happens to agree with the calculated value of Clementi[4] to almost eight significant figures. However, no theoretical values were available for comparison with the results on the two-open-shell and three-open-shell excited states.

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Exact Calculation of K-Shell and L-Shell Photoeffect*†

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An exact calculation of the atomic photoelectric effect is made. The expressions for the differential and total cross sections are developed explicitly for the K and L shells, for a pure Coulomb potential. The final electron is described by a partial-wave decomposition, and the interaction with the radiation field is treated in lowest order perturbation theory. The cross sections are evaluated numerically, and the contribution of the L shell is found to be non-negligible when compared with the K shell. The results for the K shell are compared with previous work, and agreement is obtained. The new results for the L subshells are presented and compared with the available experimental work.

I. INTRODUCTION

INVESTIGATIONS of the atomic photoelectric effect have been concerned primarily with the K shell. This is because about 80% of the total atomic effect is due to the K shell; and because the simplest picture possible, that of just a pure Coulomb potential due to a nucleus of charge Ze, is most nearly approximated by the K shell, away from threshold.[1] The assumption of any more general type of potential necessitates a numerical solution of the Dirac equation for the initial and final electron states, and such a solution was essentially impossible before the development of modern fast computers. Thus the L and higher shells have usually been neglected on the basis that the effects of screening are appreciable, so that calculations based on a pure Coulomb potential would have questionable significance.

In the original period of investigation the theoretical work was primarily nonrelativistic, except for the papers of Sauter,[2] Hall,[3] and Hulme *et al.*[4] Since the revival of interest, several years ago, all of the work has been relativistic. K-shell differential and total cross sections have been obtained in the form of analytical expressions, approximate in αZ, where α is the fine-structure constant and approximately 1/137. Some of these are valid for a general energy,[5–8] and some have been obtained for the high- or low-energy limit.[9–11] Additionally, there have been numerical evaluations in the various energy limits.[12–14] The most recent and most extensive numerical work is that of Pratt *et al.*,[15] giving differential and total K-shell cross sections for a number of Z's and for photon energies from 0.2 to 2 MeV.

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† Based in part on a doctoral dissertation submitted by one of us (W.R.A.) to the Department of Physics, the University of Notre Dame.

[1] See, for example, B. Nagel and P. Olsson, Arkiv Fysik **18**, 29 (1960).

[2] F. Sauter, Ann. Physik **11**, 454 (1931).

[3] H. Hall, Rev. Mod. Phys. **8**, 358 (1936). This article contains a comprehensive review of all of the work done up to 1936.

[4] H. R. Hulme, J. McDougall, R. A. Buckingham, and R. H. Fowler, Proc. Roy. Soc. (London) **A149**, 131 (1935).

[5] In succeeding footnotes, the symbols (HE) and (GE) indicate high energy and general energy, respectively.

[6] D. Moroi and C. J. Mullin (to be published) (GE). It has been shown here that for any initial s state, characterized by principal quantum number n, the corresponding differential and total cross sections can be written as $1/n^3$ times that for the K shell, to the neglect of relative order α^2Z^2. This result was previously obtained by R. H. Pratt, Ref. 16. This affords an easy way of determining approximate differential and total cross sections for s states of higher shells.

[7] B. Nagel, Arkiv Fysik **18**, 1 (1960) (GE).

[8] M. Gavrila, Phys. Rev. **113**, 514 (1959) (GE).

[9] F. G. Negasaka, Ph. D. thesis, University of Notre Dame, 1955 (unpublished) (HE).

[10] H. Banerjee, Nuovo Cimento **10**, 863 (1958) (HE).

[11] T. A. Weber and C. J. Mullin, Phys. Rev. **126**, 615 (1962) (HE).

[12] R. H. Pratt, Phys. Rev. **117**, 1017 (1960) (HE).

[13] B. Nagel, Arkiv Fysik **24**, 151 (1963) (HE).

[14] W. R. Alling and C. J. Mullin (to be published) (HE).

