Relativistic L-Shell Photoeffect

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(Received October 10, 1960; revised manuscript received January 17, 1961)

The expressions of the relativistic L shell photoeffect differential and total cross sections, for the case of light elements, are established. Coulomb wave functions are used for the description of the electron states in the calculation of the matrix elements, but it is shown how the results should be corrected so as to take screening effects into consideration. For the final continuum state wave function of the ejected electron, whose exact analytic form is not known, the Born approximation is used. In the case of L_{I} subshell the calculation runs similarly to the one performed previously by the author for the K shell. For the other two subshells new tedious trace evaluations have to be carried out. Thus, for the L_{I} subshell, cross sections correct to first order in αZ (inclusive) are determined, whereas in the case of the L_{II} and L_{III} subshells, only their zero-order approximation is calculated. The cross sections are discussed and compared. It is shown that they reduce in the nonrelativistic and extreme relativistic limits to results established by other means.

1. INTRODUCTION

THE nonrelativistic aspect of the photoeffect from the L shell was successfully studied a long time ago.[1] Thus, by means of a method devised together with Sommerfeld, Schur[2] has calculated the differential cross sections of the L_{I} and $L_{\mathrm{II}}+L_{\mathrm{III}}$ subshells, including retardation approximately. Equivalent results were obtained by another method for the total cross sections by Stobbe.[3] The exact integration of the nonrelativistic matrix elements was carried out separately by Fischer, Sauter, and Sommerfeld.[4] In these works Coulomb wave functions were used to describe the initial and final states of the electron; screening effects were taken into account by appropriately modifying the nuclear charge. The formulas obtained for the cross sections are in rather good agreement with the (not very accurate) experiments performed so far at low energies.[1]

However, concerning the relativistic aspect of the problem only a few remarks have been made.[5] This has been largely due to the lack of precision of the experimental results at high energies, qualitative estimates being sufficient for their interpretation. Recently, owing to the continuous advances in beta spectrometry, important progress has been made also in the study of the high-energy photoeffect from the L shell.[6] Interest has been thus stimulated for a more detailed theoretical analysis. As for the K shell, the relativistic study is extremely involved, because no analytic expression in closed form can be given for the final-state spinor of the ejected electron and because of difficulties encountered in the integration of the matrix elements. This prevents an exact analytic evaluation of the cross sections, in their dependence on energy and Z.

In the following, we set out to determine the approximate forms of the differential and total cross sections for the limiting case of light elements. The final state of the photoelectron will be described by means of the Born approximation.[7] This method was used previously by the author in the case of the K shell.[8] For the L_{I} subshell, cross sections correct to first order in αZ (inclusive) will be established. For the L_{II} and L_{III} subshells, whose contributions to absorption are of order $(\alpha Z)^2$ smaller in the high-energy region, only the zero-order approximation will be determined. The polarization of the ejected photoelectrons will not be discussed here.

Concomitantly with the present work, Pratt[9] has approached the same problem from a different point of view. He has succeeded in calculating the exact αZ dependence of the extreme relativistic form of the total cross sections. The results presented here on the energy dependence of the cross sections, combined with those of Pratt on their Z dependence, should lead to a better understanding of the high-energy photoeffect from the L shell.

The ejection of a photoelectron from an atom is in principle an involved problem of a many-electron system. However, a very good degree of accuracy could be attained under the assumption of the atom consisting of independent electrons under the influence of a central self-consistent field. In this case the differential cross section of one of the L subshells can be written

$$d\sigma_i=\frac{(2\pi)^2\alpha}{\kappa}\sum_{m\sigma}|M|^2 d\omega, \quad i=\mathrm{I, II, III}, \tag{1}$$

where the summation is to be carried out over all the

[1] See H. Bethe and E. Salpeter, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1957), Vol. 35, Part I; and H. Hall, Revs. Modern Phys. **8**, 358 (1936).
[2] G. Schur, Ann. Physik **4**, 433 (1930).
[3] M. Stobbe, Ann. Physik **7**, 661 (1930).
[4] J. Fischer, Ann. Physik **8**, 821 (1931); F. Sauter, Ann. Physik **9**, 217 (1931), and A. Sommerfeld, *Atombau und Spektrallinien* (Friedrich Vieweg und Sohn, Braunschweig, 1939), Chap. 6, Sec. 6.
[5] M. Phillips, Phys. Rev. **45**, 132 (1934); H. Hall and W. Rarita, Phys. Rev. **46**, 143 (1934).
[6] S. Hultberg, Arkiv Fysik **15**, 307 (1959). E. P. Grigoryev and A. V. Zolotavin, J. Exptl. Theoret. Phys. (U.S.S.R.) **36**, 393 (1959) [translation: Soviet Phys.—JETP **9**, 272 (1959)]. Z. Sujkowski (private communication).
[7] Similar results could be obtained by describing the final state in terms of the Sommerfeld-Maue wave function or by using an expansion in partial waves.
[8] M. Gavrila, Phys. Rev. **113**, 514 (1959); hereafter referred to as (K).
[9] R. H. Pratt, Phys. Rev. **119**, 1619 (1960).

electrons of the considered subshell (index m) and the two spin directions of the final state (index σ). The matrix element M, pertaining to a definite transition, performed under the influence of linearly polarized radiation, is given in momentum space by

$$M=\int \bar{u}_2(\mathbf{p})\mathbf{s}u_1(\mathbf{p}-\boldsymbol{\kappa})d^3p, \tag{2}$$

the notations used being the same as in (K).[10] Here u_1 and u_2 should represent the initial and final wave functions of the electron in the self-consistent field of the atom. However, such a procedure would lead to the necessity of evaluating the matrix element numerically. Instead of this, we will use in the following calculations unscreened Coulomb spinors u_1 and u_2, for which an analytic (approximate) evaluation is possible. The screening corrections to be expected will be examined in Sec. 5C.

In the equations which connect the parameters of the initial and final states of the electron we can neglect the binding energy of the L shell. Indeed, this contributes to the matrix elements and to the cross sections with terms of order $(\alpha Z)^2$ which we do not take into consideration. Hence, in our approximation we have, as in (K),

$$E=m+\kappa, \tag{3}$$

$$k^2+m^2=E^2,\quad k^2-\kappa^2=2m\kappa,\quad k^2+\kappa^2=2E\kappa. \tag{4}$$

2. L_{I} SUBSHELL

The calculations for the L_{I} subshell are to a great extent similar to those for the K shell, since the same spectral type ($S_{\frac{1}{2}}$) is involved. As in (K), we want to determine here the L_{I} matrix elements and cross sections correct to first order in αZ.

The two bound-state spinors of the L_{I} subshell (of quantum numbers $n=2$, $l=0$, $j=\frac{1}{2}$, $m=\pm\frac{1}{2}$) may be written as

$$u_1(\mathbf{p})=\frac{1}{(4\pi)^{\frac{1}{2}}}\left[G(p)+iF(p)\gamma_4\boldsymbol{\gamma}\cdot\frac{\mathbf{p}}{p}\right]\chi_1, \tag{5}$$

where χ_1 is one of the constant spinors (1,0,0,0) or (0,1,0,0) according to whether we consider the state of magnetic quantum number $m=\frac{1}{2}$ or $m=-\frac{1}{2}$. The form of the functions $G(p)$ and $F(p)$, correct to first order in αZ (whatever the ratio p/η), is[11]

$$\begin{aligned}G(p)&=\frac{2}{\pi^{\frac{1}{2}}}(2\eta)^{\frac{5}{2}}\left[p^2\left(1+\frac{\pi\alpha Z}{8}\frac{p}{m}\right)-\eta^2\right]\frac{1}{(p^2+\eta^2)^3},\\ F(p)&=\frac{2}{\pi^{\frac{1}{2}}}(2\eta)^{\frac{5}{2}}\frac{p}{2m}\frac{p^2-\eta^2}{(p^2+\eta^2)^3},\end{aligned} \tag{6}$$

where we have put $\eta=\alpha Zm/2$. It is convenient to introduce the following notation

$$\begin{aligned}u_1(\mathbf{p})&=u_{10}(\mathbf{p})+u_{11}(\mathbf{p})+u_{12}(\mathbf{p});\\ u_{10}&=N_1'\frac{p^2-\eta^2}{(p^2+\eta^2)^3}\chi_1,\\ u_{11}&=N_1'\frac{i}{2m}\frac{p^2-\eta^2}{(p^2+\eta^2)^3}\gamma_4\boldsymbol{\gamma}\cdot\mathbf{p}\chi_1,\\ u_{12}&=N_1'\frac{\pi\alpha Z}{8}\frac{p}{m}\frac{p^2}{(p^2+\eta^2)^3}\chi_1,\end{aligned} \tag{7}$$

where

$$N_1'=\frac{(2\eta)^{\frac{5}{2}}}{\pi},\quad \eta=\frac{\alpha Zm}{2}=\frac{\lambda}{2}. \tag{8}$$

For the description of the final state of the electron the second-order Born approximation will be used. This may be put into the form

$$\bar{u}_2(\mathbf{p})=\bar{u}_{20}(\mathbf{p})+\bar{u}_{21}(\mathbf{p})+\bar{u}_{22}(\mathbf{p}), \tag{9}$$

where the three terms $\bar{u}_{2j}$, corresponding to the successive Born approximations, are given by (K.15).

