7) of Section 4, when both α^2 and p^2 may be considered small. The parameters α and p consequently measure the importance of relativistic effects; but whereas frequencies may always be used so that $p \ll 1$ for any given element, the size of α is determined when the atomic number is fixed. Hence, in consideration of absorption by the K electrons of a heavy element, relativistic effects would always seem to be present, since $\alpha \cong 0.6$ for Pb 82, and is proportionately large for other heavy elements. However, although the wave functions do exhibit a

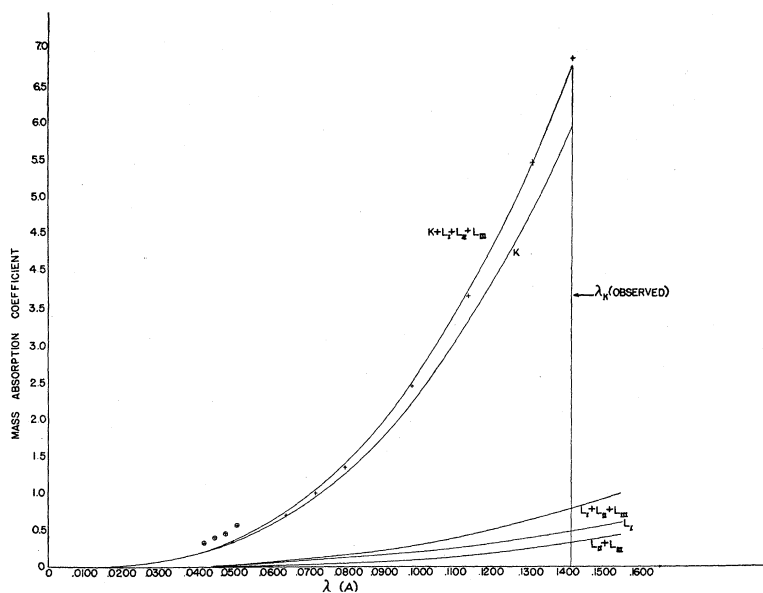


FIG. 4. Theoretical curves of the K and L mass-absorption coefficients τ/ρ for lead. + according to S. J. M. Allen, have been corrected for scattering by an amount $\sigma/\rho \sim 1$. That is, according to column 6 of Table V. \oplus according to J. Read (Proc. Roy. Soc. 152, 402 (1935)). These points were corrected by Read according to the Klein-Nishina formula ($\sigma/\rho \sim 0.085$). The coherent scattering indicates this correction should be raised somewhat.

marked and complicated effect depending on α , it turns out that τ_K itself is practically independent of α , for all frequencies ($\nu \leq 2\nu_K$) such that $p \leq 0(\alpha)$. Actual calculation also shows that the correction in p^2 , although complicated in form, contributes only a few tenths percent to τ_K , for frequencies up to twice the critical frequency. Since a frequency of $2\nu_K$, for example, ejects an electron with a momentum given by $p = \alpha \approx 0.6$ for lead, it may be considered somewhat surprising that no relativistic effects are important in this region. In fact, if the formula of Eq. (8) is used to compute the CSA of RaC ($Z=84$) for $h\nu/mc^2 = 0.692$, which corresponds to a frequency 3.7 times ν_K , one finds

$$\tau_K/N_0 = \frac{1.25 \times 10^{-17}}{Z^2} (\nu_1/\nu)^4 [1 + (4/3)(\nu/\nu_1 - 1)] \approx 4.4 \times 10^{-23} \text{ cm}^2.$$

This is to be compared with the correct value of the CSA for this case which is $6.0 \times 10^{-23} \text{ cm}^2$; according to the numerical calculation of Hulme

and his collaborators.²⁷ In view of the fact that this is in a region beyond which Eq. (8) is even here considered to be valid (for this frequency, $p \sim 1.6$, $\beta \sim 0.84!$) the discrepancy of 25 percent is satisfactory enough.

These results also seem to indicate a more gradual change in the frequency dependence of τ_K , than the theory has heretofore been thought by many writers to predict, at least for the heavy elements. For, as we have seen, starting from the series limit, $\tau_K \sim \nu^{-2.7}$. The exponent of ν is not much different for ν near $2\nu_K$; and, as we have just seen, for $\nu \sim 4\nu_K$, Eq. (8) agrees fairly well with the correct theoretical result, which is known to have a somewhat slower dependence on frequency in this region. (See Fig. 6.) One supposes therefore, since the formulas for very small and for very large frequencies join so well in the case discussed, that the exponent of ν is theoretically always less than about 3, and that τ_K

²⁷ Hulme, McDougall, Buckingham, Fowler, Proc. Roy. Soc. A149, 131 (1935).

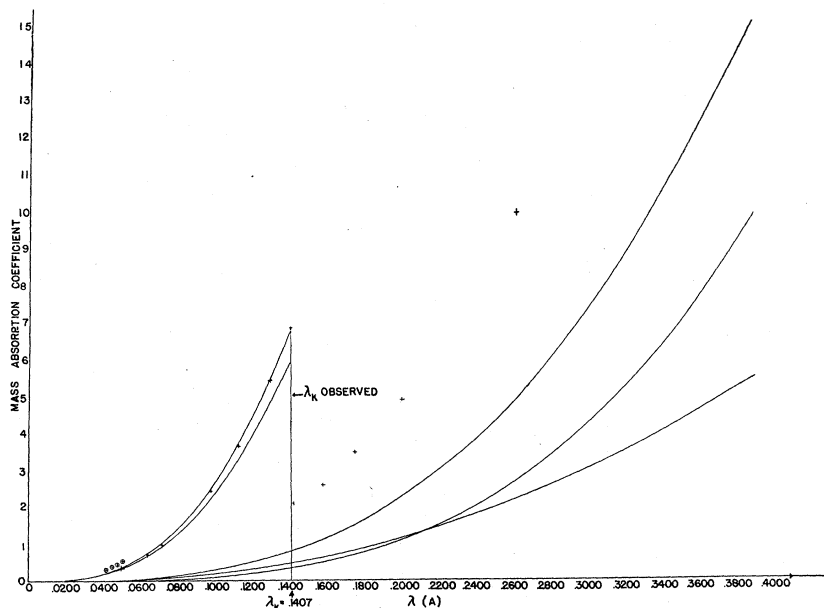


FIG. 5. Theoretical curves of the K and L mass-absorption coefficients for lead, τ_L/ρ , according to Table IV, on a different scale from Fig. 4. The points for $\lambda > \lambda_k$ obs. contain the scattering ($\sigma/\rho \sim 1$).

does not fall off as fast as $\nu^{-3.5}$, except for the lightest elements. This merely means that for heavy elements it is impossible to get far away from the K limit without being in the region where $h\nu \sim mc^2$. For light atoms however, there is

still a region where the wave-length exponent is greater than 3. This region lies between $\nu \sim 2\nu_K$ and $\nu \sim 2mc^2/h$. Hulme has calculated²⁵ the exponent of λ , under the condition $Z/137 \ll 1$, in the part of this region near $\nu = mc^2/h$, with the results:

λ	6.08×10^{-11} cm	1.22×10^{-10} cm	2.43×10^{-10} cm	6.08×10^{-10} cm	9.73×10^{-10} cm
$I \times Z^{-5}$	4.89×10^{-34}	1.87×10^{-33}	9.92×10^{-33}	1.68×10^{-31}	8.01×10^{-31}
n	1.9	2.4	3.1	3.3	

The coefficient of absorption I is written

$$I \sim Z^5 \lambda^n.$$

*The value of n under each wave-length expresses the mean variation of I between that wave-length and the one following.

10. Screening

The discussion of screening already given, applies equally well in its essential details to the results of section 9. The only difference lies in the relativistic ionization energy, which for a single bound electron is

$$h\nu_0 = mc^2 [1 - (1 - \alpha^2)^{1/2}] \cong Z^2 (1 + \alpha^2/4) Ry.$$

This is an increase over the Schrödinger value $Z^2 Ry$, and the change is such as to give good agreement with observed ionizing frequencies, when the screening constant $V_0 = (3.6Z^{4/3} - 3.3Z - 4Z^3) Ry$ of Eq. (10) is introduced. This modification gives for the ionizing frequencies, $\nu_0'' \cong Z^2 (1 + \alpha^2/4) - V_0$, which is an increase of $Z^2 \alpha^2/4$ over those computed from Eq. (10'). Ionization frequencies computed with it agree with those observed to within 4 percent for all elements from Fe 26 to U 92. The agreement is even better, being a deficit of only 2 percent, for all elements from Ag 47 to U 92. Even this small deficit of 2 percent is removed when the atomic system, with the potential given by Eq. (9), is correctly quantized. For, in the work of Roess and Kennard, this was done for Sn 50, and their result for ν_0'' exceeded $\nu_K(\text{obs})$ by only 0.3 percent.

In this way we see that a crude, but consistent, screening model may be employed to predict the ionization frequency of a K electron. When this model is applied to a Dirac electron the results

agree very satisfactorily with experiment. In Figs. (3-5) are plotted the mass-absorption coefficients for the two elements Pb 82 and Sn 50, the observed and theoretical ionization frequencies agreeing in both cases, in conformance with the remarks of this section.

In connection with apparent absorption due to scattering, for which the experimental points in these figures were partially corrected, a few remarks on the theoretical side may be proper. According to the Thomson scattering formula, one finds the mass scattering coefficient, *per atom*, to be given by $(\sigma/\rho)_{\text{atom}} \sim 0.4Z/A$, or $(\sigma/\rho)_{\text{atom}} \sim 0.17$. A rough calculation with the Fermi-Thomas field, which takes account of the fact that at least some of the atomic electrons scatter coherently, results in the formula $(\sigma/\rho)_{\text{atom}} \sim 0.17Z^3$. However, for $\nu \sim 2\nu_K$ in the case of Pb, $h\nu/mc^2 \sim \frac{1}{2}$, and this result must still be corrected by terms in $(h\nu/mc^2)$ entering the Klein-Nishina scattering formula. The first-order correction gives $(\sigma/\rho)_{\text{atom}} \sim 0.17Z^3 (1 - 2h\nu/mc^2)$, which appreciably diminishes the result where $h\nu/mc^2$ was neglected. When the higher orders are included too, we find for Pb, $(\sigma/\rho)_{\text{atom}} \sim 0.34$ at $\nu = 2\nu_K$, which is less than the scattering correction for a lighter element, near its absorption limit.

11. τ_K and τ_L in the region $h\nu/mc^2 \gg 1$

(a) The K shell

The absorption of very short wave-length radiation presents features very different from those in the problems already discussed. The chief difference may be described in terms of the coordinate system in which the wave equation is separated. For the case of an electron in a Coulomb field, the only system in which the Dirac equation is known to be separable is space polar coordinates. In this system, for energies $E > mc^2$, there are an infinite number of wave functions corresponding to a given energy, each one corresponding to a different orbital angular momentum l . In the previous sections, transitions

from the normal state, under perturbation by the light wave, were possible only to final states $l=1$, or at most $l=2$ (section 9). This came about because the wave-length of the radiation was long, or at least not small, compared to the first Bohr radius, a_0/Z . One could then expand the retardation factor $\exp i(2\pi\nu\cdot\mathbf{r}/c)$, and neglect corrections $0(2\pi\nu a_0/c)^2 \approx \alpha^2/4$ at the K absorption limit. Each higher term in the expansion of the retardation factor may be thought of as inducing transitions to final states typified by larger values of l . For frequencies so large that $h\nu/mc^2 \sim 1$, the correction term above would be $\sim (1/\alpha)^2 \gg 1$, indicating a completely different analytic character for the CSA over its behavior near the K limit. It is found actually that many terms in l contribute to the CSA when $h\nu/mc^2$ is large, the number of such terms being proportional to $h\nu/mc^2$. In fact, the behavior of these terms when $h\nu/mc^2 \gg 1$ is approximately given by the expression $\beta^3 \exp(-2lmc^2/h\nu)$, which must be summed over all l from zero to infinity. The actual problem is extremely involved in a mathematical way, due primarily to the impossibility of solving the Dirac equation in a coordinate system which embodies the symmetry (axial) of the physical problem.

Since the photoelectron may be considered to have an energy $E \gg mc^2$, when $h\nu \gg mc^2$, it would at first sight seem plausible to neglect the effect of the nucleus on it. This neglect would allow one to describe the final states in rectangular coordinates, where they are particularly simple, and contain the desired symmetry. The normal state could then be treated according to the strict Dirac equation with a Coulomb field. Such a heuristic model, however, while it leads to the correct dependence on atomic number (Z^5) and on the frequency ($1/\nu$), gives the wrong constant of proportionality.²⁸ In addition, the constant it does give, does not reduce to the correct one in the limit $\alpha \rightarrow 0$! The objection to any such model is that the errors involved in its use are uncontrolled.

Another approach to the problem was made by Sauter.²⁹ Sauter actually performed the summations over the angular momenta already dis-

cussed, under the two restrictions $h\nu \gg Z^2 Ry$, and $Z/137 \ll 1$. The first of these approximations is automatically contained in the second one when ν is large. Sauter's formula may be written

$$\tau_K = N_0 \frac{8\nu_1^3 c^2}{\pi\nu^5 Z} \frac{\beta^3}{(1-\beta^2)^{3/2}} \left[\frac{4}{3} + \frac{1-2(1-\beta^2)^{1/2}}{(1-\beta^2)^{3/2} [1+(1-\beta^2)^{1/2}]} \right] \times \left(1 - \frac{1-\beta^2}{2\beta} \log \frac{1+\beta}{1-\beta} \right),$$

where $\beta = v/c$, and is given by

$$h\nu/mc^2 + 1 = (1-\beta^2)^{-1/2}.$$

From this result

$$\tau_K = 2^7 e^2 N_0 \nu_1^{5/2} / 3mc\nu^{7/2}, \quad \text{when } \beta^2 \ll 1$$

$$\tau_K = N_0 (\alpha_0^5 Z^5 \lambda / \pi) (h/mc) = 1.16 \times 10^{-28} \lambda Z^5 N_0$$

when $\beta \sim 1$. The principal objection to the use of Sauter's formula, as we shall see, is that the effect of the approximation in α when ν is large, cannot be ignored except for the lightest elements. Even for Fe 26 this correction amounts to about 20 percent for frequencies truly far from the K limit; while for Pb 82 his result would be more than twice too large.

