THE MASS ABSORPTION COEFFICIENT OF THE K SHELL ACCORDING TO THE DIRAC RELATIVISTIC THEORY OF THE ELECTRON*

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Abstract

Taking as model an atom containing two non-interacting electrons and a fixed nucleus with charge Ze, the mass absorption coefficient is calculated by use of the proper functions of the Dirac relativistic equation. Z is determined so as to make the lowest energy level agree with the experimental value determined from the K absorption edge. The numerical calculation presented difficulty because of lack of tables of complex gamma functions. The relativistic coefficient is found to be from 0 to 40 percent smaller than the non-relativistic coefficient calculated by Nishina and Rabi, the greatest difference occurring for the heavy elements and short wave-lengths; it agrees slightly worse with experiment than the non-relativistic coefficient. The difference between theory and experiment is least for the heavy atoms, as would be expected, since for the heavy atoms (large Z) the neglected electronic interaction-field is small in comparison with the nuclear field. The variation of the relativistic coefficient with wave-length is complicated, but in the range $\frac{1}{2}\lambda_k$ to λ_k (λ_k = wave-length of K absorption edge) it is more nearly linear with λ^3 than the non-relativistic coefficient. The importance of using the relativistic equation for heavy atoms and short x-ray wavelengths is emphasized by these results, which also show that the model chosen is too approximate, even for the heavy elements.

The general normalizing factors for the discrete and continuous spectrum proper functions of a hydrogen-like atom are given.

Inroduction and Results

SEVERAL attempts[1] have been made, with classical or semi-classical theories, to calculate the atomic absorption coefficient for the K shell. More recently Wentzel[2] and Oppenheimer[3] obtained approximate formulae using non-relativistic quantum mechanics, while Nishina and Rabi[4] have given the explicit formula which follows from the Schrödinger theory. The comparison with experiment made by the latter authors shows fairly good agreement for the heavy elements and poor agreement for the light elements.

The purpose of the present paper is to calculate the mass absorption coefficient by use of the Dirac relativistic equation, and to compare the results

* Abridged Cornell Dissertation. Presented at the Cleveland Meeting of the American Physical Society, Dec. 30–31, 1930.

[1] J. J. Thomson, Conduction of Electricity. Through Gases, 2d Ed., p. 321; L. de Broglie, Journ. de Phys. et Rad. **3**, 33, (1922); A. H. Compton, Nat. Res. Council, Bul. **20**, 37, (1922); H. A. Kramers, Phil. Mag. **46**, 836, (1923).

[2] G. Wentzel, Zeits. f. Physik **40**, 574, (1926).

[3] J. R. Oppenheimer, Zeits. f. Physik **41**, 268, (1926).

[4] Y. Nishina and I. I. Rabi, Verh. d. deut. Phys. Ges. **9**. 6, (1928).

with experiment and with the non-relativistic theory. One can readily see from correspondence principle arguments that for the K electrons of the heavy atoms the relativity corrections should be important, and this is confirmed by the results.

The atom model used here as in the non-relativistic calculations consists of two non-interacting electrons in the field of a fixed nucleus with charge

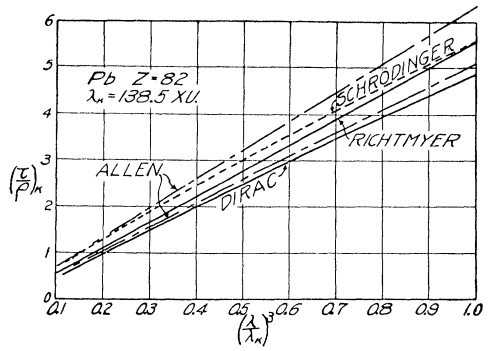

Fig. 1. The mass absorption coefficient for lead. The curves marked Allen and Richtmyer are plots of the experimental data.[7]

Z^*e, where Z^* is that charge (smaller than the true charge Z) which makes the lowest energy level of the atom model agree with the experimental value. It is obvious that this model will be most nearly correct when the interaction of the K electrons with the nucleus is large compared with their interaction with each other and with the outer electrons, i.e., for the heavy elements.

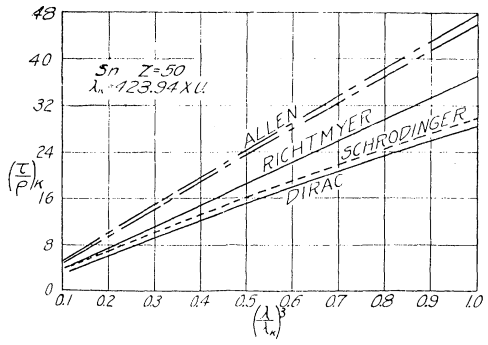

Fig. 2. The mass absorption coefficient for tin. The curves marked Allen and Richtmyer are plots of the experimental data.[7]

The calculation proceeds as follows: by use of the Dirac radiation theory[5] combined with the Dirac relativistic equation[6] the general formula for the absorption probability is derived. This formula contains a certain matrix element which is then evaluated for the case of the transition between the K

[5] P. A. M. Dirac, Roy. Soc. Proc. **A114**, 243 and 710, (1927).
[6] P. A. M. Dirac, Roy. Soc. Proc. **A117**, 610, (1928).

level and a state of the continuous spectrum corresponding to the removal of one of the K electrons. The resulting formula for the mass absorption coefficient of the K shell is then calculated numerically. The last two operations constitute what is new in the paper. The final formula is quite complicated so that the numerical calculation is very laborious, especially because of lack of tables of the gamma function of complex argument.

The results of the present calculation are collected in the Table I and Figs. 1–3. The relativistic theory gives values of the absorption coefficient which are consistently lower than those of the non-relativistic theory, the difference varying from about 40 percent for Pb at $\frac{1}{2}\lambda_k$ to less than 1 percent for Al at λ_k. The calculated absorption coefficients for Al cannot be compared with experiment because of lack of data for the long wave-lengths, but show how closely the two quantum-mechanical theories agree for the light elements.

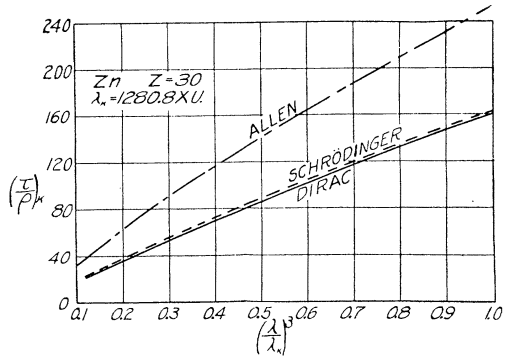

Fig. 3. The mass absorption coefficient for zinc. The curve marked Allen is a plot of the experimental data.[7]

It is found experimentally[7] that the mass absorption coefficient varies linearly with λ^n where n ranges from 2.9 to 3 and apparently changes in value with the wave-length. The classical and semi-classical theories referred to above all give a linear variation with λ^3. The quantum-mechanical theories predict a more complicated variation with λ, the non-relativistic theory indicating an exponent[8] 2.87 at $\lambda=\frac{1}{2}\lambda_k$ and 8/3 at $\lambda=\lambda_k$(λ_k=wave-length of K edge). The relativistic theory here developed gives an exponent which is somewhat closer to three for the heavy elements over the range $\frac{1}{2}\lambda_k$ to λ_k. For example, for Pb the exponent is 2.86 at $\lambda=\lambda_k$ and 3.13 at $\lambda=\frac{1}{2}\lambda_k$. For the light elements the two theories agree closely for wave-lengths which are not too short.

There are a number of reasons, aside from the inadequacy of the model, for the disagreement between theory and experiment.[9] In the first place, the

[7] F. K. Richtmyer, Phys. Rev. **27,** 1, (1926); **30,** 755, (1927). S. J. M. Allen, Phys. Rev. **28,** 907, (1926).

[8] As pointed out to me by Professor Kennard, the expression of the theoretical results in terms of these exponents is misleading, since the relation given by the quantum mechanics may be written $C(\lambda)\lambda^{n(\lambda)}$, not $K\,\lambda^{n(\lambda)}$ (K independent of λ).

[9] I wish to thank Professor F. K. Richtmyer for helpful discussions on these points.

TABLE I. *Mass absorption coefficient* $(\tau/\rho)_K$.