The matrix element of Eq. (2) may thus be itself split into three terms M_j, representing the contribution of the successive Born approximations $\bar{u}_{2j}$:

$$M=M_0+M_1+M_2. \tag{10}$$

The integration in M_0 is immediate. Taking into account the fact that at relativistic velocities β the ratio $\eta^2/(\mathbf{k}-\boldsymbol{\kappa})^2$ is of order $(\alpha Z)^2$ and hence negligible, M_0 becomes

$$M_0=N_1'N_2^*\frac{1}{(\mathbf{k}-\boldsymbol{\kappa})^4}\bar{\chi}_2\mathbf{s}\left[1+\frac{i}{2m}\gamma_4\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})+\frac{\pi\alpha Z}{8}\frac{|\mathbf{k}-\boldsymbol{\kappa}|}{m}\right]\chi_1. \tag{11}$$

This expression has the same form as the one given in Eq. (K.17), but with a different value of the coefficient N_1'.[12] With a view toward analyzing the other terms of Eq. (10) we will introduce the notation

$$M_{ij}=\int \bar{u}_{2i}(\mathbf{p})\mathbf{s}u_{1j}(\mathbf{p}-\boldsymbol{\kappa})d^3p. \tag{12}$$

The form of the matrix elements M_{10}, M_{11}, and M_{20} is given by Eqs. (K.19), (K.20), and (K.23), with the integrals $I(\lambda)$, $\mathbf{J}(\lambda)$, and $K(\lambda)$ of Eqs. (K.21), (K.22), (K.24), replaced by I', $\mathbf{J}'$, K', respectively, and the

[10] Thus, $\boldsymbol{\kappa}$ and $\mathbf{k}$ denote the photon and electron momenta, respectively, $\mathbf{s}$ the polarization vector ($\boldsymbol{\kappa}\cdot\mathbf{s}=0$, $\mathbf{s}^2=1$). Natural units are used.

[11] The functions $G(p)$ and $F(p)$ have been obtained by calculating the exact Fourier transform of the position space spinor and by subsequently retaining only the indicated order of magnitude.

[12] In Eq. (K.17), $\pi\alpha Z|\mathbf{k}-\boldsymbol{\kappa}|/8m$ should correctly stand in the place of $\alpha Z\phi(\mathbf{k}-\boldsymbol{\kappa})/2\pi^2$.

coefficient N_1 replaced by N_1'. The expressions for I', $\mathbf{J}'$, K' are

$$I'=\int \frac{1}{[(\mathbf{p}-\mathbf{k})^2+\mu^2]}\frac{ip-m}{(p^2-k^2-i\epsilon)} \times\frac{(\mathbf{p}-\boldsymbol{\kappa})^2-\eta^2}{[(\mathbf{p}-\boldsymbol{\kappa})^2+\eta^2]^3}d^3p, \quad (13)$$

$$\mathbf{J}'=\int \frac{1}{[(\mathbf{p}-\mathbf{k})^2+\mu^2]}\frac{ip-m}{(p^2-k^2-i\epsilon)} \times\frac{(\mathbf{p}-\boldsymbol{\kappa})^2-\eta^2}{[(\mathbf{p}-\boldsymbol{\kappa})^2+\eta^2]^3}(\mathbf{p}-\boldsymbol{\kappa})d^3p, \quad (14)$$

$$K'=\int\int \frac{1}{[(\mathbf{q}-\mathbf{k})^2+\mu^2]}\frac{iq-m}{(q^2-k^2-i\epsilon)} \times\frac{\gamma_4}{[(\mathbf{q}-\mathbf{p})^2+\mu^2]}\frac{ip-m}{(p^2-k^2-i\epsilon)} \times\frac{(\mathbf{p}-\boldsymbol{\kappa})^2-\eta^2}{[(\mathbf{p}-\boldsymbol{\kappa})^2+\eta^2]^3}d^3pd^3q. \quad (15)$$

The matrix element (2), correct to first order in αZ is given by

$$M=M_0+M_{10}+M_{11}+M_{20}. \quad (16)$$

The justification of this fact and the analysis of the order of magnitude of the matrix elements M_{ij} is similar to that made in (K). This time we will use, however, the following analytic form of the $\delta(\mathbf{p}-\boldsymbol{\kappa})$ function

$$\delta(\mathbf{p}-\boldsymbol{\kappa})=\frac{2}{\pi^2}\lim_{\eta\to 0}\eta\frac{p^2-\eta^2}{(p^2+\eta^2)^3}.$$

In the limit $\eta\to 0$ the integrals (13), (14), and (15) contain the function $\pi^2\delta(\mathbf{p}-\boldsymbol{\kappa})/2\eta=\pi^2\delta(\mathbf{p}-\boldsymbol{\kappa})/\lambda$ and one ascertains that the matrix elements M_{ij} are of the same order of magnitude as in the case of the K shell. Moreover, one ascertains that the terms in $1/\eta$ of the integrals I' and K' are equal, respectively, to the corresponding ones of the integrals $I(\lambda)$ and $K(\lambda)$. I' may thus be given the form of Eq. (K.26) (with $I'^{(0)}$ to replace $I^{(0)}$) and K' the form of Eq. (K.27), with essentially the same expression (K.28) for the integral L.

The matrix element M, given by Eq. (16), may be finally written

$$M=\bar{\chi}_2(P+Q)\chi_1, \quad (17)$$

P and Q being given by Eqs. (K.30) and (K.31), with $I^{(0)}$, $\mathbf{J}^{(0)}$ replaced by $I'^{(0)}$, $\mathbf{J}'^{(0)}$ and the coefficient N_1 by N_1'. We will now show that in the lowest order approximation (of the zero order terms in η or λ) the following equations hold:

$$I'^{(0)}=I^{(0)}, \quad \mathbf{J}'^{(0)}=\mathbf{J}^{(0)}. \quad (18)$$

Indeed, we have

$$I'=I(\eta)+\frac{\eta}{2}\frac{\partial I(\eta)}{\partial\eta}, \quad \mathbf{J}'=\mathbf{J}(\eta)+\frac{\eta}{2}\frac{\partial\mathbf{J}(\eta)}{\partial\eta}. \quad (19)$$

One can see that in the preceding equations the terms containing the derivatives give no zero-order contribution in η. Equations (19) then state the equality of the zero order terms in η of $I'^{(0)}$ and $I^{(0)}(\eta)$ on one hand, and of $\mathbf{J}'^{(0)}$ and $\mathbf{J}^{(0)}(\eta)$ on the other; Eqs. (18) are thus proved. Hence, in our approximation, the matrix element M of the L_{I} subshell differs from that of the K shell only by the value of the normalization coefficient N_1': $M_{\text{I}}=(N_1'/N_1)M_K$; its explicit calculation reduces entirely to the one reported in (K).