The problem of summing over l without making a critical neglect in α was successfully handled for the case of large frequencies, by a change in the order of the summation over l with certain integrations.³⁰ This treatment is discussed in Section (20). In the limit of very large frequencies it leads to the result

$$\tau_K = N_0 \frac{4\pi a_0^2 \alpha_0^8 Z^5 (mc^2/h\nu)}{\alpha^2 \alpha^2 e^{\alpha(\pi-2\alpha)}}, \quad (17)$$

$$\alpha_0 = 1/137.3, \quad \alpha = \alpha_0 Z,$$

$$a_0 = h^2 / 4\pi^2 m e^2.$$

Now to obtain a formula applicable for somewhat smaller, though still large frequencies we write finally

$$\tau_K = N_0 \frac{4\pi a_0^2 \alpha_0^8 Z^5 (mc^2/h\nu)}{\alpha^2 \alpha^2 e^{\alpha(\pi-2\alpha)}} \cdot R$$

$$= N_0 \frac{1.16 \times 10^{-28} Z^5 \lambda}{\alpha^2 \alpha^2 e^{\alpha(\pi-2\alpha)}} \cdot R, \quad (18)$$

²⁸ H. Hall and J. R. Oppenheimer, Phys. Rev. **38**, 71 (1931).

²⁹ F. Sauter, Ann. d. Physik **9**, 217 (1931).

³⁰ H. Hall, Phys. Rev. **45**, 620 (1934).

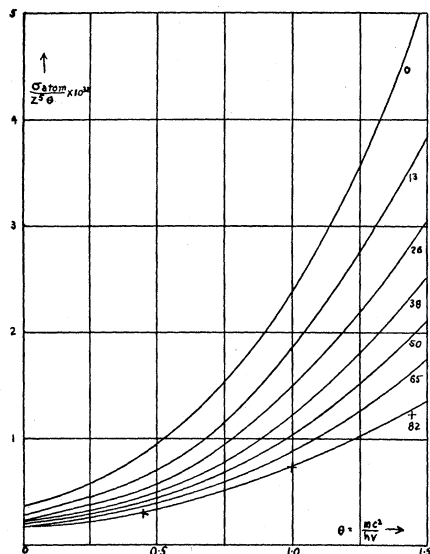


FIG. 6. Absorption coefficients for various atoms. Here the absorption coefficient per atom (σ_{atom} in Hulme's notation) is taken to be 5/4 of the absorption coefficient for the K shell.

where λ is in cm. From Sauter's formula we find, in our notation,

$$R = \left(\frac{p^3 \epsilon}{q^4} \right) \left[\frac{4}{3\epsilon} + \frac{\epsilon - 2}{\epsilon + 1} \left(1 - \frac{1}{2\epsilon p} \log \frac{\epsilon + p}{\epsilon - p} \right) \right],$$

where p and ϵ are the electron's momentum and energy in units of mc and mc^2 , respectively, and $q = h\nu/mc^2$. These quantities are related by the conservation law Eq. (16).

$$\begin{aligned} \epsilon &= q + (1 - \alpha^2)^{1/2} \cong q + 1, \\ p &= (\epsilon^2 - 1)^{1/2}. \end{aligned}$$

Formula (18) is approximately correct except for the neglect of terms α^2/ϵ . The error in it, as $\epsilon \rightarrow \infty$, (i.e., in Eq. (17)) is only a few percent for Pb, and is smaller for smaller atomic numbers.

Eq. (18) may now be used as a continuation of Eq. (6), after the latter has ceased to apply. For example, in the case of Pb for $\nu \sim 4\nu_K$, these two formulas agree to within about 20 percent, τ_K from Eq. (6) being about 15 percent smaller than the correct value as calculated by Hulme. Considering that both of these equations are here

applied outside of their respective regions of validity, the agreement is satisfactory.

The relativistic theory of absorption by a hydrogenic atom has been applied rigorously in reference 27 to compute τ_K for several different elements. The calculations were done for $h\nu/mc^2$ between 0.694 and 2.21. For frequencies greater than the latter point, Hulme used our Eq. (18) to supplement his curves. The results are shown in Fig. 6. The atomic absorption is here taken to be 5/4 that of the K shell. In Hulme's notation σ_{atom} is the atomic CSA, so that* $\sigma_{atom} = (5/4) \times (\tau/N_0)_K$. Because τ_K has the asymptotic form given by Eq. (17) Hulme plots $\sigma_{atom} \cdot Z^{-5}(h\nu/mc^2)$ against $mc^2/h\nu$. The results indicated in Fig. 7 were also found by Hulme and his collaborators. Here is shown the strong dependence of τ_K , on atomic number when the frequency is kept fixed, for two different frequencies. These numerical results for the frequency range mentioned show that Eq. (18) may be used with fair accuracy, even though it could hardly have been expected to apply for the lower frequencies.³¹ Of course when applying it here, ambiguities arise because terms of the type α^2/ϵ enter into the calculation of the correction factor R , whereas terms of this type were neglected in other parts of the derivation. This point is mentioned in the theoretical Section 20. Suffice it to say that the considerations of that section could not alter the agreement with the correct calculation for reasonably large frequencies.

(b) The L shell

The use of the factor 5/4 to obtain σ_{atom} from σ_K (our τ_K), is based on certain experimental data for a limited frequency range. Approximately the same factor may be used for all large frequencies, as may be seen from a study of the L shell. It turns out that the relatively rapid decay of $\tau_{LII} + \tau_{LIII}$ far from the ionization limit, as suggested in Section 7, persists in the relativistic theory, where most of the L absorption

* Hulme takes the ratio $\sigma_{atom} = (5/4)\sigma_K$ from Rutherford, Chadwick and Ellis, *Radiations from Radioactive Substances*, p. 464.

³¹ In reference 26 Hulme gives a table for two different frequencies and three different elements, comparing Eq. (18) with his data. For the large frequency, $h\nu/mc^2 = 2.21$ the agreement is better than 7 percent in all cases, and for the smaller one, $h\nu/mc^2 = 0.694$, it is better than 12 percent throughout.

occurs in the L_1 shell ($2S_{1/2}$ electrons). Only here the ratio between τ_L and τ_K , is no longer given by $(\frac{1}{2})^3 = \frac{1}{8}$, but is modified by effects in α^2 , so that for very heavy elements the ratio is in the neighborhood of 1/5 or 1/4.

Fig. 6, in addition to the different curves, contains three experimental points for Pb, which L. H. Gray³² previously had found, and incorporated into an empirical curve. The agreement is seen to be good. For purposes of comparison, Gray's empirical formula is given here. Gray gave for the atomic *linear* absorption coefficient, τ_{Pb} , the relation

$$\log_{10} \tau_{Pb} = 3.6505 + 1.0 \log_{10} \lambda + 0.480 (\log_{10} \lambda)^2,$$

which may be written in the form

$$\tau_{Pb} = 4.472 \times 10^{-3} \lambda^{1+0.48 \log_{10} \lambda}.$$

In these equations³³ λ is to be expressed in X.U. To obtain the CSA, τ_{Pb} must be divided by the number of atoms, N_0 , per cm^3 , where $N_0 = 3.32 \times 10^{22} \text{ cm}^{-3}$

$$(\tau_{Pb})/N_0 = 1.35 \times 10^{-25} \lambda^{1+0.48 \log_{10} \lambda} \text{ cm}^2.$$

12. Angular distribution from the K shell

The radial photoelectric current is not proportional to $\Psi\Psi^*$, but to $\Psi\alpha_4\Psi^*$ in the relativistic theory. This point was anticipated in Section 3. Using the Dirac four-component wave function we may write

$$\begin{aligned} \Psi\Psi^* &= \Psi_1\Psi_1^* + \Psi_2\Psi_2^* + \Psi_3\Psi_3^* + \Psi_4\Psi_4^*, \\ \Psi\alpha_4\Psi^* &= \Psi_1\Psi_1^* + \Psi_2\Psi_2^* - \Psi_3\Psi_3^* - \Psi_4\Psi_4^*. \end{aligned}$$

The difference between these two expressions is really negligible for small photoelectron velocities. Here the ratio of small to large components of Ψ is proportional to v/c , and consequently the above expressions differ only by terms in $(v/c)^2$. Even in this case however the angle distribution will differ slightly from the distribution $\sin^2 \theta \cos^2 \varphi$, because of relativistic effects which enter through α^2 (i.e., from retardation, and effects of the Coulomb field in both initial and final states). First, neglecting all corrections in v/c , the alteration arising from α^2 in the distribution function J is given by the result (see Section 22).

³² L. H. Gray, Proc. Camb. Phil. Soc. 27, 103 (1931).

³³ In reference 30 where $(\tau_{Pb})/N_0$ is given in this form, the first numerical factor was written in error as 1.67 instead of 1.35.

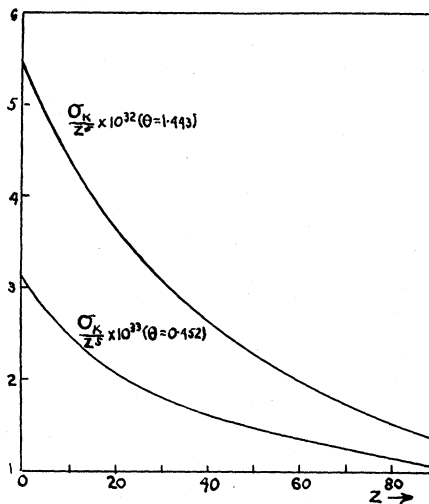


FIG. 7. The absorption coefficient as a function of atomic number for two different frequencies. ($\theta = mc^2/h\nu$).

$$J \sim \sin^2 \theta \cos^2 \varphi [1 + (0.280 \cos^2 \theta - 0.056) \alpha^2].$$

Since $\cos \theta$ enters only in the second power, there is no change due to α^2 in the angle of maximum emission, which is physically reasonable. The correction term is zero for $\cos^2 \theta = 1/5$, or $\theta = 67^\circ$; it is positive for smaller angles, and negative for larger ones. For $\theta = 30^\circ$ the correction is only $0.15 \alpha^2$, and in fact is always less than $0.22 \alpha^2$.

When the first power of $\beta = v/c$ is retained one finds:

$$J \sim \sin^2 \theta \cos^2 \varphi \times [1 + (0.280 \cos^2 \theta - 0.056) \alpha^2 + 4\beta \cos \theta]$$

in agreement with the nonrelativistic formula when $\alpha^2 \rightarrow 0$.

Now when β^2 is not to be neglected, the so-called "small components" Ψ_1, Ψ_2 contribute equally with the others. For the case $Z/137 \ll 1$ Sauter has given the distribution

$$J \sim \frac{\sin^2 \theta}{(1 - \beta \cos \theta)^4} \left[\cos^2 \varphi \{ (1 - \beta^2)^{\frac{1}{2}} - \frac{1}{2} (1 - (1 - \beta^2)^{\frac{1}{2}}) (1 - \beta \cos \theta) \} + \frac{1}{4} \frac{(1 - (1 - \beta^2)^{\frac{1}{2}})^2}{1 - \beta^2} (1 - \beta \cos \theta) \right].$$

When $\beta^2 \ll 1$ this reduces at once to Eq. (15). For the extreme relativistic region where $\beta \sim 1$, however, the term independent of the polarization vector may be of importance. The physical interpretation of this effect, in terms of the electron, is not very evident.

A NUCLEAR APPLICATION

13. Photoelectric disintegration of the deuteron³⁴

The range of the interaction between a neutron and a proton has been shown by Wigner to be smaller than the ordinary nuclear radius, which is about $2Z^{1/3} \times 10^{-13}$ cm. The argument is based on a knowledge of the mass defects of He⁴ and H². Wigner assumes a neutron-proton interaction, which was studied by Eckart³⁵ and Epstein in other connections. Wigner's treatment essentially contains the assumption that the neutron-proton force may be represented as a function of the mutual separation of the two particles. Two arbitrary constants appear in this interaction, which correspond physically to the potential energy V_0 at zero separation, and the range r_0 over which the interaction is large. Wigner found the connection between V_0 and r_0 , for a fixed energy of binding, to be given roughly by the relation $V_0 \sim r_0^{-2}$, and this relation is not very sensitive to changes in the form of the interaction. Using variational methods Wigner then found that binding energies of about 2 Mev for the deuteron, and about 30 Mev for helium are possible, and consistent with the idea of a short range ($1.0 - 1.5 \times 10^{-13}$ cm) interaction between neutron and proton.

An important feature of the short range interaction, is the appearance of the wave function which describes the stable state (deuteron). The wave function spreads over a region which is determined almost solely by the binding energy, and hardly at all by the depth of the potential hole. In the limit of $r_0 \rightarrow 0$, that is, of an interaction which is infinitely large over an infinitesimal distance, the wave function is nevertheless large at distances as great as 5×10^{-13} cm, for reasonable binding energies. This circumstance allows an elementary application of the

³⁴ See Chadwick and Goldhaber, Proc. Roy. Soc. A151, 479 (1935); Bethe and Peierls, Proc. Roy. Soc. A148, 146 (1935); Massey and Mohr, Proc. Roy. Soc. A148, 206 (1935); E. Wigner, Phys. Rev. 43, 252 (1932).

³⁵ C. Eckart, Phys. Rev. 35, 1303 (1930).

ideas of quantum mechanics to be made. One may calculate the probability of deuteron disintegration by light quanta in particular, and with considerable certainty as long as the range of interaction may be considered small enough.