λ in X.U.†	λ_k/λ	Calculated Dirac	Calculated Schröd-inger	Percent Differ-ence††	Observed Richt-myer[7]	Observed Allen[7]	Expon-ent of λ (calc.)
			Pb $Z=82$				
138.5	1.0	4.86	5.58	14.6	5.56	5.10 to 6.35	2.86
125.9	1.1	3.70	4.32	16.9	4.18	3.76 to 4.79	
115.4	1.2	2.85	3.41	19.8	3.22	3.00 to 3.72	
106.5	1.3	2.24	2.75	22.6	2.53	2.35 to 2.95	
98.9	1.4	1.79	2.24	25.4	2.03	1.89 to 2.37	
92.3	1.5	1.44	1.85	28.1	1.65	1.53 to 1.93	
86.6	1.6	1.18	1.55	30.0	1.36	1.26 to 1.62	
81.5	1.7	0.97	1.30	33.9	1.13	1.06 to 1.36	
76.9	1.8	0.81	1.11	37.0	0.95	0.89 to 1.15	
72.9	1.9	0.68	0.95	40.1	0.81	0.77 to 0.98	
69.3	2.0	0.58	0.82	42.8	0.70	0.65 to 0.86	3.13
			Sn $Z=50$				
423.94	1.0	28.5	29.8	4.6	37.0	45.9 to 47.7	2.75
385.40	1.1	21.9	23.1	5.5	27.8	34.7 to 36.1	
353.28	1.2	17.2	18.2	6.3	21.4	26.9 to 28.0	
326.11	1.3	13.7	14.7	7.4	16.9	21.4 to 22.2	
302.81	1.4	11.0	12.0	8.4	13.5	17.2 to 17.9	
282.63	1.5	9.03	9.89	9.5	11.0	13.9 to 14.6	
264.96	1.6	7.48	8.26	10.4	9.02	11.5 to 12.1	
249.38	1.7	6.24	6.97	11.7	7.52	9.6 to 10.2	
235.52	1.8	5.26	5.93	12.8	6.34	8.0 to 8.5	
223.13	1.9	4.47	5.09	14.0	5.39	6.9 to 7.4	
211.97	2.0	3.82	4.40	15.2	4.62	5.9 to 6.3	2.96
			Zn $Z=30$				
1280.8	1.0	161	163	1.5	..	254	2.67
1164.4	1.1	125	127	1.3	..	199	
1067.3	1.2	98.2	100	1.9	..	181	
985.2	1.3	78.5	80.4	2.4	..	130	
914.9	1.4	63.9	65.6	2.7	..	107	
853.9	1.5	52.6	54.2	3.2	..	90	
800.5	1.6	43.8	45.3	3.5	..	76	
753.4	1.7	37.0	38.2	3.3	..	64	
711.6	1.8	31.2	32.6	4.4	..	54	
674.1	1.9	26.6	27.9	5.1	..	46	
640.4	2.0	22.9	24.2	5.4	..	40	2.87
			Al $Z=13$				
7947.0	1.0	2453	2459	0.3	..	..	2.67
7224.5	1.1	1905	1905	0.0	..	..	
6622.5	1.2	1493	1505	0.8	..	..	
6113.1	1.3	1205	1210	0.4	..	..	
5675.4	1.4	987	987	0.0	..	..	
5298.0	1.5	811	816	0.5	..	..	
4966.9	1.6	677	682	0.7	..	..	
4674.7	1.7	571	575	0.8	..	..	
4415.0	1.8	485	490	0.9	..	..	
4182.6	1.9	416	420	1.0	..	..	
3973.5	2.0	359	363	1.2	..	..	2.87

† The values of λ_K are taken from the article by Grebe in Geiger-Scheel's Handb. d. Phys, XXI, p. 336.

†† The percent difference is calculated from the Dirac value as base.

true absorption coefficient is not measured experimentally, since scattering is always present. The scattering coefficient, though small in comparison with the true absorption coefficient over the range $\frac{1}{2}\lambda_k$ to λ_k, varies in an un-

known[10] manner with the wave-length. In the second place, the experimenter measures the absorption coefficient for all the electrons in the atom, so that one must extrapolate the absorption curve for the $L+M+N+\cdots$ electrons down to wave-lengths below the K edge and then subtract this from the total absorption in this range to get the absorption coefficient for the K electrons. Such an extrapolation, while it may introduce only a small error in the magnitude of the absorption coefficient, can easily change its variation with wave-length. Finally, even an exact model of an *isolated* atom would be incorrect, since the experimental measurements are usually made upon atoms in crystals. In the writer's opinion the above effects are not large enough to account for the discrepancy which, as already suggested by Nishina and Rabi,[4] must be due to the inadequate model. The results obtained here show clearly that for the K shell of the heavy elements the relativistic theory must be used in conjunction with the correct model.

It should be possible to use a much better model for which the discrete proper functions are obtained by the variational method which has recently been used with such success, but how one can obtain more nearly correct proper functions for the continuous spectrum remains a difficult problem.

The Probability of Absorption

According to Dirac[6] the motion of an electron in an electromagnetic field with the vector potential A and scalar potential V is described by the wave-equation

$$\left[\frac{W+eV}{c}+\rho_1\mathfrak{d}\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)+\rho_3 mc\right]\psi=0, \tag{1}$$

in which W is the energy parameter, $\boldsymbol{p}$ the momentum vector-operator with components $(h/2\pi i)(\partial/\partial x)$, $\cdots$, and ρ_1, ρ_3, and $\mathfrak{d}$ are certain matrices having four rows and columns. The probability amplitude ψ is also a matrix having four rows and only one column. We shall let V represent the field of the fixed nucleus, and choose the vector potential $\boldsymbol{A}$ of the external field so that its scalar potential vanishes.

From Eq. (1) we obtain for the Hamiltonian function of the electron

with
$$\begin{aligned} H_e &= H_0 - e\rho_1\mathfrak{d}A \\ H_0 &= -c\rho_1\mathfrak{d}\cdot\boldsymbol{p}-\rho_3 mc^2-eV. \end{aligned} \tag{2}$$

H_0 is the Hamiltonian for the motion in the nuclear field alone. We now suppose the electromagnetic field to be quantized according to the Dirac[5] scheme, and obtain with Waller,[11] taking retardation into account, the following Hamiltonian for the system atom plus field:

$$\begin{aligned} H = H_0 &+ \sum_r N_r h\nu_r \\ &- \sum_r \rho_1(\mathfrak{d}\mathfrak{U}_r)\left\{N_r^{1/2}e^{2\pi i/h[\Theta_r-(\boldsymbol{\kappa}_r\boldsymbol{x}_\cdot)]}+e^{-2\pi i/h[\Theta_r-(\boldsymbol{\kappa}_r\cdot\boldsymbol{x})]}N_r^{1/2}\right\} \end{aligned} \tag{3}$$

[10] This variation is very difficult to determine experimentally. For the most recent data see E. N. Coade, Phys. Rev. **36**, 1109, (1930).

[11] I. Waller, Zeits. f. Physik **58**, 75, (1929).

where N_r and Θ_r are operators which obey the relation

$$N_r e^{2\pi i\Theta_r/h} - e^{2\pi i\Theta_r/h} N_r = e^{2\pi i\Theta_r/h},$$

$\mathbf{x}$ is a vector with origin at the nucleus which gives the position in space, and

$$\mathfrak{y}_r = \left(\frac{e^2 h\nu_r}{2\pi c\sigma_r}\right)^{1/2} \boldsymbol{r}; \quad \kappa_r = \frac{h\nu_r}{c}\boldsymbol{n}_r, \tag{3'}$$

where $\sigma_r d\nu_r d\omega_r$ is the number of components r of the radiation field with given polarization $\boldsymbol{r}$ in the frequency interval $d\nu_r$ and with direction of motion in the element of solid angle $d\omega_r$ about $\boldsymbol{n}_r$.

If the stationary states of the atom are specified by the J''s, while N_r' is the number of photons in the component r, we obtain from the general transformation theory the Schrödinger equation corresponding to the Hamiltonian (3)[12]

$$\begin{aligned}\left[\frac{h}{2\pi i}\frac{\partial}{\partial t} + W(J'') + \sum_r N_r' h\nu_r\right]\Phi(J''; N_1', \cdots, N_r' \cdots) \\ = \sum_{J'}\sum_s \mathfrak{y}_s [N_s'^{1/2} A^s(J''J')\Phi(J'; N_1' \cdots N_{s-1}', N_s' - 1, N_{s+1}' \cdots) \\ + (N_s' + 1)^{1/2} B^s(J''J')\Phi(J'; N_1' \cdots N_{s-1}', N_s' + 1, N_{s+1}' \cdots)]\end{aligned} \tag{4}$$

with

$$\left.\begin{aligned} A^s(J''J') &= \int \psi_{J''}^*(\mathbf{x})\rho_1 \mathfrak{d}\,\psi_{J'}(\mathbf{x}) e^{-2\pi i(\boldsymbol{\kappa}_s\cdot\boldsymbol{x})/h} d\mathbf{x} \\ B^s(J''J') &= \int \psi_{J''}^*(\mathbf{x})\rho_1 \mathfrak{d}\,\psi_{J'}(\mathbf{x}) e^{+2\pi i(\boldsymbol{\kappa}_s\cdot\boldsymbol{x})/h} d\mathbf{x} \end{aligned}\right\} \tag{4'}$$

where $\psi_{J'}(\mathbf{x})$ and $W(J')$ are the characteristic function and characteristic value for the motion of the electron in the nuclear field. $|\Phi(J'; N')|^2$ gives the probability for the state $(J'; N')$ of the system, atom plus field.

In Eq. (4) the sum with respect to J' is to include an integral over the continuous spectrum if one is present. In this case the probability of finding the atom in the range $d\epsilon'$ about ϵ' is given by $|\Phi(\epsilon'; N')|^2 d\epsilon'$, where for the continuous spectrum ϵ' is used for J'.

It should be noted that the sum over J' in Eq. (4) includes the negative energy states of the atom. They do not cause difficulty in our application to absorption because here we can restrict ourselves to transitions between states having positive energy. Waller[12] has shown the importance of the negative energy states in calculating scattering and dispersion.