[15] R. H. Pratt, R. D. Levee, R. L. Pexton, and W. Aron, Phys. Rev. **134**, A898 (1964). Another numerical calculation for intermediate energies has been done by S. Hultberg, B. Nagel, and P. Olsson, Arkiv Fysik **20**, 555 (1961). We shall use HNO to refer to this latter work.

The number of calculations for the L shell has been disproportionately smaller. In the recent period of interest, there have been four: a high-energy-limit numerical calculation by Pratt[16] of the total cross sections for the various L subshells; approximate (in αZ) differential and total cross sections for the subshells for all energies by Gavrila[17] and by Moroi and Mullin[18]; and a high-energy-limit calculation of the differential cross sections which are exact in the forward direction and valid to two orders in αZ for all angles by Alling and Mullin.[14]

The experimental work has been similarly focused on the K shell.[19–23] There have been a few experiments[24,25] giving ratios such as σ_L/σ_K or σ_L/σ_A, where σ stands for the total cross section, and the subscripts L, K, and A indicate the L shell, the K shell, and the total atom, respectively. Two experimenters, Hultberg[26] and Sujkowski,[27] have investigated angular distributions for the L shell for a uranium target at different energies. Their results are given in raw form, without corrections for scattering or geometry, as there are no accurate computations with which the results may be compared.

Now the L-shell effect is a non-negligible percentage of the total atomic effect, being about 15% for uranium. Because of this, and because of the dearth of investigation of the L shell, in this paper we shall calculate the exact L-shell angular distributions and total cross sections. This will be done for a pure Coulomb potential, for arbitrary Z, and for arbitrary photon energy. Even though screening may be appreciable, use of the pure Coulomb potential represents the first meaningful calculation which can be done for the L subshells. Subsequent computations which include screening will then allow an estimate of the effects of screening to be made.

The general formalism is developed in Sec. II. In Sec. III, general expressions for the cross sections for an arbitrary shell are determined in terms of the radial parts of the matrix element, and the radial matrix elements are evaluated analytically for the K and L shells. A program has been constructed for Notre Dame's Univac-1107 Computer to numerically evaluate the analytical cross sections for the K and L shells, and for arbitrary Z and energy. Numerical results for a number of elements and energies are presented and discussed in Sec. IV, and compared with previous work.

II. GENERAL FORMALISM

The problem is the determination of the differential and total photoelectric cross sections for the K and L shells, for the case that both the initial and final electrons are considered to be moving in a pure Coulomb field. This implies that higher order radiative corrections will be neglected, and the interaction with the radiation field will be treated in lowest order perturbation theory. The momentum associated with the bound state can be appreciable for intermediate and large Z, so that the relativistic effects become important even for low energies. Consequently, the treatment will be a completely relativistic one. With these assumptions the differential cross section can be written[28]

$$d\sigma/d\Omega=(\alpha/2\pi)(pW/k)\tfrac{1}{2}\sum|M|^2, \qquad (1)$$

where $(\mathbf{p},iW)$ = four momentum of the final electron, $(\mathbf{k},ik)$ = four momentum of the incident photon, and M is the matrix element given by

$$M=\int d\mathbf{r}\psi_f{}^\dagger\boldsymbol{\alpha}\cdot\hat{\epsilon}e^{i\mathbf{k}\cdot\mathbf{r}}\psi_i\,, \qquad (2)$$

with $\boldsymbol{\alpha}=\begin{pmatrix}0\boldsymbol{\sigma}\\ \boldsymbol{\sigma}0\end{pmatrix}$, the σ_i being 2×2 Pauli matrices, $\hat{\epsilon}$ = unit vector specifying the polarization direction of the incident photon. We want to consider the incident-photon beam to be unpolarized, and we also want to count all electrons coming out, regardless of their spins. We shall thus average over polarization directions and sum over final electron spins. Since we require the cross section for either the K shell or a certain L subshell, we shall sum over all electrons in the particular shell or subshell. In Eq. (1), $\frac{1}{2}\sum$ represents the average over photon polarizations and the sum over initial and final electrons.