The work of Wigner shows that a potential box may be used to study the essential features of the deuteron problem. Bethe and Peierls have calculated the deuteron cross section according to the ideas outlined above, as have Massey and Mohr using an exponential interaction as well. Bethe and Peierls give for the deuteron CSA for gamma-rays:

$$\sigma = (he^2/6M'c)(8(\gamma-1)^3/W\gamma^3), \quad (19)$$

where W equals the binding energy of the deuteron, in ergs, and M' equals twice the reduced mass of neutron and proton. For W equal to 2.14 Mev, $h\nu = 2.62$ Mev, the CSA is

$$\sigma = 6.8 \times 10^{-28} \text{ cm}^2.$$

Chadwick and Goldhaber found experimentally a value for σ of 5×10^{-28} cm², which would seem to be in satisfactory agreement with the theoretical result, since they allow an uncertainty of a factor two.³⁶

In the light of the large uncertainty which enters experimentally, it would hardly seem necessary to improve the model of Bethe and Peierls. Nevertheless, a few definite statements may be made concerning such an improvement, and we wish to discuss some of them here. First of all, it can be said, the Bethe-Peierls result may be considered exact in the limit where the range r_0 of the interaction vanishes. Next, if the interaction be considered a constant, $-V_0$, out to a finite distance r_0 , and zero for $r > r_0$, certain changes occur in the treatment. These changes result in an *increase* of σ as given in Eq. (19).

The changes which enter, when the potential box is used, may be outlined as follows. From Eq. (33) we find the CSA in terms of the matrix integral for the electric moment.³⁷

³⁶ In this connection see Letter to the Editor by the author, Phys. Rev. 49, 401 (1936).

³⁷ The factor $r/2$ occurs in the integrand, instead of r . For if we have two particles in relative coordinates, the electric moment is given by the matrix element of $e\xi + e'\eta$, where ξ and η are the distances of the charges e and e' , respectively, from the center of mass. If charge e has the mass m , and e' the mass M we know $e\xi + e'\eta = (Me + me')r/(m+M)$, where r is the vector connecting e and e' . For $m = M$, and $e' = 0$, this gives $e\xi + e'\eta = er/2$.

$$\sigma = \frac{\pi e^2 h}{3Mc} \left| \int_0^\infty (rR_1) - \frac{r}{2}(rR_2) dr \right|^2. \quad (20)$$

The unit of energy has been taken to be

$$2m_e c^2 = 1.02 \text{ Mev.}$$

The wave functions R_1 and R_2 satisfy the differential equation

$$d^2(rR)/dr^2 + (E - V - l(l+1)/r^2)(rR) = 0, \quad (21)$$

where E is the energy in units of $2m_e c^2$, and r is the distance between neutron and proton in units of the Compton wave-length divided by $4\pi(1840)^{1/2}$. This unit of length is 6.35×10^{-13} cm. M is the reduced mass $M_P M_n / (M_P + M_n)$. The functions R_1 and R_2 are the normalized solutions of Eq. (21) for $E < 0$ (stable state-deuteron) and for $E > 0$ (state proton+neutron). If E_1 represents the binding energy of the deuteron, and E_2 the energy of the final state neutron plus proton, to conserve energy we must have³⁸

$$h\nu = E_1 + E_2.$$

Now let us represent the neutron proton interaction by the function

$$\begin{aligned} V &= -V_0 = \text{const}, & r < r_0 \\ V &= 0, & r > r_0, \end{aligned}$$

where we consider r_0 to be in the neighborhood of 1.5×10^{-13} cm, or 0.236 in terms of our unit of length.

For s states, and $E < 0$, Eq. (21) has the solution

$$\begin{aligned} rR_1 &= \sin r(V_0 - E_1)^{1/2}, & r < r_0 \\ rR_1 &= A \exp(-rE_1^{1/2}), & r > r_0. \end{aligned} \quad (22)$$

Here $E_1 = -E$, so that $E_1 > 0$. Joining the two expressions for R_1 (and the derivatives) at r_0 , gives the following conditions for the constant A , and the energy E_1

$$\begin{aligned} A &= \exp(r_0 E_1^{1/2}) \sin r_0 (V_0 - E_1)^{1/2}, \\ \tan r_0 (V_0 - E_1)^{1/2} &= -(V_0 / E_1 - 1)^{1/2}. \end{aligned}$$

³⁸ The change in momentum of the center of mass is equal to the momentum of the light quantum. This gives rise to the velocity v_0 , where $v_0/c = h\nu / (M_P + M_n)c$. Since this is small for all gamma-rays, the energy relation $h\nu = E_1 + E_2$ may be considered valid. Similarly the retardation factor $\exp(i\mathbf{k} \cdot \mathbf{r})$ may be seen to differ negligibly from unity, which validates its absence in Eq. (20). The theoretical application to the deuteron is consequently nonrelativistic in all of its essential features, and the result Eq. (33) Section 15, may be used directly with only obvious modifications in the wave functions.

The second condition requires the argument of the tangent to be $> \pi/2$. If we write $r_0(V_0 - E_1)^{1/2} = \pi/2 + \delta$, this condition becomes

$$\tan \delta = r_0 E_1^{1/2} / (\pi/2 + \delta) \quad \sim 0.2,$$

using $r_0 = 0.236(1.5 \times 10^{-13} \text{ cm})$, and a binding energy $E_1 = 2.1$ (Mev) the potential well turns out to have the depth $V_0 \sim 60$ Mev. As $r_0 \rightarrow 0$, $V_0 \rightarrow (\pi/2r_0)^2$.

Now the condition for normalizing the bound state (22) is

$$\begin{aligned} N_1^2 \left\{ \int_0^{r_0} \sin^2 \frac{r}{r_0} \left(\frac{\pi}{2} + \delta \right) \cdot dr \right. \\ \left. + \cos^2 \delta \int_{r_0}^\infty \exp(2E_1^{1/2}(r_0 - r)) dr \right\} = 1 \end{aligned}$$

and this gives, to order δ^2 ,

$$N_1^2 = 1 - \pi\delta/2 + \delta^2.$$

Now the integral in Eq. (20) we write as the sum of two integrals having the limits $0 - r_0$ and $r_0 - \infty$, respectively. One may then show that the contribution between 0 and r_0 is small (fractionally about $r_0^4/4$), and that the error in extending the limits of the second integral to $0 - \infty$, instead of $r_0 - \infty$, is also small (a fractional difference of less than $r_0^4/3$, for all γ -ray energies). The results above are a consequence of the fact that R_2 is small ($\sim r$) within the range of the interaction. The function R_2 suffers a phase shift for $r > r_0$ because of the sudden change in V , but this phase shift turns out to have no appreciable effect either (about $0.4 r_0^3$), so that the final state may really be considered unaffected by the potential V . In accordance with these remarks, we write for the normalized final state ($l=1$)

$$rR_2 = \frac{1}{\pi^{1/2} E_2^{1/2}} \left(\frac{\sin r E_2^{1/2}}{r E_2^{1/2}} - \cos r E_2^{1/2} \right)$$

and for the bound state

$$rR_1 = N_1 \cos r_0 E_1^{1/2} e^{r_0 E_1^{1/2}} \cdot e^{-r E_1^{1/2}}.$$

Using these expressions, we find from Eq. (20)

$$\sigma = \sigma_{B.P.} [1 + r_0 E_1^{1/2} + 0.6(r_0 E_1^{1/2})^2]$$

to order $(r_0 E_1^{1/2})^2$. By $\sigma_{B.P.}$ is meant the CSA as given by Eq. (19).

The effect of the correction terms in r_0 is to increase σ . This increase, for r_0 corresponding to 1.5×10^{-13} cm, and a binding energy of 2.14 Mev, is 40 percent, and results in the value $\sigma = 9.5 \times 10^{-28}$ cm².

As should be apparent from the discussion, it is not even necessary to evaluate the matrix integral to find the corrections to $\sigma_{B.P.}$, as the net correction is given by the square of the coefficient of e^{-r/a_0} in R_1 above. Consequently it would seem possible to calculate the effect of any given interaction V on the CSA, to order r_0^2 , merely by studying the wave function for the initial state. This turns out to be the case as one may see by studying the problem where

$$V = -V_0 e^{-r/r_0}.$$

The solution of Eq. (21) is then

$$rR = NJ_{2r_0 E_1}^{1/2} (2r_0 V_0)^{1/2} e^{-r/2r_0}.$$

The results of this problem are substantially the same as for the potential hole.

NONRELATIVISTIC THEORY

14. Separation of the Schrödinger equation for hydrogenic atoms

(a) Angle dependence

The Schrödinger equation for an electron in the field of an infinitely heavy nucleus, of charge Ze , is

$$\Delta\psi + (\epsilon + 2(Z/\rho))\psi = 0. \quad (23)$$

The equation is here written in simple units. That is, if r is the distance between electrons and nucleus, and if E is the energy, in c.g.s. units, then $\rho = r/a_0$, $\epsilon = E/Ry$, where $a_0 = \hbar^2/4\pi^2 m e^2$ is the radius of the first Bohr orbit for hydrogen,

and $Ry = 2\pi^2 m e^4 / \hbar^2$ is the ionization energy of hydrogen.

The well-known solution of Eq. (23) in polar coordinates may be written

$$\psi = Y_{l,m}(\theta, \varphi) R(\rho),$$

where $Y_{l,m}$ is the normalized angular function

$$Y_{l,m}(\theta, \varphi) = \left(\frac{(l-m)!}{(l+m)!} \frac{2l+1}{4\pi} \right)^{1/2} P_l^m(\cos \theta) e^{im\varphi},$$

$$P_l^m(x) = (1-x^2)^{m/2} (d^m P_l / dx^m),$$

$$P_l(x) = (1/2^l l!) (d^l (x^2-1)^l / dx^l).$$

The radial function R satisfies the differential equation

$$\frac{d^2(\rho R)}{d\rho^2} + \left(\epsilon + \frac{2Z}{\rho} - \frac{l(l+1)}{\rho^2} \right) (\rho R) = 0. \quad (24)$$

The solution is

$$R(\rho) = \rho^l e^{-\rho(-\epsilon)^{1/2}} F(l+1-Z(-\epsilon)^{-1/2}, 2l+2; 2\rho(-\epsilon)^{1/2}), \quad (25)$$

where F is the confluent hypergeometric function defined by

$$F(\alpha, \gamma; x) = 1 + \frac{\alpha}{\gamma} x + \frac{\alpha(\alpha+1)}{\gamma(\gamma+1)} \frac{x^2}{2!} + \dots$$

(b) The radial function $E < 0$

For this case the condition on R at infinity requires that $l+1-Z(-\epsilon)^{-1/2}$ = negative integer or zero. This condition will be satisfied if

$$Z(-\epsilon)^{-1/2} = n, \quad n = 1, 2, 3, \dots$$

or,

$$\epsilon = -Z^2/n^2 \quad (26)$$

for the energies of the bound states. The normalized radial function³⁰ $R_{n,l}$ for these states is

$$R_{n,l} = \frac{1}{(2l+1)!} \left(\frac{(n+l)!}{2n(n-l-1)!} \right)^{1/2} \left(\frac{2Z}{n} \right)^{1/2} \left(\frac{2Z\rho}{n} \right)^l \cdot e^{-Z\rho/n} F(l+1-n, 2l+2; 2Z\rho/n) \quad (27)$$

in our units, which we shall call Rydberg units. To obtain the normalized radial function in c.g.s. units, this expression should be multiplied by $a_0^{-1/2}$.

(c) The radial function $E > 0$

We define the quantity k by the equation

$$(-\epsilon)^{1/2} = e^{\pi i/2} k = ik.$$

³⁰ See H. Bethe, *Handbuch der Physik*, 24/1, p. 283. The normalizing factor may also be obtained directly from a term by term expansion and integration of $R_{n,l}$.

Physically, k is the ratio of two velocities: the velocity v of the state characterized by E , and $2\pi e^2/h$, the orbital velocity in the first Bohr orbit of *hydrogen*. That is, $k = v\hbar/2\pi e^2$. To simplify writing we also define

$$n = Z/k.$$

Then n is also a ratio of two velocities, which are the orbital velocity $v_0 = 2\pi e^2 Z/h$ in the ground state, and the velocity v . No confusion should arise between this n and the one defined previously for states $E < 0$, as this one always enters accompanied by the factor $\exp(\pi i/2) = i$.

We may now write, directly from Eq. (25),

$$R = N \cdot (2k\rho)^l e^{-ik\rho} F(l+1+in, 2l+2; 2ik\rho).$$

N is merely a normalizing factor which will be chosen later. A convenient integral representation for this function is⁴⁰

$$R = N \frac{\Gamma(2l+2) \exp(-i[k\rho + n \log 2k\rho - (l+1)\pi/2])}{|\Gamma(l+1+in)|^2 e^{n\pi/2}} \int_0^\infty e^{-t} t^{l+in} (1+t/2ik\rho)^{l-in} dt$$

+ the complex conjugate. (28)

This latter form is convenient for the problem of normalization, when only the asymptotic value of R for $k\rho \gg 1$ is needed. For ρ very large the integrals in Eq. (28) are particularly simple, being complex gamma functions of argument $l+1+in$ or $l+1-in$. The asymptotic expression of R turns out at once to be

$$R(\rho) \sim N \frac{\Gamma(2l+2)}{|\Gamma(l+1+in)| e^{n\pi/2}} \frac{1}{k\rho} \cos [k\rho + n \log 2k\rho - (l+1)\pi/2 - \sigma(l+1, n)], \quad (29)$$

where σ is the phase of the complex gamma function, defined by

$$e^{i\sigma(l+1, n)} = \Gamma(l+1+in) / |\Gamma(l+1+in)|.$$

The radial function

$$R \sim c/\rho \cos(k\rho + \beta)$$

(where β may vary as fast as $\log \rho$) is now normalized to $d(E/h)$ by the following condition on c :⁴¹

$$c^2 = 1/k\pi.$$

This condition determines N above in atomic units. To express N in c.g.s. units it must be multiplied by $a_0^{-1}(\hbar^2/2\pi^2 m e^4)^{1/2}$.