We want to calculate the transition probability $wd\epsilon''$ for an absorption process in which the atom jumps from an initial discrete state J' to a final state in the range $d\epsilon''$ about ϵ'' in the continuous spectrum, with absorption of a photon of definite direction (in $d\omega_s$) and definite polarization, regardless

[12] I. Waller, Zeits. f. Physik **61**, 837 (1930).

of what the final frequency state of the field may be. We suppose for the moment that the atomic states are non-degenerate.

The initial state of the field is to be taken as follows: only photons having a direction of motion within a solid angle $d\omega_s$ about n_s, a definite polarization $\mathbf{s}$, but arbitrary frequency ν_{sr}, where r expresses the variation in frequency of the component s, are to be present. For physically interesting results, the range of variation of ν_{sr} about the frequency corresponding to the atomic transition must be at least as great as the natural line breadth.

Following the well-known method,[5] we calculate the probability of the above-mentioned atomic transition with absorption of a photon of frequency ν_{sr}, and then sum over all such frequencies, obtaining finally for a time t which is large compared with the atomic period but small compared with the mean life time of the state under consideration

$$wd\epsilon'' = \frac{2\pi e^2 c^2 t}{h^2\nu^2} \left| \mathbf{s} \cdot \boldsymbol{B}^s(\epsilon''; J') \right|^2 \rho(\nu) d\omega_s d\epsilon'' \tag{5}$$

where

$$h\nu = W(\epsilon'') - W(J'), \tag{6}$$

and $\rho(\nu)$ is the spectral energy density per unit frequency range per unit solid angle for a definite polarization.

Our temporary assumption that the atomic states are non-degenerate is not true. According to the general theory of quantum mechanics, as presented by Born and Jordan,[13] when the assembly of atoms is in thermal equilibrium before the absorption process occurs, we merely add together those transition probabilities relating to transitions between the degenerate states. Therefore we obtain finally for the transition probability $wd\epsilon''$

$$wd\epsilon'' = d\omega_s \frac{2\pi e^2 c^2 t}{h^2\nu^2} \sum \left| \mathbf{s} \cdot \boldsymbol{B}^s(\epsilon''; J') \right|^2 \rho(\nu) d\epsilon'' \tag{7}$$

where the sum is to be taken over all initial states having the same energy and over all final states having the same energy.

In many practical applications we are interested in the absorption probability for arbitrary direction of motion and polarization of the absorbed photon. We can obtain this from Eq. (7) by summing over all directions of motion $d\omega_s$ and all polarizations $\mathbf{s}$. When the wave-length of the incident light is long compared with atomic dimensions, so that we can replace the exponential factor in the matrix element $\boldsymbol{B}^s$ in Eq. (4′) by unity, we can easily carry out this summation, obtaining for the absorption probability $w'd\epsilon''$ per unit time for arbitrary direction of motion and polarization of the absorbed photon

$$w'd\epsilon'' = \frac{16\pi^2 e^2 c^2}{3h^2\nu^2} \sum \left| P(\epsilon''; J') \right|^2 \rho(\nu) d\epsilon'' \tag{8}$$

[13] M. Born and P. Jordan, "Elementare Quantenmechanik," pp. 299, 321, and 329

where

$$|P|^2 = |B_x|^2 + |B_y|^2 + |B_z|^2. \tag{8'}$$

Solutions of the Dirac Equation

The solutions of Eq. (1) for the case when $\boldsymbol{A}=0$ and $V=Ze/r$ have been given by Darwin.[14] For given l and $u(=m-\frac{1}{2})$ there are two sets of solutions. We label these by introducing the quantum number j, which takes on the values $j=l\pm\frac{1}{2}$ to agree with spectroscopic notation. The two sets are:[15]

$$\begin{aligned}
j &= l+\tfrac{1}{2} & & & j &= l-\tfrac{1}{2} & & \\
\psi_1 &= -iM_\theta F_l P_{l+1}^u & & & \psi_1 &= -i(l+u)M_\theta F_{-l-1}P_{l-1}^u & & \\
\psi_2 &= -iM_\theta F_l P_{l+1}^{u+1} & & (9a) & \psi_2 &= i(l-u-1)M_\theta F_{-l-1}P_{l-1}^{u+1} & & (9b)\\
\psi_3 &= (l+u+1)M_\theta G_l P_l{}^u & & & \psi_3 &= M_\theta G_{-l-1}P_l{}^u & & \\
\psi_4 &= -(l-u)M_\theta G_l P_l{}^{u+1} & & & \psi_4 &= M_\theta G_{-l-1}P_l{}^{u+1}, & &
\end{aligned}$$

in which M_θ is the part of the total normalizing factor associated with the angular coordinates. The radial functions F_l and G_l contain their own normalizing factor.

The function $P_l{}^u(\theta, \phi)$ is a spherical harmonic defined by Darwin as follows:

$$P_l{}^u = (l-u)!\sin^l\theta\left(\frac{d}{d\cos\theta}\right)^{l+u}\frac{(\cos^2\theta-1)^l}{2^l l!}e^{iu\phi}. \tag{10}$$

The radial functions F_l and G_l satisfy the equations

$$\begin{aligned}
\frac{2\pi}{h}\left(\frac{W+eV}{c}+mc\right)F_l + \frac{dG_l}{dr} - \frac{l}{r}G_l &= 0\\
-\frac{2\pi}{h}\left(\frac{W+eV}{c}-mc\right)G_l + \frac{dF_l}{dr} + \frac{l+2}{r}F_l &= 0.
\end{aligned} \tag{11}$$

We shall use the solutions of Eq. (11) given by Gordon.[16] These are:

Discrete Spectrum: $W/mc^2<1$

$$\begin{aligned}
F_l &= \left(\frac{N_l-\rho_l-n_r}{N_l+\rho_l+n_r}\right)^{1/2} M_r(\sigma_1-\sigma_2)\\
G_l &= M_r(\sigma_1+\sigma_2)
\end{aligned} \tag{12}$$

$$\begin{aligned}
\sigma_1 &= (N_l+l+1)r^{\rho_l-1}e^{-k_0 r}{}_1F_1(-n_r;\ 2\rho_l+1;\ 2k_0 r)\\
\sigma_2 &= -n_r r^{\rho_l-1}e^{-k_0 r}{}_1F_1(-n_r+1;\ 2\rho_l+1;\ 2k_0 r)
\end{aligned} \tag{13}$$

[14] C. G. Darwin, Roy. Soc. Proc. **A118**, 654 (1928).

[15] In interpreting Eq. (9) it should be noted that in certain cases meaningless spherical harmonics are cancelled by a zero factor. Thus when $l=0$, and $u=-1$, ψ_3 in (9a) is to be taken to be zero.

[16] W. Gordon, Zeits. f. Physik **48**, 11 (1928).

where

$$
\begin{aligned}
{}_1F_1(\alpha;\beta;x) &= \sum_{n=0}^{\infty} \frac{(\alpha, n)}{(\beta, n)} x^n \\
(\alpha, n) &= \alpha(\alpha+1)\cdots(\alpha+n-1).
\end{aligned} \tag{14}
$$

M_r = radial normalizing factor.
n_r = radial quantum number.

$$\rho_l = ((l+1)^2 - \alpha^2)^{1/2}. \tag{15}$$

$$k_0 = \frac{2\pi mc}{h}\left(1 - \left(\frac{W}{mc^2}\right)^2\right)^{1/2} = \frac{1}{a_z N_l}. \tag{16}$$

$$N_l = (n_r^2 + (l+1)^2 + 2\rho_l n_r)^{1/2} \tag{17}$$

$$W = mc^2 \frac{n_r + \rho_l}{N_l} = mc^2\left\{1 + \frac{\alpha^2}{(n_r + ((j+\frac{1}{2})^2 - \alpha^2)^{1/2}}\right\}^{-1/2}. \tag{18}$$

$$a_z = \frac{h^2}{4\pi^2 me^2 Z}; \quad \alpha = \frac{2\pi e^2 Z}{hc}. \tag{19}$$

CONTINUOUS SPECTRUM: $W/mc^2 > 1$

$$F_l = -i\frac{\left(\frac{W}{mc^2} - 1\right)^{1/2}}{\left(\frac{W}{mc^2} + 1\right)^{1/2}} M_r(\sigma_1 - \sigma_2) \tag{20}$$

$$
\begin{aligned}
G_l &= M_r(\sigma_1 + \sigma_2) \\
\sigma_1 &= Ar^{\rho_l - 1}e^{-ik_0' r}\,{}_1F_1(\rho_l + iq + 1; 2\rho_l + 1; 2ik_0' r) \\
\sigma_2 &= Br^{\rho_l - 1}e^{-ik_0' r}\,{}_1F_1(\rho_l + iq; 2\rho_l + 1; 2ik_0' r)
\end{aligned} \tag{21}
$$

$$\frac{A}{B} = \frac{l + 1 + iQ}{\rho_l - iq} = \frac{\rho_l + iq}{l + 1 - iQ} \tag{22}$$

$$q = \frac{\frac{\alpha W}{mc^2}}{\left(\left(\frac{W}{mc^2}\right)^2 - 1\right)^{1/2}} = (Q^2 + \alpha^2)^{1/2} \tag{23}$$

$$k_0' = \frac{2\pi mc}{h}\left(\left(\frac{W}{mc^2}\right)^2 - 1\right)^{1/2}. \tag{24}$$

The discrete states of the Dirac electron are specified by the quantum numbers n_r, l, j, and u. These may have the following values:

$$
\begin{aligned}
n_r &= 0, 1, 2, \cdots \\
l &= 0, 1, 2, \cdots \\
j &= l \pm \tfrac{1}{2}, \geq 0
\end{aligned}
$$

(When $n_r=0$ the state $j=l-\frac{1}{2}$ is to be excluded.)

$$[-j] \leq u \leq [j],$$

where $[j]$ is the greatest integer contained in j.