The sum $\sum|M|^2$, occurring in the differential cross section (1), being performed over the same kind of transitions as in (K), will lead to the same result as there. Owing to the fact that $N_1'^2/N_1^2=\frac{1}{8}$, we finally find for the differential cross section of the photoeffect from the L_{I} subshell, correct to first order in αZ, the result

$$d\sigma_{\text{I}}=\zeta\tfrac{1}{8}d\sigma_K. \quad (20)$$

Here $d\sigma_K$ is given by Eqs. (K.92), (K.93), (K.94), and ζ is a constant introduced to take account of screening (see Sec. 5C).[13,14] The result (20) has been obtained meanwhile also by Pratt.[15]

In the usually adopted coordinate system in which $\boldsymbol{\kappa}$ points in the positive z direction, $\mathbf{s}$ in the positive x direction, the polar angles of $\mathbf{k}$ being θ and φ, by introducing the abbreviations

$$\epsilon=E/m=1/(1-\beta^2)^{\frac{1}{2}}, \quad \Theta=1-\beta\cos\theta, \quad (21)$$

$d\sigma_K$ may be given the somewhat more convenient form

$$d\sigma_K=4\alpha^6Z^5\lambda_0^2\frac{(\epsilon^2-1)^{\frac{3}{2}}}{\epsilon^4(\epsilon-1)^5}\left\{\mathfrak{F}\left(1-\frac{\pi\alpha Z}{\beta}\right)+\pi\alpha Z\mathfrak{G}\right\}d\omega, \quad (22)$$

where λ_0 is the Compton wavelength and

$$\mathfrak{F}=\sin^2\theta\left\{\cos^2\varphi\frac{1}{\Theta^4}+\tfrac{1}{2}\epsilon(\epsilon-1)[\tfrac{1}{2}(\epsilon-1)-\cos^2\varphi]\frac{1}{\Theta^3}\right\}, \quad (23)$$

$$\mathfrak{G}=\frac{\epsilon^{\frac{1}{2}}(\epsilon-1)^{\frac{1}{2}}}{2^{\frac{3}{2}}(\epsilon^2-1)}\left\{[\tfrac{1}{4}(\epsilon-1)-\cos^2\varphi]\frac{1}{\Theta^{7/2}} +[-\tfrac{1}{2}\epsilon(\epsilon-1)(\epsilon+2)+3\epsilon^2\cos^2\varphi]\frac{1}{\Theta^{\frac{5}{2}}} +[\tfrac{1}{4}\epsilon^2(4\epsilon-3)(\epsilon-1)-\epsilon^2(\epsilon+1)\cos^2\varphi]\frac{1}{\Theta^{\frac{3}{2}}}\right\} +\frac{\epsilon^2(\epsilon-1)}{4(\epsilon^2-1)^{\frac{3}{2}}}\left\{[(\epsilon-1)(\epsilon+2)-2\epsilon^2\cos^2\varphi]\frac{1}{\Theta^2} +[-\epsilon^2(\epsilon-1)+2\epsilon^2\cos^2\varphi]\frac{1}{\Theta}\right\}. \quad (24)$$

[13] When working with unscreened Coulomb wave functions as above, we have evidently $\zeta=1$.

[14] Equation (20) holds, of course, also when the photoelectron

A similar equation to (20) holds evidently also for the total cross sections, σ_K being given by Eqs. (K.98), (K.95), and (K.97). We will discuss the obtained cross sections in Sec. 5.[16] We remark however here that $d\sigma_{\rm I}$, together with $d\sigma_K$, vanish in our approximation for $\theta=0,\ \pi$.[17]

3. $L_{\rm II}$ SUBSHELL

The spinors of the $L_{\rm II}$ subshell bound states (of quantum numbers $n=2$, $l=1$, $j=\frac{1}{2}$, $m=\pm\frac{1}{2}$) may be written in split form

$$u_1(\mathbf{p})=\left[G(p)+iF(p)\gamma_4\boldsymbol{\gamma}\cdot\frac{\mathbf{p}}{p}\right]\begin{pmatrix}\vartheta_{1,\frac{1}{2},m}(\mathbf{p}/p)\\0\end{pmatrix}. \quad (25)$$

We have denoted by ϑ_{ljm} the Pauli eigenfunctions of the angular momenta $\mathbf{l}^2$, $\mathbf{j}^2$, and j_z, with the indicated eigenvalues.[18] To lowest order in αZ, the only one we are interested in, the functions $G(p)$ and $F(p)$ are given by[11,19]

$$G(p)=\frac{4}{(3\pi)^{\frac{1}{2}}}(2\eta)^{\frac{5}{2}}\left(1+\frac{3}{8}\frac{p^2}{m^2}\right)\frac{p\eta}{(p^2+\eta^2)^3},$$
$$F(p)=\frac{2}{(3\pi)^{\frac{1}{2}}}(2\eta)^{\frac{5}{2}}\frac{p}{m}\frac{p\eta}{(p^2+\eta^2)^3}. \quad (26)$$

Expression (25) may be written as

$$u_1(\mathbf{p})=\frac{1}{(4\pi)^{\frac{1}{2}}}\left[G(p)+iF(p)\gamma_4\boldsymbol{\gamma}\cdot\frac{\mathbf{p}}{p}\right]\left(\boldsymbol{\sigma}\cdot\frac{\mathbf{p}}{p}\right)\chi_1,$$

where χ_1 is one of the spinors (1,0,0,0) or (0,1,0,0) according to whether we consider the state of magnetic quantum number $m=\frac{1}{2}$ or $m=-\frac{1}{2}$. Using the relation between the σ and the γ matrices

$$\sigma_j=-i\gamma_k\gamma_l, \quad (j,k,l \text{ cycl. } 1,2,3), \quad (27)$$

and Eqs. (26), $u_1(\mathbf{p})$ becomes further

$$u_1(\mathbf{p})=\frac{N_1}{(4\pi)^{\frac{1}{2}}}\frac{1}{(p^2+\eta^2)^3}\left[1+\frac{3}{8}\frac{p^2}{m^2}+\frac{i}{2m}\gamma_4(\boldsymbol{\gamma}\cdot\mathbf{p})\right]$$
$$\times(\boldsymbol{\gamma}\cdot\mathbf{p})\gamma_1\gamma_2\gamma_3\chi_1, \quad (28)$$

where

$$N_1^2=4(2\eta)^7/3\pi, \quad \eta=\alpha Zm/2=\lambda/2. \quad (29)$$

We will describe the final-state spinor of the electron $\bar{u}_2(\mathbf{p})$ by means of the first-order Born approximation, see Eqs. (K.12) and (K.13).

We now set out to find the expression of the matrix element (2), correct to lowest order in αZ. Upon introducing the first-order Born approximation for the final state into Eq. (2) we get

$$M=M_0+M_1;$$
$$M_0=N_2^*\bar{\chi}_2\mathcal{s}u_1(\mathbf{k}-\boldsymbol{\kappa}), \quad (30)$$
$$M_1=(-ie)N_2^*\bar{\chi}_2\int\mathcal{A}(\mathbf{k}-\mathbf{p})\frac{i\mathcal{p}-m}{p^2-k^2-i\epsilon}\mathcal{s}u_1(\mathbf{p}-\boldsymbol{\kappa})d^3p.$$

With formula (28) for the initial-state spinor and the Coulomb form for the potential

$$eA_0(\mathbf{q})=-(\alpha Z/2\pi^2)(q^2+\mu^2)^{-1}$$

(with $\mu\to 0$), we can write further [neglecting $\eta^2/(\mathbf{k}-\boldsymbol{\kappa})^2$]

$$M=M_0+M_{10}+M_{11}; \quad (31)$$
$$M_0=\frac{N_1N_2^*}{(4\pi)^{\frac{1}{2}}}\frac{1}{(\mathbf{k}-\boldsymbol{\kappa})^6}\bar{\chi}_2\mathcal{s}\left[1+\frac{3}{8}\frac{(\mathbf{k}-\boldsymbol{\kappa})^2}{m^2}+\frac{i}{2m}\gamma_4\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})\right][\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})]\gamma_1\gamma_2\gamma_3\chi_1, \quad (32)$$
$$M_{10}=-\frac{\alpha Z}{2\pi^2}\frac{N_1N_2^*}{(4\pi)^{\frac{1}{2}}}(\bar{\chi}_2\gamma_4\mathbf{F}\mathcal{s}\boldsymbol{\gamma}\gamma_1\gamma_2\gamma_3\chi_1), \quad (33)$$
$$M_{11}=-\frac{\alpha Z}{2\pi^2}\frac{N_1N_2^*}{(4\pi)^{\frac{1}{2}}}\frac{i}{2m}(\bar{\chi}_2\gamma_4H\mathcal{s}\gamma_4\gamma_1\gamma_2\gamma_3\chi_1). \quad (34)$$

In the preceding equations we have introduced the abbreviations

$$\mathbf{F}=\frac{1}{4}\left(1-\frac{3\eta^2}{8m^2}\right)\operatorname{grad}_\kappa I(\eta)+\frac{3}{8m^2}\mathbf{J}(\eta), \quad (35)$$
$$H_{ij}=\tfrac{1}{4}\delta_{ij}I(\eta)+\frac{1}{4}\frac{\partial J_i(\eta)}{\partial\kappa_j}, \quad (36)$$
$$H=\sum_{i=1}^{3}H_{ii}=\tfrac{3}{4}I(\eta)+\tfrac{1}{4}\operatorname{div}\mathbf{J}(\eta), \quad (37)$$

where $I(\lambda)$ and $\mathbf{J}(\lambda)$ are given by Eqs. (K.21) and (K.22).