Due to the different behavior of the complex gamma function for very small and for very large energies E , two different forms for N are useful.

First, as we find from the condition on c^2 ,

$$N = \frac{k^{1/2} |\Gamma(l+1+in)| e^{n\pi/2}}{\pi^{1/2} \Gamma(2l+2)}, \quad (30)$$

which is useful for large energies, where n is small. With the use of the property

$$\Gamma(x)\Gamma(1-x) = \pi/\sin \pi x,$$

⁴⁰ See Whittaker and Watson, *Modern Analysis*, 4th edition, p. 337, et seq. $M_{k, m}(z) = z^{m+1/2} e^{-z/2} F(m+1/2-k, 2m+1; z)$.
⁴¹ See Mott and Massey, *Atomic Collisions*, p. 256 and H. Bethe, reference 7, p. 292. Bethe's Eq. (4.23) for R_σ should be multiplied by $2^{1/2}$, since his unit of energy is $2R_\sigma = 2 \cdot (2\pi^2 m e^4/\hbar^2)$. The exponential factor, $\exp(ikr)$ should also be changed to $\exp(-ikr)$.

since l is an integer, we may also write

$$|\Gamma(l+1+in)| = \left(\frac{\pi n}{\sinh \pi n}\right)^{\frac{1}{2}} \prod_{s=1}^l (s^2+n^2)^{\frac{1}{2}} \quad \text{and} \quad N = \frac{1}{(2l+1)!} \left(\frac{2Z}{1-e^{-2\pi n}}\right)^{\frac{1}{2}} \prod_{s=1}^l (s^2+n^2)^{\frac{1}{2}}, \quad (31)$$

which is useful for small energies, or indeed for any energies if l is not a large integer.

To summarize, the entire wave function for $E > 0$, normalized in Rydberg units, is

$$\psi_E(r, \theta, \varphi) = Y_{l, m}(\theta, \varphi) \cdot N(2k\rho)^l e^{-ik\rho} F(l+1+in, 2l+2; 2ik\rho), \quad (32)$$

where N is given by either Eq. (30) or Eq. (31). To express the wave function in c.g.s. units it should be multiplied by $a_0^{-1}(h^3/2\pi^2 m e^4)^{\frac{1}{2}}$.

15. Evaluation of the matrix element

The absorption coefficient discussed in Section 5, et seq., is given directly by the square of the matrix element of the current $j_{E, n}$ from Eq. (3B). That is, by the square of

$$\begin{aligned} J_{E, n} &= \frac{e\hbar}{im} \int \exp(i(\mathbf{\kappa} \cdot \mathbf{r})) \psi_E^*(\mathbf{A} \cdot \text{grad } \psi_n) d\tau \\ &= e2\pi i v \int \exp(i(\mathbf{\kappa} \cdot \mathbf{r})) \psi_E^*(\mathbf{A} \cdot \mathbf{r}) \psi_n d\tau. \end{aligned}$$

We consider light incident along the z axis. Then \mathbf{A} , the unit polarization vector, will be in the $x-y$ plane. Since the Schrödinger equation ignores all relativistic effects it is necessary for a consistent calculation to set $(\mathbf{\kappa} \cdot \mathbf{r})$ which enters $|J_{E, n}|$ quadratically, equal to zero. For, in the neighborhood of the first Bohr orbit, $(\mathbf{\kappa} \cdot \mathbf{r}) \sim \alpha + (v/c)^2/\alpha$ using the conservation law, and this is always of order $\alpha = Z/137$ for justifiable photoelectron velocities. It may indeed be of order unity for $(v/c)^2 \sim Z/137$, but the Schrödinger equation itself breaks down for velocities so large (except for the lightest elements where the screening model has no meaning. Hydrogen provides the single exception for which the retardation factor might be meaningfully retained).

An electron in the normal state ($n=1, l=m=0$) has the wave function

$$\psi_0 = (Z^3/\pi)^{\frac{1}{2}} e^{-Z\rho}.$$

Since $(\mathbf{A} \cdot \mathbf{r}) = A_x x + A_y y$, and x and y are proportional to $\cos \varphi, \sin \varphi$, respectively, m is determined for the final state to be ± 1 . For $m = +1$, $J_{E, n}$ is proportional to $(A_x - iA_y)$, and for $m = -1$, $J_{E, n}$ is in the same way proportional to $(A_x + iA_y)$.

We may therefore effectively sum $J_{E, n}^2$ over $m = \pm 1$, and write

$$J_{E, 0} = e2\pi i v / 2^{\frac{1}{2}} \int \psi_E^*(x+iy) \psi_0 d\tau.$$

Since $x+iy = r \sin \theta e^{i\varphi}$, l for the final state will be unity ($s-p$ transition). Then, using

$$Y_{1, 1}(\theta, \varphi) = (\frac{3}{8}\pi)^{\frac{1}{2}} \sin \theta e^{i\varphi},$$

and performing the easy angular integration, we find

$$J_{E, 0} = \frac{2Z^{\frac{3}{2}} e \cdot 2\pi i v a_0}{3^{\frac{1}{2}}} \int_0^\infty e^{-Z\rho} \rho^3 R_E d\rho. \quad (33)$$

The integral may be simply evaluated by series expansion of the integrand. One finds

$$\int_0^\infty e^{-Z\rho} \rho^4 e^{-ik\rho} F(2+in, 4; 2ik\rho) d\rho = \frac{12Z}{(Z^2+k^2)^3} \exp(-2n \cot^{-1} n).$$

Substitution of this into Eq. (4), and multiplication by a factor 2 to take account of both K electrons, leads to the absorption coefficient

$$\tau_K = 2 \cdot N_0 \frac{\hbar a_0}{mc} \frac{2^8 \pi Z^8 \exp(-4n \cot^{-1} n)}{3 (1 - e^{-2\pi n})(k^2 + Z^2)^4}$$

The conservation law, which may now be used to express τ_K as a function of ν , reads

$$\nu = Z^2 + k^2 = Z^2(1 + 1/n^2),$$

where ν is in Rydberg units.

16. Screening

We assume the atomic electron has a potential energy V in the field of the nucleus, where

$$\left. \begin{aligned} V &= -2Z/\rho + V_0 \\ &= -2/\rho \end{aligned} \right\} \text{Ry,} \quad \begin{aligned} \rho < \rho_0 &= 2(Z-1)/V_0 \\ \rho > \rho_0 & \end{aligned}$$

V_0 is of the order $3.6Z^{1/3}$, and ρ_0 consequently is of the order $\frac{1}{2}Z^{-1}$. This value of ρ_0 lies well outside of the L shell for medium heavy and heavy elements. For the bound states the energies are therefore approximately given by

$$\epsilon_n = -Z^2/n^2 + V_0, \quad n = 1, 2, 3, \dots$$

Since $V_0 - \epsilon_n$ now occurs in the bound state wave functions, in place of $-\epsilon_n$, these functions are unchanged by the presence of V_0 . The energy equation relating $\hbar\nu$, ϵ_n , and ϵ , the energy of the final state, however is changed as a result of the change in ϵ_n . It reads

$$\hbar\nu - Z^2/n^2 = \epsilon - V_0.$$

Now for the final states, $\epsilon - V_0$ occurs in place of ϵ . Since $\epsilon - V_0$ can now be negative for small photoelectron velocities, the final state wave function in this instance will have the appearance of a discrete state function of large but nonintegral total quantum number, for all $\rho < \rho_0$. Again since ρ_0 is large, and this behavior consequently persists throughout the range where the matrix integral contributes, there is no difficulty in completing the integration, as one sees by using the expression

$$R_E = N' (2(V_0 - \epsilon)^{1/2} \rho)^{1/2} e^{-\rho(V_0 - \epsilon)^{1/2}} F(l + 1 - iZ/(V_0 - \epsilon)^{1/2}, 2l + 2; 2\rho(V_0 - \epsilon)^{1/2})$$

to evaluate the integral of Eq. (33). If we let $k' = (V_0 - \epsilon)^{1/2}$, the result of this integration gives

$$\tau_{K'} = N_0 \frac{3 \cdot 2^{1/2} \pi^3 e^2 a_0^2}{hc} N'^2 \frac{\nu k'^2 Z^5}{(Z^2 - k'^2)^6} \left(\frac{1 - k'/Z}{1 + k'/Z} \right)^{2Z/k'}$$

The problem is therefore to find the normalizing factor N' , for the range $\epsilon - V_0 < 0$.

Since asymptotic formulas for functions of the type R_E above are not well known, we propose to study this normalization by means of the W.K.B. method. It will be of advantage first to see what result the W.K.B. method⁴² gives for the normalization of the pure hydrogenic function with no screening, when $\epsilon > 0$.

According to this method the solution of

$$\frac{d^2(\rho R)}{d\rho^2} + \left(\epsilon + \frac{2Z}{\rho} - \frac{l(l+1)}{\rho^2} \right) (\rho R) = 0$$

outside of the classical turning point ρ_1 , is given by

$$R_E^0 \sim \frac{1}{\pi^{1/2}} \frac{(\varphi(\rho))^{-1/2}}{\rho} \cos \left\{ \int_{\rho_1}^{\rho} \varphi^{1/2} d\rho - \frac{\pi}{4} \right\}.$$

⁴² See L. A. Young and G. E. Uhlenbeck, Phys. Rev. 36, 1154 (1930).

This function is already normalized. The quantity $\varphi(\rho)$ is defined as

$$\varphi = \left| \epsilon + \frac{2Z}{\rho} - \frac{(l + \frac{1}{2})^2}{\rho^2} \right|; \quad \varphi(\rho_1) = 0.$$

Now by joining at ρ_1 , the solution inside the turning point is given by

$$R_E^i(\rho) = \frac{1}{2\pi^{\frac{1}{2}}} \varphi^{-\frac{1}{2}} \exp \left(\int_{\rho_1}^{\rho} \varphi^{\frac{1}{2}} d\rho \right).$$

In this way the normalizing factor N (for no screening) should be approximately determined by setting

$$(2\rho\epsilon^{\frac{1}{2}})^l N = R_E^i(\rho), \quad \text{for } \rho \neq 0.$$

If we use Sterling's formula, and thereby neglect a term $1/24(l+1)$, we find from the above relation

$$N = ((2Z)^{\frac{1}{2}} n^l / (2l+1)!) \cdot (1 + \lambda^2/n^2)^{\lambda/2} \exp(n \tan^{-1} \lambda/n - \lambda).$$

If this is compared with the correct normalization as given by Eq. (31), one sees there is a fractional error here of amount $(l + \frac{1}{2})/24 \times n^2$ for small energies (large n). Nevertheless the above formula gives values accurate to within one percent for $n^2 = 3$ ($\nu/\nu_1 = 4/3$).

Now, let us consider the potential energy (in Rydberg units) to be given by

$$V = -2Z/\rho + V_0, \quad \rho < \rho_1$$

$$V = -2/\rho, \quad \rho > \rho_1 = 2(Z-1)/V_0,$$

where V_0 is a constant. The conservation law then reads

$$h\nu = Z^2 + \epsilon - V_0.$$

For the moment we shall discuss the case where $\epsilon - V_0 > 0$. Now the normalization will be found as before, that is by making the amplitude of the wave function be $1/\pi^{\frac{1}{2}} \epsilon^{\frac{1}{2}}$, for $\rho \rightarrow \infty$. But the solution of the differential equation for $V = -2/\rho$ must be joined with that for $V = -2Z/\rho + V_0$ for $\rho = \rho_1$, and consequently this will modify the amplitude inside, and therefore change the normalizing factor N somewhat. If we define

$$P = \epsilon - V_0 + \frac{2Z}{\rho} - \frac{\lambda^2}{\rho^2}; \quad P(\rho_P) = 0, \quad \lambda = l + \frac{1}{2},$$

$$Q = \epsilon + \frac{2}{\rho} - \frac{\lambda^2}{\rho^2}; \quad Q(\rho_Q) = 0,$$

$$p = \int_{\rho_P}^{\rho} P^{\frac{1}{2}} d\rho - \frac{\pi}{4},$$

$$q = \int_{\rho_Q}^{\rho} Q^{\frac{1}{2}} d\rho - \frac{\pi}{4},$$

the W.K.B. solutions may be written

$$\rho R = \frac{1}{2} (-P)^{-\frac{1}{2}} \exp \left\{ \int_{\rho_P}^{\rho} (-P)^{\frac{1}{2}} d\rho \right\}, \quad \rho < \rho_P,$$

$$\rho R = P^{-\frac{1}{2}} \cos p(\rho), \quad \rho_P < \rho < \rho_1,$$

$$\rho R = A Q^{-\frac{1}{2}} \cos [q(\rho) + \Delta], \quad \rho > \rho_1.$$

These functions represent the solution for this problem. The solution will be normalized if it is multiplied by $(A^2 \pi)^{-\frac{1}{2}}$. The two constants A and Δ are now to be found by joining the two oscillatory solutions, and their derivatives at ρ_1 . We are here not interested in the phase Δ , but only in the amplitude A . The conditions at ρ_1 give for A the relation

$$A^2 = 1 - \frac{V_0 \sin 2p(\rho_1)}{4\rho_1 P^{\frac{1}{2}}} + \left(\frac{V_0 \cos p}{4\rho_1 P^{\frac{1}{2}}} \right)^2, \quad (\rho = \rho_1)$$

in which the last term may generally be dropped. The normalization is now obtained in the same way as before, and is in fact given by

$$N = \frac{(2Z)^{\frac{1}{2}} n^l}{A(2l+1)!} \left(1 + \frac{\lambda^2}{n^2} \right)^{\lambda/2} \exp(n \tan^{-1} \lambda/n - \lambda)$$

only n is now written

$$n = Z/(\epsilon - V_0)^{\frac{1}{2}} = Z/k$$

due to the presence of V_0 . For computing A we give the expressions

$$P(\rho_1) = \epsilon + \frac{2}{\rho_1} - \frac{\lambda^2}{\rho_1^2},$$

$$p(\rho_1) = \rho_1 P^{\frac{1}{2}} + n \log \frac{\rho_1 (P^{\frac{1}{2}} + k) + n}{(n^2 + \lambda^2)^{\frac{1}{2}}}$$

$$- \lambda \cos^{-1} \frac{\lambda^2/Z\rho_1 - 1}{(1 + \lambda^2/n^2)^{\frac{1}{2}}} - \frac{\pi}{4}$$

$$= 2\rho_1 P^{\frac{1}{2}} - \lambda \cos^{-1} (\lambda^2/Z\rho_1 - 1) - \pi/4, \quad \epsilon = V_0.$$

Here $\cos^{-1}(\lambda^2/Z\rho_1 - 1/(1+\lambda^2/n^2)^{1/2})$ is in the first or second quadrant. This gives the correct phase for the limiting case $\epsilon - V_0 = 0$.