The states of the continuous spectrum are specified by W, l, j, and u, with W arbitrary but $\geq mc^2$ and l, j, and u the same as for the discrete spectrum.

Normalization of the Wave Functions
Discrete Spectrum

We require to normalize our solutions in such a way that

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi\psi^* r^2 dr \cdot \sin\theta d\theta d\varphi = 1,$$

where

$$\psi\psi^* = \psi_1\psi_1^* + \psi_2\psi_2^* + \psi_3\psi_3^* + \psi_4\psi_4^*.$$

Suppose first that $j=l+\frac{1}{2}$. Then we find from Eq. (9a) that

$$\begin{aligned}\psi\psi^* = M_\theta^2[F_lF_l^*\{P_{l+1}^u P_{l+1}^{*u} + P_{l+1}^{u+1}P_{l+1}^{*u+1}\} + G_lG_l^*\{(l+u+1)^2 P_l^u P_l^{*u} \\ + (l-u)^2 P_l^{u+1}P_l^{*u+1}\}]\end{aligned} \tag{25}$$

or

$$\psi\psi^* = M_\theta^2[F_lF_l^* + G_lG_l^*][P_{l+1}^u P_{l+1}^{*u} + P_{l+1}^{u+1}P_{l+1}^{*u+1}],$$

as may be readily demonstrated.[17]

From the known relation

$$\int_0^\pi \int_0^{2\pi} P_l^u P_l^{*u} \sin\theta d\theta d\phi = \frac{4\pi}{2l+1}(l+u)!(l-u)! \tag{26}$$

we find

$$M_\theta^2\left(l, l+\frac{1}{2}, u\right) = \frac{1}{4\pi(l+u+1)!(l-u)!}. \tag{27}$$

The integral

$$I = \int_0^\infty [F_lF_l^* + G_lG_l^*]r^2 dr$$

can be evaluated as follows: one can easily show, by use of the generating function for the Laguerre polynomials,[18] that

$$\sum_{s=0}^{\infty} \binom{s+l}{s} {}_1F_1(-s; l+1; x)t^s = \frac{e^{-\frac{xt}{1-t}}}{(1-t)^{l+1}};\ l \text{ arbitrary}. \tag{28}$$

[17] Cf. e.g., D. R. Hartree, Proc. Camb. Phil. Soc. **25**, 225 (1929).

[18] Courant and Hilbert, "Methoden der math. Physik," p. 78.

Hence

$$\sum_{r,s=0}^{\infty}\binom{r+2\rho}{r}\binom{s+2\rho}{s}\int_0^\infty x^{2\rho}e^{-x}{}_1F_1(-r;\,2\rho+1;\,x){}_1F_1(-s;\,2\rho+1;\,x)dx\cdot t^s\tau^r$$

$$=\int_0^\infty x^{2\rho}e^{-x}\frac{e^{-xt/(1-t)-x\tau/(1-\tau)}}{(1-t)^{2\rho+1}(1-\tau)^{2\rho+1}}dx$$

$$=\frac{\Gamma(2\rho+1)}{(1-t\tau)^{2\rho+1}}=\Gamma(2\rho+1)\sum_{s=0}^{\infty}\binom{s+2\rho}{s}(t\tau)^s.$$

Therefore

$$\int_0^\infty x^{2\rho}e^{-x}{}_1F_1(-r;\,2\rho+1;\,x){}_1F_1(-s;\,2\rho+1;\,x)dx=\frac{\Gamma(2\rho+1)}{\binom{s+2\rho}{s}}\delta_{rs}. \quad (29)$$

Thus from Eq. (13)

$$\int_0^\infty \sigma_1{}^2r^2dr=\frac{\Gamma(2\rho_l+1)(N_l+l+1)^2}{(2k_0)^{2\rho_l+1}\binom{n_r+2\rho_l}{n_r}}\cdot$$

$$\int_0^\infty \sigma_2{}^2r^2dr=\frac{\Gamma(2\rho_l+1)n_r{}^2}{(2k_0)^{2\rho_l+1}\binom{n_r-1+2\rho_l}{n_r-1}}\cdot$$

$$\int_0^\infty \sigma_1\sigma_2r^2dr=0.$$

Since from Eq. (12)

$$I=\frac{2M_r{}^2}{N_l+\rho_l+n_r}\int_0^\infty[N_l(\sigma_1{}^2+\sigma_2{}^2)+2\sigma_1\sigma_2(\rho_l+n_r)]r^2dr,$$

we obtain

$$M_r{}^2\left(n_r,l,l+\frac{1}{2}\right)=\frac{(N_l+\rho_l+n_r)(2k_0)^{2\rho_l+1}\Gamma(2\rho_l+n_r+1)}{n_r!2N_l[\Gamma(2\rho_l+1)]^2[(N_l+l+1)^2+n_r(n_r+2\rho_l)]}. \quad (30)$$

Now let $j=l-\frac{1}{2}$. Then from (9b) we find

$$\psi\psi^*=M_\theta{}^2[F_{-l-1}F^*_{-l-1}+G_{-l-1}G^*_{-l-1}][P_l{}^uP_l{}^{*u}+P_l{}^{u+1}P_l{}^{*u+1}], \quad (31)$$

and obtain in an exactly similar manner

$$M_\theta{}^2\left(l,l-\frac{1}{2},u\right)=\frac{1}{4\pi(l+u)!(l-u-1)!} \quad (32)$$

and

$$M_r{}^2\left(n_r,l,l-\frac{1}{2}\right)=\frac{(N+\rho+n_r)(2k_0)^{2\rho+1}\Gamma(2\rho+n_r+1)}{n_r!2N[\Gamma(2\rho+1)]^2[(N-l)^2+n_r(n_r+2\rho)]} \quad (33)$$

where in Eq. (33) the argument of N and ρ is not l, but $-l-1$. This change of argument occurs whenever $j=l-\frac{1}{2}$.

Continuous Spectrum

The angular normalizing factors are the same as for the discrete spectrum.

We first obtain an asymptotic expansion for the radial solutions, since we must here use a special normalizing method because the solutions are not quadratically integrable.

The asymptotic expansion of ${}_1F_1(\alpha;\beta;x)$ is given by[19]

$$ {}_1F_1(\alpha;\beta;x) \sim \frac{\Gamma(\beta)}{\Gamma(\alpha)} e^x x^{\alpha-\beta} + \frac{\Gamma(\beta)}{\Gamma(\beta-\alpha)}(-x)^{-\alpha}. \tag{34} $$

Using Eqs. (34) and (21), we find, omitting the prime on k_0,

$$ \begin{aligned} \sigma_1 &\sim \frac{A\Gamma(2\rho_l+1)(i)^{iq-\rho_l}}{\Gamma(\rho_l+iq+1)(2k_0)^\rho} \cdot \frac{e^{i(k_0 r + q\log 2k_0 r)}}{r} \\ \sigma_2 &\sim \frac{B\Gamma(2\rho_l+1)(-i)^{-iq-\rho_l}}{\Gamma(\rho_l-iq+1)(2k_0)^\rho} \frac{e^{-i(k_0 r + q\log 2k_0 r)}}{r}. \end{aligned} \tag{35} $$

Therefore, from Eq. (20)

$$ \begin{aligned} G_l &\sim M_r C \frac{\cos(k_0 r + q\log k_0 r - \delta_l)}{r} \\ F_l &\sim M_r C D \frac{\sin(k_0 r + q\log k_0 r - \delta_l)}{r} \end{aligned} \tag{36} $$

in which

$$ \delta_l = \rho_l \frac{\pi}{2} + \arg\Gamma(\rho_l + iq + 1) - \beta_0 - q\log 2. \tag{37} $$

$$ e^{2i\beta_0} = A/B \tag{37'} $$

$$ C = \frac{2\Gamma(2\rho_l+1)e^{-q\pi/2}|A|}{(2k_0)^\rho|\Gamma(\rho_l+iq+1)|} \cdot \left(\frac{A}{B^*}\right)^{1/2}. \tag{38} $$

$$ D = \left(\frac{\frac{W}{mc^2}-1}{\frac{W}{mc^2}+1}\right)^{1/2} = \left(\frac{q-Q}{q+Q}\right)^{1/2}. \tag{38'} $$

We shall use the Weyl normalization method.[20]

Call the radial normalization factor $M_r(W,l,j) = M(W)$. Then with proper choice of $M(W)$

$$ \begin{aligned} I &= \int_0^\infty M^*(W') r^2 dr \int_{W_1}^{W_2} M(W)\,[F_l(W)F_l^*(W') + G_l(W)G_l^*(W')]\,dW \\ &= \begin{cases} 1 & \text{when } W_1 < W' < W_2, \\ 0 & \text{when } W' \text{ lies outside the interval } (W_1, W_2). \end{cases} \end{aligned} \tag{39} $$

[19] E. W. Barnes, Trans. Camb. Phil. Soc. **20**, 253 (1906).