We must now show that Eq. (31) represents indeed the correct form of the matrix element, to lowest order

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polarization possibilities are considered. However, this simple equation (with $\zeta=1$) no longer holds to order $(\alpha Z)^2$; this can be seen on the nonrelativistic limit (references 1, 2) and also on the extreme relativistic one (reference 9).

[15] Reference 9, Sec. II. Some of the mathematical arguments produced therein are only outlined, their justification lying, in fact, in the detailed proof given above.

[16] See also the discussion given by B. Nagel [Arkiv Fysik **18**, 1 (1960), Sec. 6], for the K shell.

[17] This is contrary to what has been incorrectly stated in (K) after Eq. (K.94); see M. Gavrila, Nuovo cimento **10**, 691 (1960), and also reference 16.

[18] The form of the ϑ spinors is given, for example, in reference 1 (*Encyclopedia*), Eq. (13.19).

[19] It should be noted that the expression of $G(p)$ contains the term $3p^2/8m^2$, of relativistic origin but independent of αZ, which becomes of the order of magnitude 1 for $p\approx m$.

in αZ. The term M_0 is evidently of zero order in αZ. Contrary to appearances, the terms M_{10} and M_{11} are also of zero order. Indeed, $I(\eta)$ is of order of magnitude $1/\eta$, whereas $\mathbf{J}(\eta)$ is of zero order in η. Thus $\mathbf{F}$ and H are of order $1/\eta$ and it is only this degree of approximation we are interested in here. Since, to order $1/\eta$, $I(\eta)$ is given by [see Eq. (K.26)]

$$I(\eta)=A_0(it-m);\quad A_0=-\frac{\pi^2}{\eta}\frac{1}{(k^2-\kappa^2)(\mathbf{k}-\boldsymbol{\kappa})^2}, \tag{38}$$

where t is the four-component quantity $(\boldsymbol{\kappa},iE)$, we have

$$\mathbf{F}=\tfrac{1}{4}\operatorname{grad}_\kappa I(\eta)=\tfrac{1}{4}[(it-m)\operatorname{grad}_\kappa A_0+iA_0\boldsymbol{\gamma}], \tag{39}$$

$$H_{ij}=\tfrac{1}{4}A_0(it-m)\delta_{ij},\quad H=\tfrac{3}{4}A_0(it-m). \tag{40}$$

It is thus seen that M_{10} and M_{11} are of zero order in αZ. It may also be shown that M contains no other terms of this order of magnitude.

Hence, the matrix element (31) may be put into the form

$$M=\bar{\chi}_2 P\chi_1, \tag{41}$$

where

$$P=\frac{N_1N_2^*}{(4\pi)^{\frac{1}{2}}}\gamma_4 S\Bigg\{-\frac{1}{(\mathbf{k}-\boldsymbol{\kappa})^6}\Bigg[\frac{i}{2m}\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})+\gamma_4\Big(1+\frac{3}{8}\frac{(\mathbf{k}-\boldsymbol{\kappa})^2}{m^2}\Big)\Bigg][\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})]+\frac{\alpha Z}{8\pi^2}\Bigg[(it+m)\Big(\boldsymbol{\gamma}\operatorname{grad}_\kappa A_0+\frac{3i}{2m}A_0\gamma_4\Big)+iA_0\Bigg]\Bigg\}\gamma_1\gamma_2\gamma_3. \tag{42}$$

The differential cross section, summed up over the two electrons of the L_{II} subshell and the two possible spin orientations of the final state, is given by (1). Owing to the form (28) adopted for the initial-state spinor, which permits the matrix element to be written as in Eq. (41), the sum $\sum|M|^2$ can be performed using the formula [see (K), Sec. IV].

$$\sum_{\sigma m}|M|^2=\frac{1}{4Em}\operatorname{Sp}[P(i\boldsymbol{l}-m)\bar{P}(i\boldsymbol{k}-m)], \tag{43}$$

containing the four-vectors k $(\mathbf{k},iE)$ and l $(0,im)$, $\bar{P}$ being given by $\bar{P}=\gamma_4P^+\gamma_4$. The calculation of the traces appearing in Eq. (43) is a very tedious operation and will not be reproduced here.

We find the following formula for the differential cross section of the photoeffect from the L_{II} subshell, correct to lowest order in αZ (the notations being the same as for the L_I case):

$$d\sigma_{II}=\zeta\frac{1}{24}\alpha^8Z^7\lambda_0{}^2\frac{(\epsilon^2-1)^{\frac{1}{2}}}{\epsilon^5(\epsilon-1)^5}\Bigg\{\tfrac{1}{4}\epsilon(3\epsilon+1)\frac{1}{\Theta^4}-\tfrac{1}{16}\epsilon^2(9\epsilon^2+30\epsilon-7)\frac{1}{\Theta^3}+\tfrac{1}{8}\epsilon^3(\epsilon^3+6\epsilon^2+11\epsilon-2)\frac{1}{\Theta^2}-\tfrac{1}{16}\epsilon^4(\epsilon-1)(\epsilon+7)\frac{1}{\Theta}+\sin^2\theta\cos^2\varphi\Bigg[2(\epsilon+1)\frac{1}{\Theta^5}-2\epsilon(\epsilon+1)\frac{1}{\Theta^4}-\tfrac{1}{8}\epsilon^2(3\epsilon+1)(\epsilon^2-1)\frac{1}{\Theta^3}\Bigg]\Bigg\}d\omega. \tag{44}$$

We have again introduced here a screening factor ζ.[13] The corresponding total cross section is

$$\sigma_{II}=\zeta\frac{1}{256}\alpha^6Z^7\varphi_0\frac{(\epsilon^2-1)^{\frac{1}{2}}}{(\epsilon-1)^5}\Bigg\{9\epsilon^3-5\epsilon^2+24\epsilon-16-\frac{\epsilon^2+3\epsilon-8}{(\epsilon^2-1)^{\frac{1}{2}}}\ln[\epsilon+(\epsilon^2-1)^{\frac{1}{2}}]\Bigg\}, \tag{45}$$

where φ_0 is the Thomson scattering cross section.