Now let us consider the case $\epsilon - V_0 < 0$. Both roots of $P(\rho) = 0$ are now positive, the one moving in from $+\infty$ as $V_0 - \epsilon$ increases. We write these roots ρ_P , and $\rho_{P'}$, where

$$\rho_P = \frac{\lambda^2/Z}{1 + (1 + \lambda^2/n^2)^{1/2}}$$

$$\rho_{P'} = \frac{\lambda^2/Z}{1 - (1 + \lambda^2/n^2)^{1/2}}$$

Here as before $n^2 = Z^2/(\epsilon - V_0)$, but is now negative. The function $Q(\rho) = \epsilon + 2/\rho - \lambda^2/\rho^2$ still has only one positive root

$$\rho_Q = \lambda^2/1 + (1 + \lambda^2\epsilon)^{1/2}$$

However, in joining the solutions corresponding to $P(\rho)$ and $Q(\rho)$ at ρ_1 , where $P=Q$, we must be careful to join oscillatory solutions only if $\rho_Q < \rho_1 < \rho_{P'}$ (see Fig. 8). These conditions put a lower limit on $-n^2$, or an upper limit on ϵ which is somewhat greater than $V_0/2$, according to the particular value of Z being considered. We shall now need

$$p(\rho) = \int_{\rho_P}^{\rho} [-(V_0 - \epsilon)\rho^2 + 2Z\rho - \lambda^2]^{1/2} \frac{d\rho}{\rho} - \frac{\pi}{4}$$

$$= \int_{\rho_P}^{\rho} P^{1/2} d\rho - \frac{\pi}{4}$$

$$= \rho P^{1/2} = |n| \tan^{-1} \frac{\rho P^{1/2}}{|n|(1 + Z\rho_1/n^2)}$$

$$- \lambda \cos^{-1} \frac{\lambda^2/Z\rho - 1}{(1 + \lambda^2/n^2)^{1/2}} - \frac{\pi}{4}$$

and for continuing the solution in to $\rho = 0$ we also need

$$\int_{\rho_P}^{\rho} [\lambda^2 - 2Z\rho + (V_0 - \epsilon)\rho^2]^{1/2} \frac{d\rho}{\rho} = \int_{\rho_P}^{\rho} (-P)^{1/2} \frac{d\rho}{\rho}$$

$$= \lambda + \frac{1}{2}|n| \log \frac{1 + \lambda/|n|}{1 - \lambda/|n|} + \lambda \log \frac{Z\rho}{2\lambda^2} (1 + \lambda^2/n^2)^{1/2}$$

as $\rho \neq 0$. Now joining again at ρ_1 , and continuing

the solution in to $\rho = 0$, we again find the normalizing factor, for the energy range $\epsilon - V_0 < 0$, to be given by

$$N = \frac{(2Z)^{1/2} n^{1/2}}{A(2l+1)!} (1 + \lambda^2/n^2)^{\lambda/2} \exp(n \tan^{-1} \lambda/n - \lambda)$$

only n is now imaginary. N may be expanded in a power series in n^2 however, so that we are now prepared to give a rule for computing τ_K in the region $\nu/\nu_1 < 1$.

We omit any reference to the amplitude A for the moment. Then, since the W.K.B. method gives the same functional dependence of N on n on both sides of the ideal series limit ν_1 , it seems likely that a rigorous theory would do the same. This we shall assume. Thus we conclude that due to screening effects the result Eq. (8) for τ_K will be modified only by the factor $1/A^2$ on both sides of the ideal limit ν_1 . For energies $\epsilon - V_0 > 0$ we have found this factor to be

$$1/A^2 \cong 1 + (V_0 \sin 2p(\rho_1)/4\rho_1 P^{1/2})$$

For energies $\epsilon - V_0 < 0$ the same result follows, only in the two cases $p(\rho_1)$ is different. For $\epsilon - V_0 > 0$

$$p(\rho_1) = \rho_1 P^{1/2} + n \log \frac{\rho_1(P^{1/2} + k) + n}{(n^2 + \lambda^2)^{1/2}}$$

$$- \lambda \cos^{-1} \frac{\lambda^2/Z\rho_1 - 1}{(1 + \lambda^2/n^2)^{1/2}} - \frac{\pi}{4}$$

and for $\epsilon - V_0 < 0$

$$p(\rho_1) = \rho_1 P^{1/2} + |n| \tan^{-1} \frac{\rho_1 P^{1/2}}{|n|(1 + Z\rho_1/n^2)}$$

$$- \lambda \cos^{-1} \frac{\lambda^2/Z\rho_1 - 1}{(1 + \lambda^2/n^2)^{1/2}} - \frac{\pi}{4}$$

In both cases $P(\rho_1)$ is the same

$$P(\rho_1) = \epsilon + 2/\rho_1 - \lambda^2/\rho_1^2$$

These expressions for $p(\rho_1)$, as might have been predicted, are analytic continuations of each other as $\epsilon - V_0$ passes through the value zero.

So far little has been said concerning the effect of the amplitude A , and the corresponding phase shift Δ , on the wave functions in the integral of Eq. (33) for the matrix element. This integral is

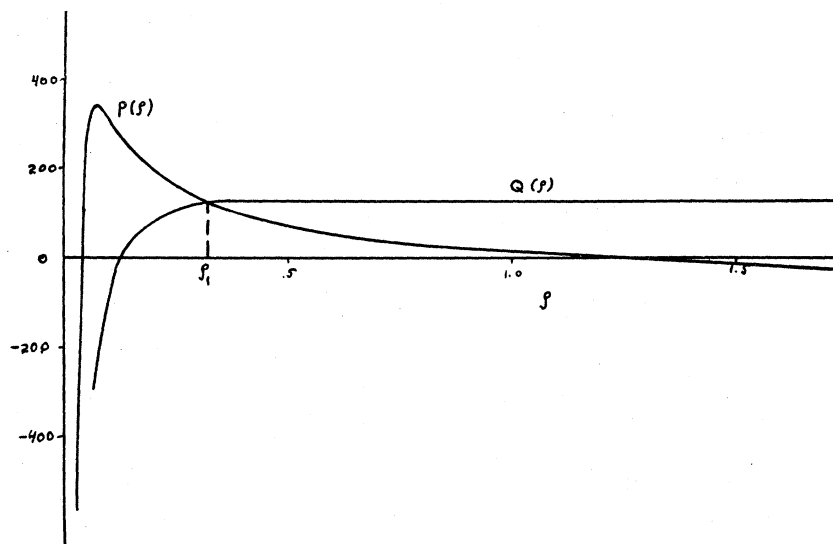


FIG. 8. Illustration of condition ($\rho_Q < \rho_1 < \rho_{P'}$) when joined radial solutions may both be oscillatory.

also subject to changes brought about in the normal state wave function due to the screening. A qualitative estimate of this effect may be made as follows. Omitting from the discussion the radial wave function of the final state, which is oscillatory, the integrand for the matrix element is

$$\rho^3 e^{-Z\rho},$$

which is a maximum for $\rho_{\max} = 3/Z$. Since the changes due to screening enter only for $\rho > \rho_1$, we may expect them to have only a slight effect if ρ_{\max} is much less than ρ_1 . This is the case for heavy elements, and is fairly well satisfied for lighter ones. If we write the condition

$$\rho_{\max} \leq \frac{1}{2}\rho_1,$$

we obtain a lower limit for Z of about 16. This should be a stringent enough condition for large energies, since the wave function begins to oscillate at about $\rho_{\max}/3$, and the contribution from beyond ρ_1 should consequently be small due to interference. For small energies the error will be greatest, since the wave-length is long here, but even for $\epsilon - V_0 = 0$ the error will be slight for heavy elements ($Z \gtrsim 26$).

In computing the phase $p(\rho_1)$ for the energy $\epsilon - V_0 = 0$, which corresponds to $\nu = \nu_1 = Z^2$, we may expand p in a series of powers of

$$\delta = [V_0/Z(Z-1)]^{\frac{1}{2}}.$$

We find

$$p(\rho_1) = 4/\delta + \lambda^2\delta/2 + \lambda^4\delta^3/96 + \dots - (\lambda + \frac{1}{4})\pi$$

and

$$1/A^2 \cong 1 + \delta \sin 2p/8(1 - \lambda^2\delta^2/4)^{\frac{1}{2}}.$$

This form for $1/A^2$ may account for the discrepancies found at $\nu = \nu_K$ for Ta Au U, as illustrated in Fig. 1, and for the discrepancies in the opposite direction for the lighter elements Fe, Cu, Ag, Sn at $\nu = \nu_K$. The phase $2p$ may fall in any quadrant, and hence $\sin 2p$ may be negative as well as positive. However, as we have already seen, the binding energy as determined from the modified Fermi-Thomas field, does not agree with ν_K (obs) unless the relativistic binding energy is used in place of the term Z^2 . This indicates that the screening should be applied to the relativistic wave functions. Nevertheless, it seems possible by physical arguments to make plausible use of the formula just derived for $1/A^2$ for the relativistic problem. The point of joining,

$\rho_1 = 2(Z-1)/V_0$, is by definition at such a distance from the nucleus that the strong nuclear field has been almost totally screened. The wave function at this point should consequently be well represented by the Schrödinger function. For the case discussed, the change in amplitude A outside of the K shell produced only the same changes on the wave function for $\rho \rightarrow 0$. In this way we found the correction $1/A^2$ to the matrix element. For the relativistic wave function we

should expect a corresponding amplitude shift to have the same effect at $\rho = 0$. On the basis of the above argument the amplitude shift would be the same as that we have found.

The corrections $1/A^2$, with V_0 determined by Eq. (10), agree qualitatively with the experimental results in Fig. 1. For Pb $1/A^2 \sim 0.96$ for $\lambda/\lambda_1 = 1$, while for Fe, Cu, Sn, $1/A^2$ is between 1.05 and 1.02 for $\lambda/\lambda_1 = 1$. The correction falls off rapidly to zero in all cases as λ/λ_1 decreases.

17. Angular distribution for K shell

From Eq. (5)

$$\Psi = \sum_{l, m} \psi^{(1)}_{E, l, m} A_{l, m} \sim \sum_{l, m} \psi^{(1)}_{E, l, m} J_{E, l, m}$$

$$\psi^{(1)}_{E, l, m} = \frac{(k\pi)^{-1/2}}{\rho} \exp \{i[k\rho + n \log 2k\rho - (\pi/2)(l+1) - \sigma(l+1, n)]\} \cdot Y_{l, m}(\theta, \varphi).$$

For long wave-lengths we have found $J_{E, l, m}$ vanishes unless $l = |m| = 1$. Therefore,

$$\Psi \sim J_{E, 1, 1} (k\pi)^{-1/2} \frac{-e^{-i\sigma(l+1, n)} (2k\rho)^{in} e^{ik\rho}}{\rho} (Y_{1, 1} + Y_{1, -1}^*),$$

consequently the current vector has only the component along ρ , or

$$\Psi^* \text{grad } \Psi - \Psi \text{grad } \Psi^* \sim \cos \varphi \sin \theta.$$

The angle distribution is given by the square of this component.

$$J \sim \cos^2 \varphi \sin^2 \theta.$$

RELATIVISTIC THEORY

18. The Dirac equation⁴³ for hydrogenic atoms

(a) *Form of solutions and angle dependence*

The relativistic wave equation, including the effect of spin and change of mass with velocity, of an electron in the electromagnetic field ($A_0; A_1, A_2, A_3$), is

$$\left[\frac{E}{c} + \frac{e}{c} A_0 + \left(\alpha, \mathbf{p} + \frac{e}{c} \mathbf{A} \right) + \alpha_4 mc \right] \psi = 0. \tag{34}$$

The state ψ is characterized by the energy E . The operators in the equation are: $p = -i\hbar \text{grad}$, and

$$\alpha_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \alpha_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

where $\alpha_i \alpha_k + \alpha_k \alpha_i = 2\delta_{ik}$ ($i, k = 1, 2, 3, 4$).

⁴³ P. A. M. Dirac, Proc. Roy. Soc. A117, 610 (1928).