[20] H. Weyl, Math. Ann. **68**, 220 (1910).

If we write down Eqs. (11) for the energy value W, and their complex conjugates for the energy value W', multiply each of the resulting equations by r^2, then multiply the first equation for W by $F^*(W')$, the second by $-G^*(W')$, the first for W' by $-F(W)$, and the second by $G(W)$, and finally add, we obtain the equation

$$\frac{2\pi}{hc}\cdot(W - W')r^2[F(W)F^*(W') + G(W)G^*(W')] = \frac{\partial}{\partial r}r^2[G^*(W')F(W) - G(W)F^*(W')]. \quad (40)$$

Substituting Eq. (40) in Eq. (39), we get

$$I = \int_0^\infty M^*(W')dr \int_{W_1}^{W_2} \frac{hc}{2\pi}\frac{M(W)}{W' - W}\frac{\partial}{\partial r}[r^2G(W)F^*(W') - G^*(W')F(W)]dW$$

$$= \lim_{R\to\infty} \frac{hc}{2\pi}M^*(W')\int_{W_1}^{W_2}\frac{M(W)}{W'-W}R^2[G(W,R)F^*(W',R) - G^*(W',R)F(W,R)]dW$$

since $r^2GF=0$ when $r=0$.

We may therefore use our asymptotic expansions for F and G. From Eq. (36) we can write

$$I = \lim_{R\to\infty}\frac{hc}{2\pi}M^*(W')C^*(W')\int_{W_1}^{W_2}\frac{M(W)}{W' - W}[C(W)D(W')\cos Ru.\sin Ru' - C(W)D(W)\sin Ru\cdot\cos Ru']dW,$$

where

$$Ru = k_0R + q\log k_0R - \delta_l,$$

or

$$u(W) = \frac{2\pi mc}{h}\cdot\left(\left(\frac{W}{mc^2}\right)^2 - 1\right)^{1/2} + \frac{\alpha}{\left(1 - \left(\frac{mc^2}{W}\right)^2\right)^{1/2}}\frac{1}{R}\log\frac{2\pi mc}{h}R\left(\left(\frac{W}{mc^2}\right)^2 - 1\right)^{1/2} - \frac{\delta_l}{R}\cdot \quad (41)$$

We can choose R large enough so that $u(W)$ for $W_1 \leqq W \leqq W_2$ is an increasing function of W, and so can find the inverse function $W=f(u)$, which is continuous and possesses a continuous derivative for $W>mc^2$. We make a simple rearrangement in I and change variables from W to u, obtaining

$$I = \lim_{R\to\infty}\frac{hc}{2\pi}M^*(W')C^*(W')\int_{u_1}^{u_2}\frac{M[f(u)]C[f(u)]}{f(u') - f(u)}[D[f(u')]\sin R(u' - u) + \{D[f(u')] - D[f(u)]\}\sin Ru\cdot\cos Ru']f'(u)du,$$

$$= \lim_{R\to\infty}\frac{hc}{2\pi}M^*(W')C^*(W')(I_R' + I_R'').$$

Consider

$$\lim_{R\to\infty} I_R'' = \lim_{R\to\infty} \cos Ru' \int_{u_1}^{u_2} M[f(u)]C[f(u)]f'(u)\frac{D[f(u')] - D[f(u)]}{f(u') - f(u)} \sin Ru.\, du.$$

Now $D'(W)$ exists for $W > mc^2$, and the remaining functions in the integrand are continuous, so that we can apply the well-known result[21] that

$$\lim_{n\to\infty} \int_a^b \psi(t) \sin nt\, dt = 0$$

when $\psi(t)$ is integrable in (a, b). This gives us

$$\lim_{R\to\infty} I_R'' = 0.$$

By the same argument we can show that $\lim_{R\to\infty} I_R' = 0$ when W' is not in the interval (W_1, W_2). When $W_1 < W' < W_2$, we can write, putting $u' - u = y$,

$$\begin{aligned} I_R' &= D(W') \int_{u'-u_1}^{u'-u_2} M[f(u' - y)]C[f(u' - y)]f'(u' - y)\frac{\sin Ry}{f(u' - y) - f(u')}dy \\ &= D(W') \int_{u'-u_2}^{u'-u_1} M[f(u' - y)]C[f(u' - y)]\frac{\sin Ry}{y}dy\frac{f'(u' - y)}{f'(u')} \\ &+ D(W') \int_{u'-u_1}^{u'-u_2} M[f(u' - y)]C[f(u' - y)]f'(u' - y)\left[\frac{1}{f(u' - y) - f(u')}\right. \\ &\left. - \frac{1}{f'(u')y}\right] \sin Ry \cdot dy = I_R''' + I_R^{IV}. \end{aligned}$$

Since the function in the square brackets in I_R^{IV} is finite at $y = 0$, the same argument as above shows that $\lim_{R\to\infty} I_R^{IV} = 0$. Further,

$$\lim_{R\to\infty} I_R''' = D(W')M(W')C(W')\pi$$

by the Dirichlet integral.[22]

Finally, therefore,

$$I = \tfrac{1}{2}hc\,|\,M(W')\,|^2\,|\,C(W')\,|^2\,D(W'),$$

and we must take

$$M_r^2(W, l, l + \tfrac{1}{2}) = 2/hcD\,|\,C\,|^2. \tag{42}$$

Since the above calculation has not made use of a particular value for j, we have also

$$M_r^2(W, l, l - \tfrac{1}{2}) = 2/hcD\,|\,C\,|^2, \tag{43}$$

where in Eq. (43) the argument of ρ and A is $-l-1$, not l.

[21] See K. Knopp, Unendliche Reihen, p. 363.

[22] Knopp, reference 21, p. 366.

Selection Rules

The selection rules for the matrix elements B^s in Eq. (4′), when retardation is neglected, have been shown by Darwin[14] to be

$$\begin{aligned} \Delta l &= 1, \\ \Delta j &= 0, \pm 1, \\ \Delta u &= 0, \pm 1. \end{aligned} \tag{44}$$

The table below gives the possible transitions:

Initial State				Initial State			
n_r	l	$l+\frac{1}{2}$	u	n_r	l	$l-\frac{1}{2}$	u
Final State				Final State			
n_r'	$l+1$	$l+3/2$	u'	n_r'	$l+1$	$l+\frac{1}{2}$	u'
n_r'	$l+1$	$l+\frac{1}{2}$	u'	n_r'	$l-1$	$l-\frac{1}{2}$	u'
n_r'	$l-1$	$l-\frac{1}{2}$	u'	n_r'	$l-1$	$l-3/2$	u'

(45)

with $u'=u$, $u\pm1$, and arbitrary n_r'. The only degeneracy of the possible final states of the discrete spectrum is that with respect to u'. If n_r' stands for the energy W of a state in the continuous spectrum, all possible final states having this value W fall together.

The Mass Absorption Coefficient of the K Shell

The atomic absorption coefficient τ_ν for a given energy jump is defined as follows:

$$\tau_\nu I(\nu)d\nu = \text{energy absorbed per second} = h\nu \cdot w'dW \tag{46}$$

where $w'dW$ ($=w'd\epsilon''$ of Eq. (8)) is the transition probability for the energy jump under consideration, and $I(\nu)d\nu$ is the intensity of the incident radiation in the range $d\nu$. Thus

$$(\tau_\nu)_K I(\nu)d\nu = h\nu \cdot w'(W; 0, 0, \tfrac{1}{2})dW,$$

since in the K shell $n_r=l=0$, and $j=\frac{1}{2}$.

The formula for the mass absorption coefficient $(\tau_\nu/\rho)_K$[23] becomes, since $dW=h.d\nu$,

$$\left(\frac{\tau_\nu}{\rho}\right)_K = \frac{Nh^2\nu}{AI(\nu)}w'\left(W; 0, 0, \frac{1}{2}\right) = \frac{Nh^2\nu}{A8\pi c\rho(\nu)}w'\left(W; 0, 0, \frac{1}{2}\right), \tag{47}$$

where N is Avogadro's number, A is the atomic weight, and $\rho(\nu)$ is defined in connection with Eq. (5).

[23] The ρ in τ_ν/ρ is not to be confused with $\rho(\nu)$. The former is the mass of an atom, while the latter is energy density.