4. L_{III} SUBSHELL

The four bound-state spinors of the L_{III} subshell (of quantum numbers $n=2$; $l=1$; $j=\frac{3}{2}$; $m=\pm\frac{1}{2},\pm\frac{3}{2}$) may be given the following form[18]:

$$u_1(\mathbf{p})=\Big[G(p)+iF(p)\gamma_4\boldsymbol{\gamma}\cdot\frac{\mathbf{p}}{p}\Big]\begin{pmatrix}\vartheta_{1,\frac{3}{2},m}(\mathbf{p}/p)\\0\end{pmatrix}. \tag{46}$$

In the lowest order approximation in αZ we are interested in, the functions $G(p)$ and $F(p)$ are given by[11]

$$G(p)=\frac{4}{(3\pi)^{\frac{1}{2}}}(2\eta)^{\frac{5}{2}}\frac{p\eta}{(p^2+\eta^2)^3},\quad F(p)=\frac{p}{2m}G(p). \tag{47}$$

It is convenient to transform expression (46). To this end we use the equality, which can be easily checked by direct calculation,

$$\frac{1}{(8\pi)^{\frac{1}{2}}}\Big(-\frac{p_1}{p}\sigma_1-\frac{p_2}{p}\sigma_2+2\frac{p_3}{p}\sigma_3\Big)\chi_1=\begin{pmatrix}\vartheta_{1,\frac{3}{2},m}(\mathbf{p}/p)\\0\end{pmatrix},\quad m=\pm\tfrac{1}{2}, \tag{48}$$

where χ_1 is the spinor (1,0,0,0) or (0,1,0,0) according to whether we have $m=\frac{1}{2}$ or $m=-\frac{1}{2}$, respectively. Similarly, we have also

$$\Big(\frac{3}{8\pi}\Big)^{\frac{1}{2}}\Big(\frac{p_1}{p}\sigma_1-\frac{p_2}{p}\sigma_2\Big)\chi_1=\begin{pmatrix}\vartheta_{1,\frac{3}{2},m}(\mathbf{p}/p)\\0\end{pmatrix},\quad m=\pm\tfrac{3}{2}, \tag{49}$$

where χ_1 is the spinor (1,0,0,0) or (0,1,0,0) according to whether we have $m=-\frac{3}{2}$ or $m=\frac{3}{2}$, respectively.

We now introduce the following notation: given a vector $\mathbf{q}(q_1,q_2,q_3)$ we shall denote by $\mathbf{q}'$ the vector of components $(-q_1,-q_2,2q_3)$ and by $\mathbf{q}''$ the vector of components $(q_1,-q_2,0)$. We will distinguish with similar superscripts the (nonvector) quantities pertaining to the case $m=\pm\frac{1}{2}$, from those pertaining to $m=\pm\frac{3}{2}$.

Taking advantage of this notation and using Eqs. (27), (47), and (49), the initial-state spinors (46) may be given the form

$$u_1(\mathbf{p})=\frac{N_1'}{(4\pi)^{\frac{1}{2}}}\frac{1}{(p^2+\eta^2)^3}\left(1+\frac{i}{2m}\gamma_4\boldsymbol{\gamma}\cdot\mathbf{p}\right)(\boldsymbol{\gamma}'\cdot\mathbf{p})\times\gamma_1\gamma_2\gamma_3\chi_1,\quad m=\pm\tfrac{1}{2},\tag{50}$$

$$u_1(\mathbf{p})=\frac{N_1''}{(4\pi)^{\frac{1}{2}}}\frac{1}{(p^2+\eta^2)^3}\left(1+\frac{i}{2m}\gamma_4\boldsymbol{\gamma}\cdot\mathbf{p}\right)(\boldsymbol{\gamma}''\cdot\mathbf{p})\times\gamma_1\gamma_2\gamma_3\chi_1,\quad m=\pm\tfrac{3}{2},\tag{51}$$

where

$$N_1'^2=\tfrac{1}{2}N_1^2,\quad N_1''^2=\tfrac{3}{2}N_1^2,\quad N_1^2=4(2\eta)^7/3\pi.\tag{52}$$

For the description of the final state of the electron, the first-order Born approximation [see Eqs. (K.12) and (K.13)] will again be used. Hence the matrix element (2), which describes an individual transition, takes the form (30). Upon introducing into Eq. (30) the expressions (50) and (51) for the initial-state spinors, two types of matrix elements appear, according to whether we consider the case $m=\pm\frac{1}{2}$ or $m=\pm\frac{3}{2}$. In the case of $m=\pm\frac{1}{2}$, the matrix element correct to lowest order in αZ (the only one we are interested in) is given by

$$M'=M_0'+M_{10}'+M_{11}',\tag{53}$$

where

$$M_0'=\frac{N_1'N_2^*}{(4\pi)^{\frac{1}{2}}}\frac{1}{(\mathbf{k}-\boldsymbol{\kappa})^6}\bar{\chi}_2\boldsymbol{s}\left[1+\frac{i}{2m}\gamma_4\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})\right]\times[\boldsymbol{\gamma}'\cdot(\mathbf{k}-\boldsymbol{\kappa})]\gamma_1\gamma_2\gamma_3\chi_1,\tag{54}$$

$$M_{10}'=-\frac{\alpha Z}{2\pi^2}\frac{N_1'N_2^*}{(4\pi)^{\frac{1}{2}}}(\bar{\chi}_2\gamma_4\mathbf{F}\boldsymbol{s}\boldsymbol{\gamma}'\gamma_1\gamma_2\gamma_3\chi_1),\tag{55}$$

$$M_{11}'=-\frac{\alpha Z}{2\pi^2}\frac{N_1'N_2^*}{(4\pi)^{\frac{1}{2}}}\frac{i}{2m}(\bar{\chi}_2\gamma_4H_{ij}\boldsymbol{s}\gamma_4\gamma_i\gamma_j'\gamma_1\gamma_2\gamma_3\chi_1),\tag{56}$$

$\mathbf{F}$ and H_{ij} being defined as in Eqs. (39) and (36). The analysis of the order of magnitude of the terms contained in Eq. (53) is carried out similarly as for the L_{II} subshell. In the present case, however, the term M_{11}' of Eq. (56) is of first order in αZ and hence negligible. Indeed, from Eq. (40) we have to order $1/\eta$

$$H_{ij}\boldsymbol{s}\gamma_4\gamma_i\gamma_j'=\tfrac{1}{4}A_0(it-m)\boldsymbol{s}\gamma_4(\delta_{ij}\gamma_i\gamma_j')=0,\tag{57}$$

which shows that M_{11}' has no zero-order term in αZ.

Further, because $\boldsymbol{\gamma}'\cdot\boldsymbol{\gamma}=-\gamma_1^2-\gamma_2^2+2\gamma_3^2=0$, we may write

$$\mathbf{F}\boldsymbol{s}\boldsymbol{\gamma}'=\tfrac{1}{4}[-\boldsymbol{s}(it+m)(\boldsymbol{\gamma}'\cdot\mathrm{grad}_\kappa A_0+2iA_0(\boldsymbol{\gamma}'\cdot\mathbf{s})].$$

With this the matrix element (53) can be put into the form

$$M'=\bar{\chi}_2Q\chi_1,\tag{58}$$

where Q stands for

$$Q=\frac{N_1'N_2^*}{(4\pi)^{\frac{1}{2}}}\gamma_4\boldsymbol{s}\left\{-\frac{1}{(\mathbf{k}-\boldsymbol{\kappa})^6}\left[\frac{i}{2m}\boldsymbol{\gamma}\cdot(\mathbf{k}-\boldsymbol{\kappa})+\gamma_4\right]\times[\boldsymbol{\gamma}\cdot(\mathbf{k}'-\boldsymbol{\kappa}')]+\frac{\alpha Z}{8\pi^2}[(it+m)(\boldsymbol{\gamma}\cdot\mathrm{grad}_\kappa' A_0)-2iA_0\boldsymbol{s}(\boldsymbol{\gamma}\cdot\mathbf{s}')]\right\}\gamma_1\gamma_2\gamma_3.\tag{59}$$

The close similarity of the expressions (50) and (51) for the initial-state spinors permits a completely analogous treatment for the $m=\pm\frac{3}{2}$ case. Thus, the matrix element M'' will be given by equations similar to Eqs. (53)–(56). Also here, on account of the equation corresponding to (57) (since again $\boldsymbol{\gamma}''\cdot\boldsymbol{\gamma}=\gamma_1^2-\gamma_2^2=0$), the term M_{11}'' is of first order in αZ and thus negligible. Hence, the matrix element M'' may be expressed as in Eqs. (58) and (59), where now any quantity q' has to be replaced by q''.

The sum $\sum|M|^2$ occurring in the formula for $d\sigma_{III}$ of Eq. (1) may be split into two parts, one containing the terms with $m=\pm\frac{1}{2}$, the other containing the terms with $m=\pm\frac{3}{2}$:

$$\sum_{\sigma,m}|M|^2=\sum_{\sigma,m=\pm\frac{1}{2}}|M'|^2+\sum_{\sigma,m=\pm\frac{3}{2}}|M''|^2.\tag{60}$$

Given the form (58) in which we have written the matrix elements in both cases, as well as the definition of the spinors χ_1 and $\bar{\chi}_2$, each of the two sums of Eq. (60) may be performed using formula (43). The traces which appear in both cases are of the same kind as those for the L_{II} subshell.