* The relations between the components of ψ , defined by the Dirac α matrices, and the components defined by Weyl's s' matrices (see H. Weyl, *Gruppen-theorie und Quantenmechanik* (Hirzel, 1928); p. 172) are given by

$$(\psi_1, \psi_2, \psi_3, \psi_4)_{\text{Weyl}} = (\psi_1 + \psi_3, \psi_2 + \psi_4, \psi_1 - \psi_3, \psi_2 - \psi_4)_{\text{Dirac}}.$$

The wave function ψ is itself a matrix of a single column

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}.$$

The solutions of Eq. (34) for a Coulomb field may be written as follows:

$$\begin{array}{l|l} j=l-\frac{1}{2} & j=l+\frac{1}{2} \\ \psi_1 = \left(\frac{l+m-\frac{1}{2}}{2l-1}\right)^{\frac{1}{2}} if(r) Y_{l-1, m-1} & \psi_1 = \left(\frac{l-m+\frac{3}{2}}{2l+3}\right)^{\frac{1}{2}} if(r) Y_{l+1, m-1} \\ \psi_2 = \left(\frac{l-m-\frac{1}{2}}{2l-1}\right)^{\frac{1}{2}} if(r) Y_{l-1, m+1} & \psi_2 = \left(\frac{l+m+\frac{3}{2}}{2l+3}\right)^{\frac{1}{2}} if(r) Y_{l+1, m+1} \\ \psi_3 = \left(\frac{l-m+\frac{1}{2}}{2l+1}\right)^{\frac{1}{2}} g(r) Y_{l, m-1} & \psi_3 = -\left(\frac{l+m+\frac{1}{2}}{2l+1}\right)^{\frac{1}{2}} g(r) Y_{l, m-1} \\ \psi_4 = -\left(\frac{l+m+\frac{1}{2}}{2l+1}\right)^{\frac{1}{2}} g(r) Y_{l, m+1} & \psi_4 = \left(\frac{l-m+\frac{1}{2}}{2l+1}\right)^{\frac{1}{2}} g(r) Y_{l, m+1} \end{array}$$

The projection of the angular momentum on the z axis is here denoted by m (a half-integer). The two sets of solutions correspond to the two possible values of the total angular momentum j . The radial functions f and g satisfy two first-order simultaneous equations. In this section we write

$$\begin{aligned} \rho &= 2\pi mcr/h = r \cdot 2\pi/\text{Compton wave-length}, \\ \epsilon &= E/mc^2, \end{aligned}$$

where r is the radius vector, and E the energy in c.g.s. units. The equations for f and g may then be written

$$\begin{aligned} [\epsilon+1+\alpha/\rho]f + [dg/d\rho + (1-k)g/\rho] &= 0, \\ [\epsilon-1+\alpha/\rho]g - [df/d\rho + (1+k)f/\rho] &= 0. \end{aligned} \quad (35)$$

Here, as before, $\alpha = 2\pi e^2 Z/hc \approx Z/137$. We have also that

$$\begin{aligned} k = j + \frac{1}{2} = l + 1, & \quad \text{when } j = l + \frac{1}{2}, \\ k = -(j + \frac{1}{2}) = -l, & \quad \text{when } j = l - \frac{1}{2}. \end{aligned}$$

The Eqs. (35) may now be solved at once by series substitution, after splitting off an exponential factor. Only the result will be given here as the procedure is straightforward. Except for a normalizing factor we find,⁴⁴

⁴⁴ See H. Bethe, reference 7, for similar results. The functions f and g are customarily written as a linear combination of two other confluent hypergeometric functions,

$$F\left(\gamma+1 - \frac{\alpha\epsilon}{(1-\epsilon^2)^{\frac{1}{2}}}, 2\gamma+1\right), \quad \text{and} \quad F\left(\gamma - \frac{\alpha\epsilon}{(1-\epsilon^2)^{\frac{1}{2}}}, 2\gamma+1\right).$$

Our solution is of course equivalent to these others, but in form is much more convenient for calculations in the continuum ($\epsilon > 1$), since our $G(\rho)$, although involving $i = (-1)^{\frac{1}{2}}$, is itself real.

The other independent solutions of Eqs. (35) (which are inadmissible as wave functions, and hence are omitted) are obtained from those above by changing the sign of $\gamma = (k^2 - \alpha^2)^{\frac{1}{2}}$ throughout. This change, unlike the corresponding one in l for solutions of the Schrödinger equation, actually does give the other independent solutions, since $-\gamma$ is never a negative integer, and the series for $F(a, -2\gamma)$, for example, consequently exists.

$$f = \frac{\alpha}{k+\gamma} G_\gamma(\rho) + \frac{k+\gamma}{\alpha} A \cdot G_{\gamma+1}(\rho), \quad g = G_\gamma(\rho) + A \cdot G_{\gamma+1}(\rho). \quad (36)$$

Where

$$\gamma = (k^2 - \alpha^2)^{\frac{1}{2}}, \quad A = \frac{\alpha}{(1 - \epsilon^2)^{\frac{1}{2}}} \frac{k\epsilon - \gamma}{2\gamma(2\gamma + 1)(k + \gamma)}$$

and

$$G_\gamma(\rho) = (2\rho(1 - \epsilon^2)^{\frac{1}{2}})^{\gamma-1} e^{-\rho(1 - \epsilon^2)^{\frac{1}{2}}} F(\gamma - \alpha\epsilon/(1 - \epsilon^2)^{\frac{1}{2}}, 2\gamma; 2\rho(1 - \epsilon^2)^{\frac{1}{2}}).$$

(b) *The radial functions for $E < mc^2$*

When $\epsilon < 1$ the confluent hypergeometric functions defining f and g become infinite as $\rho \rightarrow \infty$, unless

$$\gamma - \alpha\epsilon/(1 - \epsilon^2)^{\frac{1}{2}} = \text{a negative integer, or zero.}$$

We write

$$\alpha\epsilon/(1 - \epsilon^2)^{\frac{1}{2}} - \gamma = n', \quad n' = 0, 1, 2, \dots$$

This determines the discrete energies

$$\epsilon = [1 + (\alpha/(\gamma + n'))^2]^{-\frac{1}{2}}. \quad (37)$$

For each n' there are two values of ϵ . One is obtained by putting $k = l + 1$ ($j = l + \frac{1}{2}$), and the other by putting $k = -l$ ($j = l - \frac{1}{2}$). Since k can never be zero an exception is found for the case $l = 0$ (e.g., the normal state), when ϵ has only one value.

The normalizing factor for discrete states is determined by the condition

$$\int_0^\infty (f^2 + g^2) \rho^2 d\rho = 1.$$

It is generally easy to find directly. The complete, normalized solutions for the normal state only will be given here. For $k = 1$, $n' = 0$, which characterize the normal state functions, we find

$$f = [\alpha/(1 + \gamma_1)] [(1 + \gamma_1)/2\Gamma(1 + 2\gamma_1)]^{\frac{1}{2}} (2\alpha)^{\gamma_1 + \frac{1}{2}} \rho^{\gamma_1 - 1} e^{-\alpha\rho},$$

$$g = 1 \cdot [(1 + \gamma_1)/2\Gamma(1 + 2\gamma_1)]^{\frac{1}{2}} (2\alpha)^{\gamma_1 + \frac{1}{2}} \rho^{\gamma_1 - 1} e^{-\alpha\rho}.$$

(c) *The radial functions for $E > mc^2$*

The solutions for this case are formally the same as before. We write

$$f = N \cdot \left(\frac{\alpha}{k+\gamma} G_\gamma + \frac{k+\gamma}{\alpha} A \cdot G_{\gamma+1} \right), \quad g = N(G_\gamma + A G_{\gamma+1}) \quad (38)$$

We make the definitions, $p = (\epsilon^2 - 1)^{\frac{1}{2}}$, $n = \alpha\epsilon/p$. Then

$$A = \frac{\alpha}{p} \frac{k\epsilon - \gamma}{2\gamma(2\gamma + 1)(k + \gamma)}, \quad \text{and} \quad G_\gamma(\rho) = (2p\rho)^{\gamma-1} e^{-ip\rho} F(\gamma + in, 2\gamma; 2ip\rho) = \text{real.}$$

As written, p is the momentum of the electron, in units of mc .

Now $G_\gamma(\rho)$ behaves very much like the nonrelativistic function R for very large ρ , as may be seen by reference to Eq. (28). We may write

$$G_\gamma(\rho) \sim \frac{2\Gamma(2\gamma)}{|\Gamma(\gamma + in)| e^{n\pi/2}} \frac{1}{2p\rho} \cos \left[p\rho + n \log 2p\rho - \frac{\pi\gamma}{2} - \sigma(\gamma, n) \right].$$

From this it may be shown that

$$f \sim -\frac{c}{\rho}(\epsilon-1)^{\frac{1}{2}} \sin \nu, \quad g \sim -\frac{c}{\rho}(\epsilon+1)^{\frac{1}{2}} \cos \nu, \tag{39}$$

where $\nu = p\rho + n \log 2p\rho - \pi\gamma/2 - \sigma(\gamma, n) - \tan^{-1} \frac{\alpha}{k+\gamma} \left(\frac{\epsilon-1}{\epsilon+1}\right)^{\frac{1}{2}}$

and
$$c = \frac{N}{[2(k+\gamma)(k\epsilon+\gamma)]^{\frac{1}{2}}} \cdot \frac{\Gamma(2\gamma+1)}{|\Gamma(\gamma+in)| e^{\pi n/2}}$$

The normalizing condition is

$$\lim_{\Delta E \rightarrow 0} \int_0^{\infty} f \left\{ \int_{(E-\Delta E)/h}^{(E+\Delta E)/h} f d(E/h) \right\} \rho^2 d\rho + \text{same for } g = 1.$$

This condition requires c to be given by the expression, $c = (\pi p)^{-\frac{1}{2}}$ using our units of length and energy. In this way N is determined. From the condition on c we find

$$N = \left[\frac{2p}{\pi} (k+\gamma)(k\epsilon+\gamma) \right]^{\frac{1}{2}} \cdot \frac{|\Gamma(\gamma+in)| e^{\pi n/2}}{\Gamma(2\gamma+1)}.$$

If we write f and g , instead of as in Eqs. (38), as

$$\begin{aligned} f &= \frac{N}{(\epsilon+1)^{\frac{1}{2}} \cos \Gamma} (\epsilon-1)^{\frac{1}{2}} \left(\sin \Gamma \cdot G_{\gamma} + \frac{\gamma \cos \Gamma + n \sin \Gamma}{2\gamma(2\gamma+1)} G_{\gamma+1} \right) \\ g &= \frac{N}{(\epsilon+1)^{\frac{1}{2}} \cos \Gamma} (\epsilon+1)^{\frac{1}{2}} \left(\cos \Gamma \cdot G_{\gamma} + \frac{n \cos \Gamma - \gamma \sin \Gamma}{2\gamma(2\gamma+1)} G_{\gamma+1} \right) \end{aligned} \tag{40}$$

where $\tan \Gamma = \frac{\alpha}{k+\gamma} \left(\frac{\epsilon+1}{\epsilon-1}\right)^{\frac{1}{2}}$ then the quantity

$$\frac{N}{(\epsilon+1)^{\frac{1}{2}} \cos \Gamma} = \frac{2 |\Gamma(\gamma+1+in)| e^{\pi n/2}}{\Gamma(2\gamma+1)} \left(\frac{p}{\pi}\right)^{\frac{1}{2}}$$

may be considered as the normalizing factor. The advantage of this symmetrical form is that the above quantity remains unchanged for states where $k < 0$.

Asymptotic forms for f and g when $k < 0$, similar to those in Eqs. (39) for $k < 0$, are sometimes useful. They are given by

$$f = -\frac{c}{\rho}(\epsilon-1)^{\frac{1}{2}} \sin \nu', \quad g = -\frac{c}{\rho}(\epsilon+1)^{\frac{1}{2}} \cos \nu',$$

where $c = (\pi p)^{-\frac{1}{2}}$, and

$$\nu' = p\rho + n \log 2p\rho - \pi(\gamma+1)/2 - \sigma(\gamma, n) - \tan^{-1} \frac{\alpha}{|k|+\gamma} \left(\frac{\epsilon+1}{\epsilon-1}\right)^{\frac{1}{2}}.$$

The phase ν' differs from ν only by a constant.

19. The relativistic absorption coefficient

The two normal states are of the same energy, $\epsilon = \gamma_1$. They are specified by the numbers: $j = \frac{1}{2}$, $k = 1$, $m = \pm \frac{1}{2}$. The wave functions are:

$$\begin{array}{l}
 \mathbf{m} = \frac{1}{2} \quad (\alpha) \quad \psi_1^0 = \frac{1}{2\pi^{\frac{1}{2}}} \cdot if \cos \theta \\
 \psi_2^0 = \frac{1}{2\pi^{\frac{1}{2}}} if \sin \theta e^{i\varphi} \\
 \psi_3^0 = \frac{1}{2\pi^{\frac{1}{2}}} \cdot (-g) \\
 \psi_4^0 = 0
 \end{array}
 \quad \left| \quad
 \begin{array}{l}
 \mathbf{m} = -\frac{1}{2} \quad (\beta) \quad \psi_1^0 = \frac{1}{2\pi^{\frac{1}{2}}} \cdot (-if) \sin \theta e^{-i\varphi} \\
 \psi_2^0 = \frac{1}{2\pi^{\frac{1}{2}}} \cdot if \cos \theta \\
 \psi_3^0 = 0 \\
 \psi_4^0 = \frac{1}{2\pi^{\frac{1}{2}}} \cdot g
 \end{array}$$

where f and g are as given in section 18b.

The problem is now to evaluate

$$J_{E, n} = \int \exp(i\mathbf{k} \cdot \mathbf{r})(\mathbf{A} \cdot \mathbf{j}_{E, n}) d\tau, \quad \text{where } \mathbf{j}_{E, n} = -ce\psi_E^* \boldsymbol{\alpha} \psi_n.$$

The light may be considered again incident along the z axis, so that \mathbf{A} lies in the x, y plane; say in the direction of the x axis. Only for large frequencies, which we shall consider, $\exp i(\mathbf{k} \cdot \mathbf{r})$ must be retained. This factor of course complicates the analysis.