Consulting the table (45) of possible transitions, we see that the sum over the degenerate states in Eq. (8) extends over the initial values of u, the final values u', and $j=\frac{1}{2}$, $3/2$, the only possible final l being 1. We thus obtain

$$\left(\frac{\tau_\nu}{\rho}\right)_K = \frac{2\pi e^2 cN}{3A\nu}\left[\sum_{u,u}{}' \left| P\left(W,1,\frac{3}{2},u';0,0,\frac{1}{2},u\right)\right|^2 + \sum_{u,u}{}' \left| P\left(W,1,\frac{1}{2},u';0,0,\frac{1}{2},u\right)\right|^2\right]. \quad (48)$$

Carrying out the angular integrations indicated by the definitions (8′) and (4′) of the P's, and using the angular normalizing factors given by Eqs. (27) and (32), and finally summing over u and u', we easily obtain

$$\left(\frac{\tau_\nu}{\rho}\right)_K = \frac{4\pi e^2 cN}{3A\nu}\left[\frac{8}{3}\left|\int_0^\infty F_0 G_1 r^2 dr\right|^2 + 3\left|\int_0^\infty F_{-2}G_0 r^2 dr + \frac{1}{3}\int_0^\infty F_0 G_{-2} r^2 dr\right|^2\right]. \quad (49)$$

Writing $\rho=(1-\alpha^2)^{1/2}$, $\rho'=(4-\alpha^2)^{1/2}$, $a=k_0'/k_0$, and taking

$$A = \frac{((l+1)^2+Q^2)^{1/2}}{Q} e^{i\tan^{-1}Q/(l+1)}$$
$$B = \frac{((l+1)^2+Q^2)^{1/2}}{Q} e^{-i\tan^{-1}q/\rho'} \quad (50)$$

we find for the functions F_0, G_0, G_1, G_{-2}, and F_{-2}, using Eqs. (12), (13), (20), (21), (30), (42), (43), (38), and (38′),

$$F_0 = (2k_0)^\rho \left(\frac{(1-\rho)k_0}{\Gamma(2\rho+1)}\right)^{1/2} r^{\rho-1}e^{-k_0 r}. \quad (51)$$

$$G_0 = (2k_0)^\rho \left(\frac{(1+\rho)k_0}{\Gamma(2\rho+1)}\right)^{1/2} r^{\rho-1}e^{-k_0 r} \quad (52)$$

$$G_1 = \frac{(2ak_0)^{\rho'}\,|\,\Gamma(\rho'+iq+1)\,|\,e^{q\pi/2}}{2\Gamma(2\rho'+1)}\left(\frac{2}{hc}\right)^{1/2}\left(\frac{q-Q}{q+Q}\right)^{-1/4}\cdot \left[e^{i[\tan^{-1}Q/2-ak_0r]}r^{\rho'-1}{}_1F_1(\rho'+iq+1;2\rho'+1;2iak_0r) + e^{-i[\tan^{-1}q/\rho'+ak_0r]}r^{\rho'-1}{}_1F_1(\rho'+iq;2\rho'+1;2iak_0r)\right]. \quad (53)$$

$$G_{-2} = \frac{(2ak_0)^{\rho}\,|\,\Gamma(\rho+iq+1)\,|\,e^{q\pi/2}}{2\Gamma(2\rho+1)}\left(\frac{2}{hc}\right)^{1/2}\left(\frac{q-Q}{q+Q}\right)^{-1/4}\cdot \left[e^{i[\tan^{-1}Q/-1-ak_0r]}r^{\rho-1}{}_1F_1(\rho+iq+1;2\rho+1;2iak_0r) + e^{-i[\tan^{-1}q/\rho+ak_0r]}r^{\rho-1}{}_1F_1(\rho+iq;2\rho+1;2iak_0r)\right]. \quad (54)$$

$$F_{-2} = \frac{(2ak_0)^{\rho}\,|\,\Gamma(\rho+iq+1)\,|\,e^{q\pi/2}}{i2\Gamma(2\rho+1)}\left(\frac{2}{hc}\right)^{1/2}\left(\frac{q-Q}{q+Q}\right)^{1/4}.$$

$$\cdot \left[e^{i[\tan^{-1}Q/-1-ak_0r]}r^{\rho-1}{}_1F_1(\rho+iq+1;2\rho+1;2iak_0r)\right. \tag{55}$$
$$\left. - e^{-i[\tan^{-1}q/\rho+ak_0r]}r^{\rho-1}{}_1F_1(\rho+iq;2\rho+1;2iak_0r)\right].$$

Integrating and rearranging, we obtain

$$\int_0^\infty F_0G_1r^2dr = 2^{\rho'+\rho}a^{\rho'}\cdot\left(\frac{1-\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2}\frac{|\Gamma(\rho'+iq+1)|\,e^{q\pi/2}}{(1-ia)^{\rho'+\rho+1}}\left(\frac{q-Q}{q+Q}\right)^{-1/4}\cdot$$
$$\cdot\frac{\Gamma(\rho'+\rho+1)}{\Gamma(2\rho'+1)}\cdot\left[e^{-i\tan^{-1}Q/2}\,{}_2F_1\left(\rho'+\rho+1,\rho'-iq+1;2\rho'+1;-\frac{2ia}{1-ia}\right)\right. \tag{56}$$
$$\left.+e^{i\tan^{-1}q/\rho'}{}_2F_1\left(\rho'+\rho+1,\rho'-iq;2\rho'+1;-\frac{2ia}{1-ia}\right)\right].$$

$$\int_0^\infty F_0G_{-2}r^2dr = 2^{2\rho}a^{\rho}\cdot\left(\frac{1-\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2}\frac{|\Gamma(\rho+iq+1)|\,e^{q\pi/2}}{(1-ia)^{2\rho+1}}\left(\frac{q-Q}{q+Q}\right)^{-1/4}\cdot$$
$$\cdot\left[e^{i\tan^{-1}Q/-1}\cdot{}_2F_1\left(2\rho+1,\rho-iq+1;2\rho+1;-\frac{2ia}{1-ia}\right)\right. \tag{57}$$
$$\left.+e^{i\tan^{-1}q/\rho}\cdot{}_2F_1\left(2\rho+1,\rho-iq;2\rho+1;-\frac{2ia}{1-ia}\right)\right].$$

$$\int_0^\infty F_{-2}G_0r^2dr = i2^{2\rho}a^{\rho}\cdot\left(\frac{1+\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2}\frac{|\Gamma(\rho+iq+1)|\,e^{q\pi/2}}{(1-ia)^{2\rho+1}}\left(\frac{q-Q}{q+Q}\right)^{1/4}\cdot$$
$$\cdot\left[e^{-i\tan^{-1}Q/-1}\cdot{}_2F_1\left(2\rho+1,\rho-iq+1;2\rho+1;-\frac{2ia}{1-ia}\right)\right. \tag{58}$$
$$\left.-e^{i\tan^{-1}q/\rho}\cdot{}_2F_1\left(2\rho+1,\rho-iq;2\rho+1;-\frac{2ia}{1-ia}\right)\right].$$

The two hypergeometric functions in (56) cannot be readily evaluated in their present form because of very slow convergence or non-convergence of the usual series. There are two possible methods of evaluating them numerically. One method is to express them as definite integrals and then to integrate numerically. Because $\rho'-\rho-1$ is so small, the numerical integration will be inaccurate or laborious if no further transformation of the resulting integrals is made. A convenient transformation which is satisfactory over the range of values of a and q which corresponds to $\frac{1}{2}\lambda_k \leqq \lambda \leqq \lambda_k$, is that which results in the integral J defined by Eq. (62) below.

Using the relationship

$${}_2F_1(\alpha,\beta;\gamma;x) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)}\int_0^1 u^{\alpha-1}(1-u)^{\gamma-\alpha-1}(1-ux)^{-\beta}du, \tag{59}$$

and making some simple transformations, we can write

$$ {}_2F_1\left(\rho'+\rho+1,\ \rho'-iq+1;\ 2\rho'+1;\ -\frac{2ia}{1-ia}\right) $$

$$ =\left(\frac{1+ia}{1-ia}\right)^{iq-\rho-1}\left\{1+\frac{J^*}{B(\rho'-\rho,\ \rho'+\rho+1)}\right\} \tag{60} $$

$$ {}_2F_1\left(\rho'+\rho+1,\ \rho'-iq;\ 2\rho'+1;\ -\frac{2ia}{1-ia}\right) $$

$$ =\left(\frac{1+ia}{1-ia}\right)^{iq-\rho'}\left\{1+\frac{J}{B(\rho'-\rho,\ \rho'+\rho+1)}\right\} \tag{61} $$

where

$$ J=\int_{-1/2}^{+1/2}\left(\frac{1}{2}-t\right)^{\rho'+\rho}\left(\frac{1}{2}+t\right)^{\rho'-\rho-1}dt\left[\left(\frac{1+ia}{1-2iat}\right)^{\rho'-iq}-1\right] \tag{62} $$

and

$$ B(\alpha,\beta)=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}. \tag{63} $$

The other method of evaluating the hypergeometric functions in Eq. (56) is to transform them to another combination of hypergeometric functions which do converge fairly rapidly. By use of the transformation[24] connecting Y_1 with Y_3 and Y_4 one finds readily from Eq. (60) that

$$ B(\rho'-\rho,\ \rho'+\rho+1)+J=\frac{(1+a^2)^{\rho'}}{(2a)^{2\rho'}}e^{i\rho'\pi}\left[B(\rho-iq,\ \rho'-\rho)\left(\frac{1-ia}{1+ia}\right)^{\rho}\cdot\right. $$

$$ \cdot\ {}_2F_1\left(-\rho'-\rho,\ 1+iq-\rho';\ 1+iq-\rho;\ \frac{1+ia}{1-ia}\right) \tag{64} $$

$$ +B(-\rho+iq,\ \rho'+\rho+1)\left(\frac{1-ia}{1+ia}\right)^{iq}\cdot $$

$$ \left.\cdot\ {}_2F_1\left(1+\rho-\rho',\ -\rho'-iq;\ \rho-iq+1;\ \frac{1+ia}{1-ia}\right)\right]. $$

The series for the hypergeometric functions in Eq. (64) converge fairly rapidly for any range of wave-length. The chief difficulty in the use of this formula is the calculation of the gamma functions. High accuracy can be obtained from this formula with less work than from numerical integration, but for three-figure accuracy the latter is much quicker. All the calculations in this paper were performed by numerical integration.