The formula we find for the differential cross section of the photoeffect from the L_{III} subshell, correct to lowest order in αZ, is[13]

$$d\sigma_{III}=\zeta_{\frac{1}{12}}\alpha^8Z^7\lambda_0^2\frac{(\epsilon^2-1)^{\frac{1}{2}}}{\epsilon^5(\epsilon-1)^5}\left\{-\tfrac{1}{4}\epsilon(3\epsilon-1)\frac{1}{\Theta^4}+\tfrac{1}{2}\epsilon^2(3\epsilon^2-1)\frac{1}{\Theta^3}+\tfrac{1}{2}\epsilon^3(\epsilon^3-3\epsilon^2+2\epsilon+1)\frac{1}{\Theta^2}-\tfrac{1}{4}\epsilon^4(\epsilon-2)(\epsilon-1)\frac{1}{\Theta}+\sin^2\theta\cos^2\varphi\left[2(\epsilon+1)\frac{1}{\Theta^5}-\epsilon(\epsilon+1)(3\epsilon-1)\frac{1}{\Theta^4}+\epsilon^2(\epsilon^2-1)\frac{1}{\Theta^3}\right]\right\}d\omega.\tag{61}$$

We get for the total cross section

$$\sigma_{III}=\zeta\tfrac{1}{32}\alpha^6Z^7\varphi_0\frac{(\epsilon^2-1)^{\frac{1}{2}}}{(\epsilon-1)^5}\left\{4\epsilon^3-6\epsilon^2+5\epsilon+3-\frac{\epsilon^2-3\epsilon+4}{(\epsilon^2-1)^{\frac{1}{2}}}\ln[\epsilon+(\epsilon^2-1)^{\frac{1}{2}}]\right\}. \quad (62)$$

5. DISCUSSION

A. Differential Cross Sections

We will discuss in the following the differential cross sections (20), (44), (61), and their energy dependence. To obtain their form in the low-energy limit we will expand these formulas in powers of β, neglecting order β^2. Since in this approximation $\epsilon\rightarrow 1$, we find for the L_I subshell

$$d\sigma_I^{NR}=\zeta\sqrt{2}\alpha^6Z^5\lambda_0^2\left(1-\pi\frac{Ze^2}{\hbar v}\right)\left(\frac{mc^2}{h\nu}\right)^{7/2}\times\sin^2\theta\cos^2\varphi(1+4\beta\cos\theta)d\omega. \quad (63)$$

In the case of the L_{II} and L_{III} subshells we get

$$d\sigma_{II}^{NR}=\tfrac{1}{3}d\sigma_{II+III}^{NR},\quad d\sigma_{III}^{NR}=\tfrac{2}{3}d\sigma_{II+III}^{NR}, \quad (64)$$

where we have put

$$d\sigma_{II+III}^{NR}=\zeta\frac{\sqrt{2}}{8}\alpha^8Z^7\lambda_0^2\left(\frac{mc^2}{h\nu}\right)^{9/2}\times(1+2\beta\cos\theta+4\beta\cos\theta\sin^2\theta\cos^2\varphi)d\omega. \quad (65)$$

Equations (63) and (65) contain, apart from *second-order* terms in $(Ze^2/\hbar v)$, just the angular distributions Schur determined by a direct, nonrelativistic calculation[20] (from the nonrelativistic point of view the L_{II} and L_{III} subshells cannot be distinguished). It should be noted that the ratio $(d\sigma_{II}^{NR}/d\sigma_{III}^{NR})=\frac{1}{2}$ is equal to the ratio of the number of electrons in the subshells considered.[21]

In the extreme relativistic limit $\beta\rightarrow 1$ $(\epsilon\rightarrow\infty)$, the negative powers of Θ are rapidly decreasing functions of the angle θ and this determines a similar behavior for the differential cross sections. Thus, at very high energies of the incident photons, practically all the photoelectrons are ejected in forward directions. The range in which the differential cross sections are appreciably different from zero is more concentrated around $\theta=0$, the larger the value of ϵ. In this range one can approximate

$$\frac{1}{\Theta}\simeq\frac{2\epsilon^2}{1+\epsilon^2\theta^2}.$$

Introducing this into Eqs. (20), (44), (61), taking into account that $\Theta^{-p-1}=\mathcal{O}(\epsilon^2)\cdot\Theta^{-p}$, and retaining only the highest powers of ϵ, we obtain[22]

$$d\sigma_I^{ER}=\zeta\tfrac{1}{8}d\sigma_K^{ER}=\zeta\tfrac{1}{2}\alpha^6Z^5\lambda_0^2\frac{1}{\epsilon^6}\times\{\mathfrak{F}(1-\pi\alpha Z)+\pi\alpha Z\mathfrak{G}\}d\omega, \quad (66)$$

$$\mathfrak{F}=2\epsilon^7\frac{\epsilon^2\theta^2}{(1+\epsilon^2\theta^2)^3},\quad \mathfrak{G}=-\epsilon^7\frac{\epsilon^2\theta^2}{(1+\epsilon^2\theta^2)^{7/2}};$$

$$d\sigma_{II}^{ER}=\zeta\frac{1}{48}\alpha^8Z^7\lambda_0^2\epsilon\frac{16-7\epsilon^2\theta^2+\epsilon^4\theta^4}{(1+\epsilon^2\theta^2)^4}d\omega; \quad (67)$$

$$d\sigma_{III}^{ER}=\zeta\tfrac{1}{6}\alpha^8Z^7\lambda_0^2\epsilon\frac{1+8\epsilon^2\theta^2+\epsilon^4\theta^4}{(1+\epsilon^2\theta^2)^4}d\omega. \quad (68)$$

Remark that in this limit all three cross sections are independent of the polarization of the absorbed photon.

We will now discuss the angular dependence of the cross sections for the case of unpolarized incident radiation. Given the cross section for linearly polarized radiation in the form $d\sigma=[J_1(\theta)+2J_2(\theta)\cos^2\varphi]d\omega$, the cross section for the unpolarized case may be written $d\sigma=J(\theta)d\omega$, where $J=J_1+J_2$.

In our approximation the angular distribution $J(\theta)$ of the L_I subshell is the same as for the K shell, vanishing for $\theta=0$, π and presenting a maximum at an angle smaller than $\pi/2$. In the nonrelativistic limit, Eq. (63) shows that the maximum occurs for $\theta_m=(\pi/2)-2\beta$. As the photon energy increases, the maximum moves towards smaller angles. At very high energies it is seen from formulas (66) that θ_m is proportional to $1/\epsilon$.[23]

In the nonrelativistic limit the L_{II} and L_{III} subshells have the same angular distribution $J(\theta)$, yielded by Eq. (65):

$$J(\theta)\sim 1+2\beta\cos\theta+2\beta\cos\theta\sin^2\theta.$$

This is nearly isotropic; it presents a slight maximum for the β-independent angle of $\theta_m\simeq 36°$, for which $J(\theta_m)/J(0)=1+0.16\beta$ (and a minimum symmetrically situated with respect to $\pi/2$).[24]

At the intermediate energy of $h\nu/mc^2=0.4$, the

[20] Reference 2, Eq. (17). The exact consideration of retardation in the calculation of the *nonrelativistic* matrix elements (reference 4) is, in fact, meaningless. Indeed, the corrective terms to the Schur angular distributions thus found, being of order β^2 (or $h\nu/mc^2$), lie beyond the limits of validity of the calculation and are physically incorrect.

[21] See also M. Phillips, reference 5.

[22] Concerning $\mathfrak{G}$ see also the discussion of reference 17, Sec. 2; the expression given there in Eq. (7) is equivalent to the one given above.

[23] Considering only $\mathfrak{F}$ one finds $\theta_m=1/\epsilon\sqrt{2}$. See also reference 16, Sec. 6.

[24] When also the binding energy I_L of the electron in the L shell is taken into account, the formula of Schur [reference 2, Eq. (17)] yields a θ_m lying between 36° and $\pi/2$, depending on the value of the ratio $I_L/h\nu$.