ψ_i is the wave function for the initial bound electron and the solution of the Dirac equation for energy $W_B<m$. $\psi_f{}^\dagger$ is the Hermitian adjoint of the final state ψ_f which is a continuum solution of Dirac's equation for energy $W>m$ and which must have the well-known asymptotic form of a plane wave plus an incoming spherical wave. As such it cannot be written in closed form; instead it occurs as an infinite sum of partial waves.

The nucleus is considered to be infinitely heavy so that it can absorb an arbitrary amount of momentum. However, energy is conserved among the photon and the initial and final electrons. This is expressed as

$$k+W_B=W. \qquad (3)$$

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[16] R. H. Pratt, Phys. Rev. **119**, 1619 (1960).

[17] M. Gavrila, Phys. Rev. **124**, 1132 (1961).

[18] Reference 6. It has also been shown here that, to the neglect of relative order α^2Z^2, the differential and total cross sections for an $nP_{1/2}$ and $nP_{3/2}$ initial state are equal to $32(n^2-1)/3n^5$ times the corresponding quantities for the $2P_{1/2}$ and $2P_{3/2}$ states, respectively. (Previously obtained by Pratt, Ref. 16.)

[19] S. Colgate, Phys. Rev. **87**, 592 (1952).

[20] A. Hedgran and S. Hultberg, Phys. Rev. **94**, 498 (1954).

[21] S. Hultberg, Arkiv Fysik **9**, 245 (1955).

[22] G. White Grodstein, Natl. Bur. Std. (U. S.), Circ. No. 583 (1957); also R. T. McGinnies, Natl. Bur. Std. (U. S.), Suppl. to Circ. No. 583 (1959).

[23] S. Hultberg and R. Stockendal, Arkiv Fysik **15**, 355 (1959).

[24] G. D. Latyshev, Rev. Mod. Phys. **19**, 132 (1947).

[25] E. P. Grigor'ev and A. V. Zolotavin, Zh. Eksperim. i Teor. Fiz. **36**, 393 (1959) [English transl.: Soviet Phys.—JETP **9**, 272 (1959)].

[26] S. Hultberg, Arkiv Fysik **15**, 307 (1959).

[27] Z. Sujkowski, Arkiv Fysik **20**, 269 (1961).

[28] We shall use natural units with $\hbar=c=1$. A unit vector is denoted by $\hat{a}=\mathbf{a}/|\mathbf{a}|$.

III. EXACT CROSS SECTIONS FOR ARBITRARY ENERGY

1. General Expressions for the Cross Sections for an Arbitrary Energy

Using Eqs. (1) and (2), we want to determine the analytical expressions for the relativistic differential and total cross sections, for an arbitrary atomic shell. No restriction will be placed on the energy of the incident photon beam. However, when the resulting expressions are to be evaluated numerically, a practical limit must be imposed. This is owing to the fact that the relative contributions of successive partial waves decrease less rapidly for increasing energy, so that more partial waves must be included as the energy increases. The method, however, is practical for the beta-spectroscopically important region, and this is the very region where a more exact analysis is needed. The expressions will be given in terms of the radial parts of the matrix element, which can be evaluated upon specification of the atomic shell. Their evaluation will be carried out in the subsequent section for the K and L shells.

The wave functions in the matrix elements, ψ_i and ψ_f representing the initial and final electron states, may be written as

$$\psi_i=\begin{pmatrix} ig_{x_2}\Omega_{x_2m_2}(\hat{r}) \\ f_{x_2}\Omega_{-x_2m_2}(\hat{r}) \end{pmatrix}$$

and

$$\psi_f=4\pi\sum_{x_1m} P_{x_1m_1}(\hat{p},S)\begin{pmatrix} ig_{x_1}{}^{(i)}(pr)\Omega_{x_1m_1}(\hat{r}) \\ f_{x_1}{}^{(i)}(pr)\Omega_{-x_1m_1}(\hat{r}) \end{pmatrix},$$

where $\mathbf{p}$ is the linear momentum of the final electron, and S indicates its spin.