The hypergeometric functions occurring in Eqs. (57) and (58) can be reduced to elementary functions by the use of the relation

$$ {}_2F_1(\alpha,\beta;\alpha;x)=(1-x)^{-\beta} \tag{65} $$

[24] E. W. Barnes, Proc. Lond. Math. Soc. (2), **6**, 141 (1908).

Making these transformations and noting that $Q=1/a$, we obtain for the three integrals

$$\int_0^\infty F_0 G_1 r^2 dr = 2^{\rho'+\rho} a^{\rho'} \left(\frac{1-\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2} \frac{|\Gamma(\rho'+iq+1)|\, e^{q(\pi/2-2\tan^{-1}a)}}{\Gamma(\rho'-\rho)(1+a^2)^{(\rho'+\rho+1)/2}} \left(\frac{q-Q}{q+Q}\right)^{-1/4} \cdot$$

$$\cdot \left[e^{-i[\tan^{-1}Q/2-(\rho'-\rho-1)\tan^{-1}a]} \cdot \{B(\rho'-\rho,\rho'+\rho+1)+J^*\}\right. \tag{66}$$

$$\left. + e^{i[\tan^{-1}q/\rho'-(\rho'-\rho-1)\tan^{-1}a]} \cdot \{B(\rho'-\rho,\rho'+\rho+1)+J\}\right].$$

$$\int_0^\infty F_0 G_{-2} r^2 dr = 2^{2\rho} a^\rho \cdot \left(\frac{1-\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2} \frac{|\Gamma(\rho+iq+1)|\, e^{q(\pi/2-2\tan^{-1}a)}}{(1+a^2)^{\rho+1/2}} \left(\frac{q-Q}{q+Q}\right)^{-1/4} \cdot$$

$$\cdot \left[ie^{-2i\tan^{-1}a} + e^{i[\tan^{-1}q/\rho+\tan^{-1}a]}\right] \tag{67}$$

$$\int_0^\infty F_{-2} G_0 r^2 dr = 2^{2\rho} a^\rho \cdot \left(\frac{1+\rho}{2hck_0\Gamma(2\rho+1)}\right)^{1/2} \frac{|\Gamma(\rho+iq+1)|\, e^{q(\pi/2-2\tan^{-1}a)}}{(1+a^2)^{\rho+1/2}} \left(\frac{q-Q}{q+Q}\right)^{1/4} \cdot$$

$$\cdot \left[e^{-2i\tan^{-1}a} - ie^{i[\tan^{-1}q/\rho+\tan^{-1}a]}\right]. \tag{68}$$

Substituting in Eq. (49) we obtain finally for the mass absorption coefficient for the K shell

$$\left(\frac{\tau_\nu}{\rho}\right)_K = \frac{N}{AZ} \frac{h\lambda}{3\pi mc} \frac{2^{2\rho} e^{q(\pi-4\tan^{-1}a)}}{\Gamma(2\rho+1)(1+a^2)^{\rho+1}} \left[\frac{8}{3} \frac{(2a)^{2\rho'}(1-\rho)}{(1+a^2)^{\rho'}} \cdot\right.$$

$$\cdot \frac{|\Gamma(\rho'+iq+1)|^2}{[\Gamma(\rho'-\rho)]^2} \left(\frac{q-Q}{q+Q}\right)^{-1/2} |B(\rho'-\rho,\rho'+\rho+1)+J|^2(1+\cos\phi)$$

$$+ 3\frac{(2a)^{2\rho}|\Gamma(\rho+iq+1)|^2}{(1+a^2)^\rho} \left\{(1+\rho)\left(\frac{q-Q}{q+Q}\right)^{1/2}(1+\sin\delta)\right. \tag{69}$$

$$\left. \left. + \frac{1-\rho}{9}\left(\frac{q-Q}{q+Q}\right)^{-1/2}(1-\sin\delta) + \frac{2}{3}(1-\rho^2)^{1/2}\cdot\cos\delta\right\}\right].$$

in which

$$\phi = \tan^{-1}\tfrac{1}{2}Q + \tan^{-1}q/\rho' - 2(\rho'-\rho-1)\tan^{-1}a + 2\tan^{-1}\chi.$$

$$\chi = \arg\,[B(\rho'-\rho,\rho'+\rho+1)+J]$$

$$\delta = 3\tan^{-1}a + \tan^{-1}q/\rho$$

$$a^2 = x\frac{2+xy}{2-y};\ Q = \frac{1}{a};\ q^2 = Q^2+\alpha^2;\ \alpha^2 = y(2-y);$$

$$x = \lambda_k/\lambda - 1;\ \text{and}\ y = h/mc\lambda_k.$$

The two expressions in Eq. (69) which are most difficult to calculate are the absolute value of the gamma function of complex argument, and the

integral J. The gamma function can be most conveniently calculated from the asymptotic expansion

$$\log|\Gamma(x+iy)| \sim \tfrac{1}{2}(x-\tfrac{1}{2})\log(x^2+y^2) - y\tan^{-1}y/x - x + \tfrac{1}{2}\log 2\pi + \sum_{n=1}^{\infty}\frac{B_{2n}}{2n(2n-1)}\frac{\cos[(2n-1)\tan^{-1}y/x]}{(x^2+y^2)^{n-1/2}}. \quad (70)$$

where the B_{2n} are the well-known Bernoulli numbers. By taking x large and using the difference equation satisfied by the gamma function, Eq. (70) forms a relatively easy method of calculation.

Under adverse circumstances, the calculation of the integral J could be very laborious. Fortunately, when the wave-length is confined to the range $\frac{1}{2}\lambda_k$ to λ_k, the integrand of Eq. (62) does not change rapidly and has no important oscillations, so that an approximate formula of integration may be expected to give sufficient accuracy. The formula used is one given by Woolhouse,[25] namely,

$$\int_0^1 f(x)dx = \frac{7}{390}[f(0)+f(1)] + \frac{16,807}{133,380}[f(1/14)+f(13/14)] + \frac{128}{570}[f(1/4)+f(3/4)] + \frac{71}{270}f(\tfrac{1}{2}). \quad (71)$$

It would be very difficult to obtain a numerical value for the error involved in using this formula when evaluating an integral as complicated as J. However, the writer has tried the formula in evaluating known integrals of functions which have closely the same shape as the actual integrand in J, and from these trials he is convinced that in the wave-length range mentioned above at least three- and very probably four-figure accuracy can be expected. This is further supported by the close agreement of the results for Al ($Z=13$) with those calculated from the Nishina-Rabi formula, an entirely independent procedure. The effect on the absorption coefficient of an error in calculating J depends of course upon the relative magnitude of the two parts of Eq. (69). In the range under consideration the term containing J is from 2 to 3 times as large as the other term.

Mass Absorption Coefficient at the Absorption Edge

At the absorption edge, where $\lambda=\lambda_k$, Eq. (69) cannot be used to calculate the absorption coefficient because there $a=0$ and $q=Q=\infty$. A limiting process is necessary, and it is most convenient to pass to the limit for the individual proper functions and then to integrate, instead of passing to the limit directly in Eq. (69). Another more simple method if only the form of the proper functions is necessary, is to solve the radial differential Eqs. (11) when $W=mc^2$, but this has the disadvantage for our purpose of requiring another normalization using Weyl's method.

[25] Woolhouse, Journ. Inst. Act. **27**, 122, (1888). Cf. Whittaker and Robinson, "Calculus of Observations," p. 158.

We want to find $\lim_{a\to o} F_l$ and $\lim_{a\to o} G_l$. To do this we consider separately the radial normalizing factor and the functions σ_1 and σ_2 (see Eq. 21)). From the well-known Stirling formula, we can write[26]

$$|\Gamma(\rho' + iq + 1)| \sim (2\pi)^{1/2} a^{-\rho'-1/2} e^{-q\pi/2},$$

also

$$|A| \sim 1, \quad \text{and} \quad (2k_0')^{\rho'} = (2k_0)^{\rho'} a^{\rho'},$$

so that from Eq. (38)

$$|C| \sim 2\Gamma(2\rho' + 1)(2k_0)^{-\rho'}(a/2\pi.)^{1/2} \tag{72}$$

Also, from Eq. (38′),

$$D = \left(\frac{q-Q}{q+Q}\right)^{1/2} = \left(\frac{(1+a^2\alpha^2)^{1/2} - 1}{(1+a^2\alpha^2)^{1/2} + 1}\right)^{1/2} \sim \tfrac{1}{2}a\alpha \tag{73}$$

since $q^2 = Q^2 + \alpha^2 = 1/a^2 + \alpha^2$. Therefore, from Eq. (42),

$$M_r = \frac{1}{|C|}\left(\frac{2}{hcD}\right)^{1/2} \sim \left(\frac{2\pi}{hc\alpha}\right)^{1/2} \frac{(2k_0)^{\rho'}}{\Gamma(2\rho'+1)} \frac{1}{a} = \frac{(2k_0)^{\rho'}}{e(Z)^{1/2}\Gamma(2\rho'+1)} \frac{1}{a}, \tag{74}$$

using Eq. (19).