TABLE I. Energy dependence of the relativistic L shell total cross sections.[a]

$h\nu/mc^2$	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{2}$	1	4
$\sigma_I/\zeta\varphi_0\alpha^4Z^5$	393.3	99.2	10.1	1.30	0.078
$\sigma_{II}/\zeta\varphi_0\alpha^6Z^7$	409.1	78.75	5.62	0.56	0.020
$\sigma_{III}/\zeta\varphi_0\alpha^6Z^7$	763.8	144	10.1	1.05	0.055

[a] See references 29 and 31.

numerical evaluation of $J(\theta)$, based on the complete formulas (44) and (61), reveals the following situation. For both the L_{II} and L_{III} subshells the J_1 functions present a monotonic decrease in the angle θ from their maximum for $\theta=0$, whereas the J_2 functions increase from zero for $\theta=0$ to a maximum for θ of about 20°, decreasing afterwards. In the case of the L_{II} subshell, $J=J_1+J_2$ results as a monotonically decreasing function of θ, beginning from a maximum for $\theta=0$. In the case of the L_{III} subshell, the increase of J_2 compensates the decrease of J_1, so that J increases from a minimum for $\theta=0$ to a maximum for $\theta_m\simeq 20°$, decreasing afterwards; one finds $J(\theta_m)/J(0)=1.27$, θ_m being much smaller than the corresponding angle for the K and L_I shells (in Suter's approximation).

Passing on to higher energies the general aspect of the angular distributions remains unchanged, for the L_{II} as well as for the L_{III} subshell. Thus, in the extreme relativistic limit Eq. (67) yields for the L_{II} case a $J(\theta)$ which is a rapidly decreasing function of θ, beginning from its maximum for $\theta=0$; indeed $J(1/\epsilon)/J(0)=0.04$. In the L_{III} case Eq. (68) yields a $J(\theta)$ which increases, from a minimum for $\theta=0$ to a maximum[25] for $\theta_m=0.42/\epsilon$, to decrease afterwards; one finds $J(\theta_m)/J(0)=1.28$, θ_m being smaller than the corresponding angle for the K and L_I shells (equal to $1/\epsilon\sqrt{2}$ in the same approximation).

B. Total Cross Sections

In the nonrelativistic limit our total cross sections become, if use is made also of Eq. (64),

$$\sigma_I^{NR}=\zeta\frac{1}{\sqrt{2}}\alpha^4Z^5\varphi_0\left(1-\pi\frac{Ze^2}{\hbar\nu}\right)\left(\frac{mc^2}{h\nu}\right)^{7/2},$$
$$\sigma_{II+III}^{NR}=\zeta\frac{3\sqrt{2}}{16}\alpha^6Z^7\varphi_0\left(\frac{mc^2}{h\nu}\right)^{9/2}. \tag{69}$$

These formulas agree to first and zero order, respectively, with the ones found by Stobbe.[26] In the extreme relativistic limit, by keeping only the lowest order in $1/\epsilon$ (or $mc^2/h\nu$) one finds[27]

$$\sigma_I^{ER}=\zeta\frac{1}{8}\left(1-\frac{19}{15}\pi\alpha Z\right)\sigma_0,$$
$$\sigma_{II}^{ER}=\zeta\frac{3}{128}(\alpha Z)^2\sigma_0,\quad \sigma_{III}^{ER}=\zeta\tfrac{1}{12}(\alpha Z)^2\sigma_0, \tag{70}$$

where

$$\sigma_0=\tfrac{3}{2}\alpha^4Z^5\varphi_0mc^2/h\nu. \tag{71}$$

Equations (70) agree, to the corresponding degree of approximation, with the ones obtained by Pratt, by another method.[28]

Table I contains the numerical results calculated for the total relativistic cross sections, correct to lowest order in αZ,[29] for different values of the energy of the incident photon. In comparison to the nonrelativistic formulas (69), the relativistic ones yield a more gradual decrease with increasing photon energy. [As seen from Eq. (70), in contradistinction to Eq. (69), for very high energies the decline is proportional to $mc^2/h\nu$.] The comparison of the nonrelativistic and relativistic formulas, in the zero-order approximation, can be followed in Table II,[30] at the same time with the variation of the ratio of the relativistic cross sections σ_{II} and σ_{III}.

TABLE II. Energy dependence of ratios of relativistic and nonrelativistic total cross sections.[a]

$h\nu/mc^2$	NR	$\frac{1}{6}$	$\frac{1}{4}$	$\frac{1}{2}$	1	4	ER
σ_{II}/σ_{III}	0.500	0.535	0.546	0.558	0.531	0.366	0.281
σ_I^{NR}/σ_I	1	0.95	0.91	0.79	0.54	0.07	0
$\sigma_{II+III}^{NR}/(\sigma_{II}+\sigma_{III})$	1	0.72	0.61	0.38	0.16	0.007	0

[a] See references 30 and 31.

C. Extrapolation to Large Z and Screening

The results presented so far should be discussed and corrected in two respects. First, since the cross sections have been evaluated with Coulomb wave functions *approximate in* αZ their validity should be delimited in this direction and the possibility of extrapolation to large Z considered. Next, the corrections should be examined which stem from the departure (owing to screening) of the self-consistent wave functions of the photoelectron from the Coulomb form.

Concerning the *magnitude* of our cross sections, this is correct only for light elements. This can be understood by noting that the nonrelativistic formulas of Stobbe for the total cross sections,[26] as well as the

[25] In contrast to the case of the lower energies, the maximum is no longer due to J_2, but to J_1 (now $J=J_1$).

[26] See reference 1 (*Encyclopedia*), Eqs. (71.14) and (71.15).

[27] Formulas (70) can be obtained also by direct integration of the differential cross sections (66), (67), (68), and by retaining again only the lowest order terms in $1/\epsilon$.

[28] Reference 9, Sec. IV.

[29] σ_I is calculated with the zero order approximation [putting $\pi\alpha Z=0$ in Eq. (22)] and σ_{II}, σ_{III} with Eqs. (45), (62).

[30] Table II is based on the data of Table I and using the nonrelativistic formulas (69). For the sake of simplicity we have put $\zeta=1$.

extreme relativistic ones of Pratt,[28] contain the ("Coulomb") exponential factor $\exp[\alpha Z(\pi+2\tau)/\beta]$ where $-\pi\leqslant\tau\equiv\arctan[2k\eta/(k^2-\kappa^2-\eta^2)]\leqslant 0$. Since the coefficient $(\pi+2\tau)/\beta$ of αZ is generally large, the αZ expansion of the exponential converges slowly and its first terms represent a good approximation only for low Z. (In the case of the $L_{\rm I}$ subshell we have taken into account the first two terms, whereas for the $L_{\rm II}$ and $L_{\rm III}$ cases only the zero-order term.)

Nevertheless, it may be expected that the *angular dependence* of our differential cross sections as well as the *energy dependence* of our total ones yield good approximations even for medium Z.[31] If so, one could obtain adequate expressions for the cross sections for larger Z, by multiplying them with convenient factors $f(\alpha Z)$,[32] which depend on the subshell considered. Thus Pratt[28] has proposed interpolation formulas for the cross sections of the $L_{\rm I}$ subshell, by combining our result Eqs. (20)–(24) with a function $f(\alpha Z)$ which he obtained from the study of the extreme relativistic limit. In the case of the $L_{\rm II}$ and $L_{\rm III}$ subshells (for which the present work has not determined the αZ corrective terms to the cross sections), at sufficiently high energies, interpolation formulas of the type $\sigma_i'=C_i f_i(\alpha Z)\sigma_i(\epsilon)$ could tentatively be used; here $f_i(\alpha Z)$ should be given by Table II of Pratt,[28,33] $\sigma_i(\epsilon)$ by formula (45) or (62) [with $\zeta=1$], and $C_{\rm II}=128/3(\alpha Z)^2$, $C_{\rm III}=12/(\alpha Z)^2$. It should be noted however that in the case of the L shell the efficiency of any interpolation formulas cannot be checked, because there exist no exact numerical computations for comparison (such as those of Hulme *et al.*[34] for the K shell).