Integration over the angles presents no difficulties, but then a radial integration remains. We shall here summarize the results after completing the angular integration which is straightforward. We find.

$$\begin{aligned}
 \tau_{K \text{ shell}} &= 2 \cdot \frac{1}{2} (\tau_\alpha + \tau_\beta) \\
 &= N_0 \frac{4\pi}{h\nu c} \sum_{l=0}^{\infty} [J_\alpha^2(k) + J_\alpha^2(-k) + J_\beta^2(k) + J_\beta^2(-k)].
 \end{aligned} \tag{41}$$

To express the J 's, let us split off the common factor

$$\frac{1}{2} e N_0 N (h\pi/m)^{\frac{1}{2}},$$

where $N_0 = [(2\alpha)^{2\gamma_1+1}/2(1+\gamma_1)\Gamma(1+2\gamma_1)]^{\frac{1}{2}}$, $N = 2(p/\pi)^{\frac{1}{2}} e^{\pi n/2} |\Gamma(\gamma+1+i^n)|/\Gamma(2\gamma+1)$.

We further define integrals involving the radial function g (and similarly for ones in f).

$$g(\mu-1, k+1) = \int_0^\infty e^{-\alpha\rho} e^{-i q \rho} F(k+1, 2k+2; 2i q \rho) \rho^{\mu-\gamma} g d\rho,$$

where $q = h\nu/mc^2$, and g of the integrand is given by Eqs. (40). That is, omitting the normalizing factor written above.

$$f = (\epsilon-1)^{\frac{1}{2}} \left(\sin \Gamma \cdot G_\gamma + \frac{\gamma \cos \Gamma + n \sin \Gamma}{2\gamma(2\gamma+1)} G_{\gamma+1} \right), \quad g = (\epsilon+1)^{\frac{1}{2}} \left(\cos \Gamma \cdot G_\gamma + \frac{n \cos \Gamma - \gamma \sin \Gamma}{2\gamma(2\gamma+1)} G_{\gamma+1} \right).$$

The functions f' and g' will indicate that the sign of k is to be changed in f and g , respectively. The change in the sign of k will affect only the coefficients $\sin \Gamma$, $\cos \Gamma$ of G_γ , $G_{\gamma+1}$, since only here does k occur nonquadratically. We had

$$\tan \Gamma = \frac{\alpha}{k+\gamma} \left(\frac{\epsilon+1}{\epsilon-1} \right)^{\frac{1}{2}}, \quad \text{so that} \quad \tan \Gamma' = -\frac{k+\gamma}{\alpha} \left(\frac{\epsilon+1}{\epsilon-1} \right)^{\frac{1}{2}}$$

Then we may write

$$\left. \begin{aligned}
 J_\alpha(k) &= \frac{[k(k^2-1)]^{\frac{1}{2}}}{\Gamma(k+\frac{1}{2})} (iq/2)^{k-2} \alpha g(\mu-2, k), \\
 J_\alpha(-k) &= \frac{[k(k^2-1)]^{\frac{1}{2}}}{\Gamma(k+\frac{3}{2})} (iq/2)^{k-1} \alpha g'(\mu-1, k+1), \\
 J_\beta(k) &= \frac{k^{\frac{1}{2}}(iq/2)^{k-2}}{2\Gamma(k+\frac{3}{2})} \{ \alpha(k-1)(2k+1)g(\mu-2, k) - \alpha q^2 g(\mu, k+1) - (1+\gamma_1)q^2 f(\mu, k+1) \}, \\
 J_\beta(-k) &= -\frac{2k^{\frac{1}{2}}(iq/2)^{k-1}}{\Gamma(k+\frac{1}{2})} \left\{ \alpha \frac{k+1}{2k+1} g'(\mu-1, k+1) - \alpha g'(\mu-1, k) - (1+\gamma_1)f'(\mu-1, k) \right\},
 \end{aligned} \right\} (42)$$

where we have written $\mu = k + \gamma + \gamma_1$. Every term in each of these equations is real.

Now the fundamental integral occurring here is

$$S(\mu-2, k, \gamma+in) = \int_0^\infty e^{-\rho(\alpha+ip+iq)} \rho^{\mu-2} F(k, 2k; 2iq\rho) F(\gamma+in, 2\gamma; 2ip\rho) \cdot d\rho.$$

We have defined S explicitly only as a function of those parameters which change from term to term in Eqs. (42). This integral was treated⁴⁶ by the author in connection with the same problem. The method indicated in that treatment can be extended, due to the partial symmetry between the two confluent hypergeometric functions in the integrand, to find two forms for the integral. One of these forms is convenient for $h\nu/mc^2 \gg 1$, and the other for $h\nu/mc^2 < 1$. Again because the work is straightforward as indicated in the reference, we shall write down the two forms. The parameters μ, k, γ may, with certain obvious restrictions, be considered as arbitrary.

I.

$$\begin{aligned}
 S(\mu-2, k, \gamma+in) &= \Gamma(\mu-1) e^{-n\beta'} \left(\frac{x}{4pq} \right)^k \frac{1}{B(k, k)} \int_0^1 \frac{(u-u^2)^{k-1}}{(1-xu)^k} a^{-in} \\
 &\quad \cdot \left(\frac{a^{-\frac{1}{2}} e^{i\beta'/2} - a^{\frac{1}{2}} e^{-i\beta'/2}}{2i\beta} \right)^{\mu-2k-1} (ae^{-i\beta'})^{(2\gamma+1-\mu)/2} F(\gamma-in, 2\gamma+1-\mu, 2\gamma; 1-ae^{-i\beta'}) \cdot du.
 \end{aligned}$$

We have here made the following definitions to avoid writing.

$$x = \frac{2p}{\epsilon+p} < 1; \quad a = \frac{1-xu}{(1-x)^{\frac{1}{2}}}; \quad \beta' = 2 \tan^{-1} \frac{1+\gamma_1 p}{\epsilon+1 \alpha}.$$

This form is convenient for investigation near the series limit, where n may be very large, because of the way in which confluence occurs in the integrand when $n \rightarrow \infty, x \rightarrow 0$.

II. The second form is

$$\begin{aligned}
 S(\mu-2, k, \gamma+in) &= \frac{\Gamma(\mu-1) e^{n\beta} q^{2\gamma+1-\mu}}{B(\gamma+in, \gamma-in) |[\alpha+i(p+q)]^{in}|^2} \left(\frac{x}{4pq} \right)^\gamma \\
 &\quad \cdot \int_0^1 \frac{u^{\gamma-1-in} (1-u)^{\gamma-1+in}}{(1-xu)^\gamma (1-x)^{in/2}} \left(\frac{a^{-1} e^{i\beta} - a e^{-i\beta}}{4i} \right)^{\mu-k-\gamma-1} \left(\frac{\eta}{i} \right)^{k-\gamma} F\left(\frac{2k+1-\mu}{2}, \frac{2k+2-\mu}{2}, k+\frac{1}{2}; -\left(\frac{\eta}{i} \right)^2 \right) \cdot du.
 \end{aligned}$$

⁴⁶ H. Hall, Phys. Rev. 38, 66 (1931).

Here we have written

$$\beta = \tan^{-1} \frac{\alpha}{\gamma_1}; \quad \eta = \frac{a^{-\frac{1}{2}}e^{i\beta/2} - a^{\frac{1}{2}}e^{-i\beta/2}}{a^{-\frac{1}{2}}e^{i\beta/2} + a^{\frac{1}{2}}e^{-i\beta/2}}$$

and a is the same as in case I. This is the same form, except for slightly different writing, that has already been used for the problem of very large energies.⁴⁶

The two integrals just given to define S may be studied in the following manner. The range of integration $0 \leq u \leq 1$ is divided into two ranges $0-u_0$, and u_0-1 , where $u_0 = [1 + (1-x)^{\frac{1}{2}}]^{-1}$ is the point where $u(1-u)/(1-xu)$ is a maximum. Let u_1 designate points in the first range, so that $0 \leq u_1, u_1 \leq u_0$; and u_2 points in the second range, so that $u_0 \leq u_2 \leq 1$. Then, if we set $y = xu(1-u)/(1-xu)$, it follows that $u_2 + u_1 = 1 + y$, $u_2 - u_1 = 2[((1+y)/2)^2 - y/x]^{\frac{1}{2}}$. Then we find $u_2 u_1 = y/x$

$$a_1 = (1-xu_1)/(1-x)^{\frac{1}{2}} = [u_1(1-u_1)/u_2(1-u_2)]^{\frac{1}{2}},$$

$$a_2 = 1/a_1$$

and in the same way

$$[(1-u_1)/u_1(1-x)^{\frac{1}{2}}]^{in} = [(1-u_2)/u_2(1-x)^{\frac{1}{2}}]^{-in}.$$

A brief inspection of the integrands in I and II will now show that the integrals are real, as they must be. We write then

$$P = \int_0^1 \left(\frac{xu(1-u)}{1-xu} \right)^{k-1} \frac{f(a(u))}{1-xu} du = \int_0^{u_0} + \int_{u_0}^1$$

$$= \left\{ \int_0^{u_0} - \int_1^{u_0} \right\} \frac{y^{k-1} f(a)}{1-xu} du$$

$$= \int_{y_0}^0 \left[\frac{f(a(u_2))}{1-xu_2} \frac{du_2}{dy} - \frac{f(a(u_1))}{1-xu_1} \frac{du_1}{dy} \right] y^{k-1} dy,$$

$$y_0 = \frac{xu_0(1-u_0)}{1-xu_0} = \frac{1-(1-x)^{\frac{1}{2}}}{1+(1-x)^{\frac{1}{2}}}$$

Now for the cases here presented $f(a_2) = f^*(a_1)$. This follows at once in form II. In I it may be seen by using the relation

$$F(\alpha, \beta, \gamma, x) = (1-x)^{-\beta} F(\gamma - \alpha, \beta, \gamma, -x/(1-x)).$$

We find further from the definitions

$$u_1 = (1+y)/2 - [((1+y)/2)^2 - y/x]^{\frac{1}{2}}, \quad u_2 = (1+y)/2 + [((1+y)/2)^2 - y/x]^{\frac{1}{2}},$$

that $du_2/dy = -(1-xu_2)/x(u_2-u_1), \quad du_1/dy = (1-xu_1)/x(u_2-u_1).$

It therefore follows that

$$P = - \int_{y_0}^0 \frac{f_2 + f_2^*}{2} \frac{y^{k-1}}{[(1+y/2)^2 - y/x]^{\frac{1}{2}}} dy.$$

This form is very convenient for a large class of integrals, including our I and II, because nearly all the contribution to the integral comes for y near y_0 , unless of course the behavior of f dominates over that of y^{k-1} .

⁴⁶ H. Hall, Phys. Rev. 45, 622 (1934).

In case I, when an expansion, for small energies, in p^2 is needed, the substitution

$$y = y_0 e^{-\tau/k}$$

results in the expression

$$P = \frac{y_0^k}{x u_0 k (1-x)^{1/2}} \int_0^\infty \frac{f_2 + f_2^*}{2} \frac{e^{-\tau}}{[t/k + (y_0 t / 2 u_0 k (1-x)^{1/2})^2]^{1/2}} d\tau,$$

where $t = k(1 - e^{-\tau/k})$. The integrand may now be expanded in powers of $\tau^{1/2}$, and due to the $e^{-\tau}$ factor few terms are needed. The actual calculations for the absorption coefficient are tedious and long, and are hardly worth repeating here. In computing the relativistic absorption coefficient near the series limit, it suffices to say, all terms α^2 , $p^2 = (v/c)^2$, and larger ones were retained, with the results as outlined in section 9. There is no appreciable change due to relativistic effects, even for Pb, for frequencies as large as $\nu \sim 2\nu_K$, unless they come from higher terms in α^2 , p^2 .

20. Discussion of τ_K when $h\nu/mc^2 \gg 1$

In this case, many terms in the angular momentum contribute to the sum of Eq. (41). We shall here give an evaluation of the J 's, based on the treatment of the last section, which will lead to the correct value of the CSA in the limit $h\nu/mc^2 \rightarrow \infty$. This means that γ may be set equal to k , since the main contribution will be for k of the order E . The difference between γ_1 and unity will however be maintained, so that the final result will be correct for all α when $h\nu/mc^2 \rightarrow \infty$. This order of approximation allows us to write

$$[k(k^2 - 1)]^{1/2} k^{-\delta_1} = \left[\frac{\Gamma(k + 2 - 2\delta_1)}{(k - 2)!} \right]^{1/2}, \quad \text{where } \delta_1 = 1 - \gamma_1 \sim \alpha^2/2.$$

This allows us to express the J 's in a fairly simple form. We omit a common factor which is independent of k . Then we find

$$\begin{aligned} J_\alpha(k) &= \left[\frac{\Gamma(k + 2 - 2\delta_1)}{(k - 2)!} \right]^{1/2} \int_0^{y_0} y^{k-1} f_1 dy \\ J_\alpha(-k) &= \left[\frac{\Gamma(k + 2 - 2\delta_1)}{(k - 2)!} \right]^{1/2} \int_0^{y_0} y^{k-1} f_4 dy, \\ J_\beta(k) &= \left[\frac{\Gamma(k + 2 - 2\delta_1)}{(k - 2)!} \right]^{1/2} \int_0^{y_0} y^{k-1} \left\{ f_1 - 2f_2 - \frac{2(1 + \gamma_1)}{\alpha} f_3 \right\} dy, \\ J_\beta(-k) &= \left[\frac{\Gamma(k + 2 - 2\delta_1)}{(k - 2)!} \right]^{1/2} \int_0^{y_0} y^{k-1} \left\{ \frac{2(1 + \gamma_1)}{\alpha} f_6 + f_4 - 2f_5 \right\} dy, \end{aligned} \tag{43}$$

where

$$\begin{aligned} f_1 &= \left[\left(\frac{1+y}{2} \right)^2 - \frac{y}{x} \right]^{-1/2} \text{Real} \left(\frac{1-u}{u(1-x)^{1/2}} \right)^{in} \left(\frac{a^{-1/2} e^{i\beta/2} - a^{1/2} e^{-i\beta/2}}{2i} \right)^{-\delta_1} \left(\frac{a^{-1/2} e^{i\beta/2} + a^{1/2} e^{-i\beta/2}}{2} \right)^{-\delta_1}, \\ f_2 &= \left[\quad \quad \quad \right]^{-1/2} \text{Real} \left(\quad \quad \quad \right)^{in} \left(\quad \quad \quad \right)^{2-\delta_1} \left(\quad \quad \quad \right)^{-\delta_1}, \\ f_3 &= \left[\quad \quad \quad \right]^{-1/2} \text{Real} \left(\quad \quad \quad \right)^{in} \left(\quad \quad \quad \right)^{1-\delta_1} \left(\quad \quad \quad \right)^{1-\delta_1}, \end{aligned}$$

$$\begin{aligned}
 f_4 &= \left[\quad \right]^{\frac{1}{2}} \text{Real} \left(\quad \right)^{in} \left(\quad \right)^{-\delta_1} \left(\quad \right)^{-\delta_1}, \\
 f_5 &= \left[\quad \right]^{\frac{1}{2}} \text{Real} \left(\quad \right)^{in} \left(\quad \right)^{-\delta_1} \left(\quad \right)^{2-\delta_1}, \\
 f_6 &= \left[\quad \right]^{\frac{1}{2}} \text{Real} \left(\quad \right)^{in} \left(\quad \right)^{1-\delta_1} \left(\quad \right)^{1-\delta_1}.
 \end{aligned}$$

The empty spaces in the brackets here are to be filled with the quantities in the corresponding brackets of f_1 .