It is a known property[27] of the degenerate hypergeometric function that

$$\lim_{\epsilon\to\infty} \frac{(\frac{1}{2}z)^{\alpha}}{\Gamma(\alpha+1)} {}_1F_1\left(\frac{1}{\epsilon}; \alpha+1; -\epsilon z^2/4\right) = J_\alpha(z), \tag{75}$$

where $J_\alpha(z)$ is the ordinary Bessel function. It is evident, therefore, that

$$\begin{aligned} \lim_{a\to 0} \sigma_2 &= \lim_{a\to 0} Br^{\rho'-1} e^{-iak_0 r} {}_1F_1(\rho' + iq; 2\rho' + 1; 2iak_0 r) \\ &= -i\Gamma(2\rho'+1)(2k_0)^{-\rho'} r^{-1} J_{2\rho'}((8k_0 r)^{1/2}). \end{aligned} \tag{76}$$

It can easily be shown that

$$\begin{aligned} {}_1F_1(\rho' + iq + 1; 2\rho' + 1; 2ik_0' r) &= \frac{2\rho'}{\rho' + iq} {}_1F_1(\rho' + iq; 2\rho'; 2ik_0' r) \\ &\quad - \frac{\rho' - iq}{\rho' + iq} {}_1F_1(\rho' + iq; 2\rho' + 1; 2ik_0' r). \end{aligned} \tag{77}$$

With Eqs. (77) and (21), we find

$$\begin{aligned} \sigma_1 \pm \sigma_2 = r^{\rho'-1} e^{-ik_0' r} \Bigg[& A \frac{2\rho'}{\rho' + iq} {}_1F_1(\rho' + iq; 2\rho'; 2ik_0' r) \\ & + \left[\pm B - A\frac{\rho' - iq}{\rho' + iq}\right] {}_1F_1(\rho' + iq; 2\rho' + 1; 2ik_0' r)\Bigg]. \end{aligned} \tag{78}$$

[26] The symbol $\backsim$, as used in this section, has the following significance. if $f(a) \backsim g(a)$ then $\lim_{a\to 0} f(a)/g(a) = 1$.

[27] G. N. Watson, "Bessel Functions," p. 154.

From Eqs. (78), (76), and (50), we find after some calculation

$$(\sigma_1 + \sigma_2) \sim a \cdot r^{-1}\Gamma(2\rho' + 1)(2k_0)^{-\rho'}\left[J_{2\rho'-1}((8k_0r)^{1/2}) \cdot (2k_0r)^{1/2} + (l + 1 - \rho')J_{2\rho'}((8k_0r)^{1/2})\right],$$

$$\lim_{a\to 0}(\sigma_1 - \sigma_2) = 2ir^{-1}\Gamma(2\rho' + 1)(2k_0)^{-\rho'}J_{2\rho'}((8k_0r)^{1/2}),$$

so that finally, with Eqs. (20) and (74),

$$\lim_{a\to 0} F_l = \alpha/e(Z)^{1/2}r \cdot J_{2\rho'}((8k_0r)^{1/2}) \tag{79}$$

$$\lim_{a\to 0} G_l = 1/e(Z)^{1/2}r \cdot \left[(2k_0r)^{1/2}J_{2\rho'-1}((8k_0r)^{1/2}) + (l+1 - \rho')J_{2\rho'}((8k_0r)^{1/2})\right]. \tag{80}$$

After some simple calculations, using the formula[28]

$$\int_0^\infty J_\nu(at)\exp(-p^2t^2)t^{\mu-1}dt = \frac{\Gamma\left(\frac{\nu+\mu}{2}\right)\left(\frac{a}{2p}\right)^\nu}{2p^\mu\Gamma(\nu+1)}\exp(-a^2/4p^2)\,{}_1F_1\left(\frac{\nu-\mu}{2}+1;\nu+1;a^2/4p^2\right),$$

we find for the mass absorption coefficient at the absorption edge

$$\left(\frac{\tau_\nu}{\rho}\right)_{K\text{'edge}} = \frac{h^2N\lambda_k}{3\pi me^2A}\frac{2^{2\rho}\exp(-4)}{Z^2\Gamma(2\rho+1)}\left[\frac{8}{3}2^{2\rho'}(1-\rho)\left[\frac{\Gamma(\rho'+\rho+1)}{\Gamma(2\rho'+1)}\right]^2 \cdot [2\rho'\,{}_1F_1(\rho'-\rho-1;2\rho';2) + (2-\rho')\,{}_1F_1(\rho'-\rho;2\rho'+1;2)]^2 + 3\cdot 2^{2\rho}\left[\alpha(1+\rho)^{1/2} - \frac{3-\rho}{3}(1-\rho)^{1/2}\right]^2\right]. \tag{81}$$

Eqs. (69) and (81) for the mass absorption coefficient have been derived for a one-electron atom. Actually, of course, the K shell contains two electrons, so that one might expect, in the absence of interaction between the electrons, merely to multiply the values for the one-electron atom by two. This is incorrect. In the one-electron atom the lowest energy level is doubly degenerate since there are two possible directions for the "spin" magnetic moment of the electron, represented analytically by $u=0$ or -1. In the two-electron atom, however, the lowest state is non-degenerate. If the Pauli exclusion principle were not in force, the degeneracy of the lowest state would be four, since in the absence of interaction each electron may have the values $u=0$ or -1. Since, however, no two electrons may have the same quantum numbers, and because of the identity of the electrons,[29] three of the degener-

[28] Watson, reference 27, p. 394.

[29] W. Heisenberg, Zeits. f. Physik **38**, 411 (1926).

ate states are ruled out, so that multiplying by two for the two K electrons and dividing by two because there is no degeneracy leaves Eqs. (69) and (81) unchanged.

Since the completion of this paper an article by Stobbe[30] has appeared in which the mass absorption coefficient is calculated by means of the non-relativistic quantum mechanics. Stobbe uses a screening constant for the K electrons which is considerably smaller than that necessary to make the energy of the model agree with that experimentally determined from the K edge. He justifies this procedure by pointing out that in the final state with one K electron ejected, the energy of the remaining electrons is different from that in the initial state, so that the absorbed frequency does not correspond exactly to the change in energy of the ejected K electron alone.

The present calculations can easily be adapted to a model with a smaller screening constant by lowering Z to compensate for the decrease in s; the results then apply to different atoms, for instance to gold (79) instead of lead (82) if s is changed from 4.512 to 1.512. With the smaller screening constant, however, the λ_k' of the model will no longer agree with the experimental value. We want the abscissas of the computed and observed curves to coincide at the experimental λ_k. Now the absorption coefficient depends on a matrix element which is a function of λ_k' and W, the energy of the ejected electron. In the present calculations W was connected with a wave-length λ' of the incident x-rays given by $W=mc^2+h(\nu'-\nu_k')=mc^2+hc(1/\lambda'-1/\lambda_k')$. In the adapted calculations ν_k' is replaced by ν_k corresponding to the actual absorption edge and so W must be connected with a wave-length λ given by $W=mc^2+hc(1/\lambda-1/\lambda_k)$. We must now use λ and not λ' in Eq. (47) since the factor multiplying the matrix element in this equation arose originally from the change in energy of the atom as a whole. The new absorption coefficient is therefore

$$\frac{\tau}{\rho}(\lambda)=\frac{\lambda}{\lambda'}\cdot\frac{\tau}{\rho}(\lambda'),$$

where

$$\frac{1}{\lambda}-\frac{1}{\lambda_k}=\frac{1}{\lambda'}-\frac{1}{\lambda_k'}.$$

When one calculates this new absorption it turns out, however, that the agreement with experiment is worse. This does not mean that if one calculated the absorption coefficient for gold using a larger screening constant that one would find better agreement with experiment, but merely that the use of a large screening constant for lead agrees better with experiment than the use of a small one with gold, and is probably to be attributed to the rapid loss of accuracy of the model as Z is decreased.

That the agreement with experiment is worse can be seen roughly from the following considerations. At the absorption edge $\lambda/\lambda'=(Z'/Z)^2$ by Moseley's law, where Z' is the atomic number used in the calculation and Z

[30] M. Stobbe, Ann. d. Physik (5), **7**, 661 (1930).

that of the atom to which it is now applied. But the observed absorption coefficients are closely in the ratio $(Z'/Z)^3$ at the edge; and the theoretical values are already too low. It is therefore not thought worth while to publish the modified values.

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