We will now examine the screening corrections to the matrix elements. Pratt[28] has suggested that these could be obtained multiplying the Coulomb matrix elements by a certain constant. We will show in the following that this is indeed true for the lowest order approximations in αZ. In this case the matrix elements of all three subshells are of the form (30), where $u_{1s}(\mathbf{p})$ now represents the initial-state spinor of the electron in the central self-consistent field of the atom (subscript s has been introduced to emphasize this), for which the Fourier transform of the potential is denoted by $A_0(\mathbf{p})$.[35]

The term M_0 of Eq. (30) contains $u_{1s}(\mathbf{k}-\boldsymbol{\kappa})$. For functions such as $\psi_{1s}(\mathbf{r})$, the value of the Fourier transform $u_{1s}(\mathbf{p})$ at point $\mathbf{p}$ is determined by the form of $\psi_{1s}(\mathbf{r})$ over a radial distance in the neighborhood of the origin $0<r\lesssim 3/|\mathbf{p}|$.[36] Since in the present case $\mathbf{p}=\mathbf{k}-\boldsymbol{\kappa}$, the interesting range is $0<r\lesssim 3\lambda_0$.[37] Now, for not too large values of Z this range lies well inside the first Bohr orbit; in it, the self-consistent potential $A_0(r)$ practically coincides with the unscreened one generated by the nucleus. Then, near the origin, $\psi_{1s}(\mathbf{r})$ is proportional to the Coulomb function $\psi_{1c}(\mathbf{r})$ for unscreened Z,[38]

$$\psi_{1s}(\mathbf{r})=\zeta^{\frac{1}{2}}\psi_{1c}(\mathbf{r}). \tag{72}$$

It follows that $u_{1s}(\mathbf{k}-\boldsymbol{\kappa})=\zeta^{\frac{1}{2}}u_{1c}(\mathbf{k}-\boldsymbol{\kappa})$ and that the term M_0 of Eq. (30) should be corrected for screening by multiplication with $\zeta^{\frac{1}{2}}$.

M_1 of Eq. (30) may be written as

$$M_1=\int\varphi(\mathbf{p})u_{1s}(\mathbf{p})d^3p. \tag{73}$$

As shown in Secs. 2, 3, and 4, in the Coulomb case the leading term of the integral comes, whatever $\mathbf{k}$ and $\boldsymbol{\kappa}$, from the contribution of the neighborhood of the origin $\mathbf{p}\simeq 0$, where $u_{1c}(\mathbf{p})$ is large. The same situation occurs also in the screened case.[39] Then, to obtain the leading term of M_1 we expand $\varphi(\mathbf{p})$ near the origin

$$M_1\simeq\int\Big[\varphi(0)+\sum p_j\Big(\frac{\partial\varphi}{\partial p_j}\Big)_0 +\tfrac{1}{2}\sum p_ip_j\Big(\frac{\partial^2\varphi}{\partial p_i\partial p_j}\Big)_0+\cdots\Big]u_{1s}(\mathbf{p})d^3p. \tag{74}$$

The successive terms of Eq. (74) contain the derivatives of $\psi_{1s}(\mathbf{r})$ at $\mathbf{r}=0$. Owing to Eq. (72), we can write

$$M_1\simeq\zeta^{\frac{1}{2}}(2\pi)^{\frac{3}{2}}\Big[\varphi(0)\psi_{1c}(0)+(-i)\sum\Big(\frac{\partial\varphi}{\partial p_j}\Big)_0\Big(\frac{\partial\psi_{1c}}{\partial x_j}\Big)_0 +\frac{(-i)^2}{2}\sum\Big(\frac{\partial^2\varphi}{\partial p_i\partial p_j}\Big)_0\Big(\frac{\partial^2\psi_{1c}}{\partial x_i\partial x_j}\Big)_0+\cdots\Big]. \tag{75}$$

Because of the behavior of the Coulomb functions at the origin, only the lowest order terms of expansion (75) will give a determined contribution to M_1. Indeed, as we work in the Pauli approximation, the large components being of quantum number l, these will yield a

[31] The results of Tables I and II should then be applicable also to medium Z.

[32] In the case of the K shell, the interpolation formulas of this type proposed by Hall (reference 1) and by R. H. Pratt [Phys. Rev. **117**, 1017 (1960), Sec. VI] give satisfactory results.

[33] When taking screening into account, $f_i(\alpha Z)$ should be taken from Table IV of reference 9.

[34] H. Hulme *et al.*, Proc. Roy. Soc. (London) **A149**, 131 (1935).

[35] The self-consistent field of the initial state is actually slightly different from that of the final state $A_0(\mathbf{p})$.

[36] To lowest order, the function $u_{1s}(\mathbf{p})$ is in fact proportional to its large components; these are defined as the product of a spin-angle dependent factor $\mathfrak{d}$ multiplied by the Fourier-Bessel transform $G(p)$ of the nonrelativistic radial function [see for instance Eqs. (46) and (47)], now of the Hartree type. J. C. Slater, Phys. Rev. **42**, 33 (1932), has shown that the numerical radial functions of Hartree can be well approximated by analytic forms $R(r)=\sum cr^ne^{-\lambda r}$. Now, for such functions it may be shown directly that the value of the Fourier-Bessel transform $G(p)$ at p is determined by the form of $R(r)$ for $0<r\lesssim\pi/p$ (or less).

[37] Indeed, with Eq. (4),

$$1/|\mathbf{k}-\boldsymbol{\kappa}|\leqslant 1/(k-\kappa)=[1+(1+2m/\kappa)^{\frac{1}{2}}]/2m.$$

For *relativistic* κ/m it ensues that $1/|\mathbf{k}-\boldsymbol{\kappa}|\lesssim\lambda_0$.

[38] For all the L subshells the factors $\zeta^{\frac{1}{2}}$ may be taken from calculations of M. E. Rose *et al.*; they are given by H. Brysk and M. E. Rose, Revs. Modern Phys. **30**, 1169 (1958), Fig. 10.

[39] This may be seen by considering the Fourier transforms $\bar{u}_{1s}(\mathbf{p})$ of the screened Slater functions (see reference 36).

nonvanishing and determined contribution only to the term containing the derivatives of order l, whereas the small components to the term with the $(l-1)$ derivatives. The two contributions are of the same order of magnitude in αZ. The expansion (75) cannot be used beyond these terms, since derivatives of higher order than the indicated ones do not exist at $\mathbf{r}=0$.[40]

Further, $\varphi(\mathbf{p})$ and its derivatives at $\mathbf{p}=0$ contain $A_0(\mathbf{k}-\boldsymbol{\kappa})$ and its derivatives with respect to κ_j. Now, the value of the Fourier transform $A_0(\mathbf{k}-\boldsymbol{\kappa})$ is determined by the form of the self-consistent potential $A_0(r)$ in the range $0<r\lesssim 3/|k-\boldsymbol{\kappa}|\simeq 3\lambda_0$. As in this range (for not too big values of Z) screening effects are negligible, $A_0(\mathbf{k}-\boldsymbol{\kappa})$ should be taken of Coulomb form. Then the square bracket of Eq. (75) represents the Coulomb form for M_1 and it is seen that this should be corrected for screening by multiplication with $\zeta^{\frac{1}{2}}$.

It follows that, to lowest order in αZ, all three L subshell relativistic cross sections should be corrected for screening by introducing the ζ factors.[38,41] As regards the effects of screening on the higher order αZ approximations of the cross sections (calculated with Coulomb functions), these are difficult to estimate; nevertheless it appears that the screening procedure discussed above should apply to some extent also in their case.

So far no conclusive comparison of the formulas obtained in the present work with the existing experimental results[6] can be made, since experiments have been performed only for heavy elements and mostly at low energies; neither have true angular distributions been determined as yet for the L shell.[42]

6. ACKNOWLEDGMENTS

The author expresses his gratitude to Dr. R. H. Pratt for stimulating and instructive correspondence. It is a pleasure for him to thank Professor S. Titeica for his kind interest in this work.

[40] In the Coulomb case the square bracket of Eq. (75) represents an alternative method for calculating M_1. It may be checked that it leads to the same results as obtained in Secs. 2, 3, 4.

[41] The preceding arguments do not apply at nonrelativistic energies (see reference 36), where different values must be used for ζ.

[42] See however the discussion of reference 9, Sec. IV.