One point connected with the derivation of Eqs. (43) we may mention here. When terms in $1/\epsilon$, or what is the same thing, when terms in $1/k$ are dropped, we may omit the first terms of f and g' , and the second terms of f' and g . That is, we may write, from Eqs. (40),

$$\begin{aligned}
 f &= N \cdot \frac{1}{2(2k+1)} G_{k+1}(\rho), & \text{when } k > 0, \\
 g &= N \cdot G_k(\rho), \\
 f' &= -N \cdot G_k(\rho), \\
 g' &= N \cdot \frac{1}{2(2k+1)} G_{k+1}(\rho) & \text{when } k < 0.
 \end{aligned}$$

In the case of f' , g' , the sign of k has already been changed, of course, so that the absolute value of k is intended here.

We see $f_1=f_4$, $f_3=f_6$. The expression $a(u)$ is the same as in the last section. It is seen that $y \cong y_0 \cong 1 - 1/\epsilon < 1$. Hence it will be permissible to square the J 's, obtaining a double integral for each one, and then to change the order of summing and integrating. We proceed in this manner. In the double integral resulting, after the sum over $k=2, 3, \dots$, is completed, there will be two variables of integration, y_1 and y_2 say. If the substitutions $y_1=y_0(1-2u/\epsilon)$, $y_2=y_0(1-2v/\epsilon)$ are made, and finally we go to the limit $\epsilon \rightarrow \infty$, we find after some work

$$\begin{aligned}
 \tau_K &= N_0 \cdot 4\pi a_0^2 \alpha_0^3 \frac{Z^5 (1 - \frac{2}{3}\delta_1) \exp(-\pi\alpha + 2\alpha \tan^{-1} \alpha/\gamma_1)}{\epsilon (1 - \delta_1/2) \alpha^{2\delta_1}} \frac{3}{8} \\
 &\cdot \int_0^\infty \int_0^\infty dudv \frac{[(\cos^2(\beta/2) + u)(4 \sin^2(\beta/2) + 4u) \cdot (\cos^2(\beta/2) + v)(4 \sin^2(\beta/2) + 4v)]^{-\delta_1/2}}{[u(1+u)v(1+v)]^{\frac{1}{2}}(1+u+v)^{4-2\delta_1} \{ \quad \}^{-1}}.
 \end{aligned}$$

All factors have been restored in τ_K . Here $\sin \beta = \alpha$, so that $\sin^2 \beta/2 = \delta_1/2$, etc. The bracket, left blank in the integral, is

$$\begin{aligned}
 \{ \quad \} &= \{ \cos \varphi(u) \cos \varphi(v) + [(1+2u) \cos \varphi(u) - 2 \cot \beta/2 (u+u^2)^{\frac{1}{2}} \sin \varphi(u)] \\
 &\quad \cdot [(1+2v) \cos \varphi(v) - 2 \cot \beta/2 (v+v^2)^{\frac{1}{2}} \sin \varphi(v)] \},
 \end{aligned}$$

where

$$\varphi(u) = \alpha \log \frac{(1+u)^{\frac{1}{2}} + u^{\frac{1}{2}}}{(1+u)^{\frac{1}{2}} - u^{\frac{1}{2}}} - \delta_1 \tan^{-1} \frac{2\gamma_1 (u+u^2)^{\frac{1}{2}}}{\alpha (1+2u)}.$$

This formulation is exact for the limit $\epsilon \rightarrow \infty$.

Now let us consider the double integral above, for the case $\alpha=0$. It may then be written

$$\int_0^\infty \int_0^\infty \frac{dudv \left\{ 1 + \left[1 + 2u - 4(u+u^2)^{\frac{1}{2}} \log \frac{(1+u)^{\frac{1}{2}} + u^{\frac{1}{2}}}{(1+u)^{\frac{1}{2}} - u^{\frac{1}{2}}} \right] \cdot [\text{same for } v] \right\}}{[(u+u^2)(v+v^2)]^{\frac{1}{2}}(1+u+v)^4}. \tag{44}$$

Partial integration shows that we may write in the integral

$$\{ \quad \} = 1 + (1+2u)(1+2v) = 2(1+u+v+2uv). \quad (45)$$

One may now prove that the integral above, where α is neglected, is equal to $8/3$. Because of the factor $(1+u+v)^{-4}$, the chief value of the integral is contributed for rather small values of u, v . Thus, if in the factors depending on α, u and v are set equal to zero, one obtains Eq. (17) at once on replacing the expression

$$\frac{1 - \frac{2}{3}\delta_1 \exp(2\alpha \tan^{-1} \alpha/\gamma_1)}{1 - \delta_1/2} \frac{\alpha^{2\delta_1}}{\alpha^{2\delta_1}}$$

by the approximate expression $e^{2\alpha^2/\alpha^2}$, and by making a similar change in the removed factor.

Now although the important values of u and v are small, a somewhat better result than Eq. (17) can be obtained by another approximation of $u_{\alpha v}, v_{\alpha v}$. An inspection of expression (44) shows that u and v can be set equal to about $1/7$ in the slowly varying factors, and the correct result $8/3$ will be found. Consequently, if we set $u=v=1/7$ in the part of the original integral depending on α , we find approximately

$$\tau_K = \tau_K^0 \cdot \frac{1 - \frac{2}{3}\delta_1 \exp(-\pi\alpha + 2\alpha \tan^{-1}(\alpha/\gamma_1))}{1 - \delta_1/2} \frac{\alpha^{2\delta_1}}{\alpha^{2\delta_1}} \left[\frac{(1+2/7)^2}{(1+1/7)(\alpha^2+4/7)} \right]^{\delta_1} \left(1 + 0.05\alpha \tan^{-1} \frac{0.63}{\alpha} \right),$$

where τ_K^0 represents the value obtained for τ_K from Eq. (17) by setting $\alpha=0$. We rewrite the above expression for τ_K in the form

$$\tau_K = \frac{\tau_K^0}{\alpha^{2\delta_1} e^{\alpha\pi - 2\alpha}} \cdot \frac{1 - \frac{2}{3}\delta_1 \exp[2\alpha(\tan^{-1}(\alpha/\gamma_1) - \alpha)]}{1 - \delta_1/2} \frac{\alpha^{4\delta_1 - 2\alpha^2}}{\alpha^{4\delta_1 - 2\alpha^2}} \left(\frac{81}{8(7+4/\alpha^2)} \right)^{\delta_1} \left(1 + 0.05\alpha \tan^{-1} \frac{0.63}{\alpha} \right).$$

The factor by which this differs from τ_K in Eq. (17) may now be computed. For $\alpha=0.6$ (Pb), we find it to be about 0.96, or only 4 percent lower. A more careful determination of the error in Eq. (17) due to α could now be made along similar lines, but due to the small part τ_K plays in the *total* absorption for large frequencies, this hardly seems worth while. Particularly since our estimate of the error above proves it is not large.

Concerning the relative contribution of the J 's to τ_K when $h\nu/mc^2 \gg 1$, we see that $J_\alpha(k)$ and $J_\alpha(-k)$ contribute equally and $J_\beta(k)$ and $J_\beta(-k)$ contribute equally. In expression (45), $1+(1+2u)(1+2v)$, $J_\alpha(+k)$ and $J_\alpha(-k)$ may be considered to be responsible for $\frac{1}{2}$ each; $J_\beta(k)$, $J_\beta(-k)$ for $(1+2u)(1+2v)/2$ each. Or, it may be stated, the spin states α and β contribute approximately the fractions $\frac{3}{8}$ and $\frac{5}{8}$, respectively, to τ_K .

21. Discussion for τ_L when $h\nu/mc^2 \gg 1$

The $L_I(2S_{1/2})$ shell contains two electrons, which, in the notation of section 18, are typified by the quantum members $j=\frac{1}{2}$, $m=\pm\frac{1}{2}$, $k=1$. The corresponding wave functions are

$$\begin{array}{l|l} m = \frac{1}{2} & \begin{array}{l} \psi_1 = i(\frac{1}{3})^{1/2} f Y_{1,0} \\ \psi_2 = i(\frac{2}{3})^{1/2} f Y_{1,1} \\ \psi_3 = -g Y_{0,0} \\ \psi_4 = 0 \end{array} \\ \hline m = -\frac{1}{2} & \begin{array}{l} \psi_1 = i(\frac{2}{3})^{1/2} Y_{1,-1} \\ \psi_2 = i(\frac{1}{3})^{1/2} f Y_{1,0} \\ \psi_3 = 0 \\ \psi_4 = g Y_{0,0} \end{array} \end{array}$$

The energy of both electrons is the same, being given by $\epsilon = (1 - \delta_{1/2})^{\frac{1}{2}}$. The functions f and g can be found at once from Eqs. (36). The absorption coefficient can now be written out from Eqs. (42) by making the appropriate changes in the bound state. This is true because the components ψ_i have the same angle dependence as those for the *normal state*.

The work is thenceforth about the same as for the K shell, and we shall not give any of the details. We find approximately,

$$\tau_{L_1}/\tau_K = \frac{1}{8} \cdot 2^{2\alpha^2}.$$

This gives for the ratio, 0.20 for Pb, 0.15 for Sn.

22. Angular distribution for the K shell

To find the contribution to the angle distribution from one normal state (α), we must sum the product

$$\psi_{m, l, j} J_{m, l, j; \alpha}$$

over all values of m, l, j to which transitions occur. This gives

$$\Psi_\alpha = \sum \psi_{m, l, j} J_{m, l, j; \alpha}.$$

The angle distribution (radial current) will then be given by

$$s_r^\alpha = \Psi_\alpha^* \alpha_i \Psi_\alpha.$$

To this must be added s_r^β , obtained in the same way using J_β . We find then

$$\Psi_\alpha = \sum_{m, l} \{ \psi_{m, l}^{a'} J_{m, l; \alpha}^{a'} + \psi_{m, l}^{b'} J_{m, l; \alpha}^{b'} \},$$

$$\Psi_\beta = \sum_{m, l} \{ \psi_{m, l}^{a'} J_{m, l; \beta}^{a'} + \psi_{m, l}^{b'} J_{m, l; \beta}^{b'} \},$$

$$J_{m, l; \alpha}^{a'} = J_\alpha^{\frac{1}{2}}(-k) + J_\beta^{-\frac{1}{2}}(-k),$$

$$J_{m, l; \alpha}^{b'} = J_\alpha^{\frac{1}{2}}(k) - J_\beta^{-\frac{1}{2}}(k),$$

$$J_{m, l; \beta}^{a'} = J_\alpha^{-\frac{1}{2}}(-k) + J_\beta^{\frac{1}{2}}(-k),$$

$$J_{m, l; \beta}^{b'} = -J_\alpha^{-\frac{1}{2}}(k) + J_\beta^{\frac{1}{2}}(k).$$

We then find

$$\Psi_\alpha = \sum_l \{ \psi_{l, 3/2}^{a'} J_\alpha(-k) + \psi_{l, -1/2}^{a'} J_\beta(-k) + \psi_{l, 3/2}^{b'} J_\alpha(k) - \psi_{l, -1/2}^{b'} J_\beta(k) \},$$

$$\Psi_\beta = \sum_l \{ \psi_{l, -3/2}^{a'} J_\alpha(-k) + \psi_{l, 1/2}^{a'} J_\beta(-k) - \psi_{l, -3/2}^{b'} J_\alpha(k) + \psi_{l, 1/2}^{b'} J_\beta(k) \}.$$

where $J_\alpha(\pm k)$, $J_\beta(\pm k)$ are now given by Eqs. (42). If we now neglect all terms in $(v/c)^2$, s_r^α and $\Psi_\alpha \Psi_\alpha^*$ are equivalent expressions for the current. Even when the first power in v/c is neglected the calculations are tedious, and the net effect of α^2 is small. We shall omit all details and merely state the result for $(v/c) = 0$.

$$\Psi_\alpha \Psi_\alpha^* \sim \sin^2 \theta [\cos^2 \varphi - \alpha^2 \{ (0.086 - 0.428 \cos^2 \theta) \cos^2 \varphi + (\pi/8) \sin 2\varphi \}],$$

$$\Psi_\beta \Psi_\beta^* \sim \sin^2 \theta [\cos^2 \varphi - \alpha^2 \{ (0.026 - 0.132 \cos^2 \theta) \cos^2 \varphi - (\pi/8) \sin 2\varphi \}].$$

The sum of these expressions gives the radial current as already presented in Section 12.

$$J \sim \sin^2 \theta \cos^2 \varphi [1 - \alpha^2 (0.056 - 0.280 \cos^2 \theta)].$$

The contributions from the two spin states α and β are observed here to differ, particularly in the $\sin 2\varphi$ term. This latter difference however is of course impossible to observe.