$$P_{x_1m_1}(\hat{p},S)=(\Omega_{x_1m_1}(\hat{p}),v(s)),$$

where $v(s)$ is the large component of the plane-wave spinor:

$$u=\left(\frac{W+m}{2W}\right)^{1/2}\begin{pmatrix} v \\ w \end{pmatrix};\quad v^\dagger v=1,\quad w=\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{W+m}v.$$

The Ω_{xm}'s are two-component functions given by

$$\Omega_{xm}=\sum_u C(l\tfrac{1}{2}j;m-u,u)Y_{l,m-u}(\hat{r})X^u \tag{4}$$

and

$$\Omega_{-xm}=\Omega_{xm}(l\rightarrow l'),$$

where $C(l_al_bl_c;m_am_b)$ is the Clebsch-Gordan coefficient (referred to hereafter as C coefficient), $Y_{l,m}$ is the spherical harmonic of order l, and the X^u are two-component Pauli spinors.[29] The quantities j, l, and l' are obtained from x by

$$K=|x|,\quad j=K-\tfrac{1}{2},\quad l=j-\tfrac{1}{2}\quad x<0$$
$$=j+\tfrac{1}{2}\quad x>0,\quad l'=2j-l.$$

g_{x_2}, f_{x_2} and $g_{x_1}{}^{(i)}$, $f_{x_1}{}^{(i)}$ are the radial parts of the bound and continuum functions, respectively; the normalization of the latter being chosen to give the proper asymptotic form.

Following Hulme,[30] we expand the retardation factor as

$$e^{i\mathbf{k}\cdot\mathbf{r}}=4\pi\sum_{lm} i^l j_l(kr)Y_{l,m}{}^*(\hat{k})Y_{l,m}(\hat{r}),$$

where the $j_l(kr)$ are spherical Bessel functions of order l. Inserting this and the expressions for the wave functions into the matrix element (2), defining the radial parts of the matrix element as

$$I_{x_1lx_2}=i^l\int_0^\infty r^2dr g_{x_1}{}^{(i)*}(pr)f_{x_2}(r)j_l(kr),$$
$$J_{x_1lx_2}=i^l\int_0^\infty r^2dr f_{x_1}{}^{(i)*}(pr)g_{x_2}(r)j_l(kr), \tag{5}$$

and the angular parts by

$$\epsilon_{m_1-m-m_2}{}^*A_{\pm x_1m_1lm\mp x_2m_2}=\int d\Omega_r\Omega_{\pm x_1m_1}{}^\dagger(\hat{r})\boldsymbol{\sigma}\cdot\hat{\epsilon}\Omega_{\mp x_2m_2}(\hat{r})Y_{l,m}(\hat{r}),$$

we obtain

$$\tfrac{1}{2}\sum_{\epsilon,S,m_2}|M|^2=\frac{(4\pi)^4}{2}\sum_{\substack{x_1m_1\\ \bar{x}_1\bar{m}_1,}}\sum_{\substack{lm\\ \bar{l}\,\bar{m}}}\sum_{\substack{\epsilon S\\ m_2}} P_{\bar{x}_1\bar{m}_1}(\hat{p},S)P_{x_1m_1}{}^\dagger(\hat{p},S)Y_{l,m}{}^*(\hat{k})Y_{\bar{l},\bar{m}}(\hat{k})\epsilon_{m_1-m-m_2}{}^*\epsilon_{\bar{m}_1-\bar{m}-m_2}$$
$$\times(A_{x_1m_1lm-x_2m_2}I_{x_1lx_2}-A_{-x_1m_1lmx_2m_2}J_{x_1lx_2})(A_{\bar{x}_1\bar{m}_1\bar{l}\bar{m}-x_2m_2}I_{\bar{x}_1\bar{l}x_2}{}^*-A_{-\bar{x}_1\bar{m}_1\bar{l}\bar{m}x_2m_2}J_{\bar{x}_1\bar{l}x_2}{}^*). \tag{6}$$

$\epsilon^*_{m_1-m-m_2}$ represents the complex conjugate of the components of $\hat{\epsilon}$ in a spherical basis. The components are

$$\epsilon_1=(-1/\sqrt{2})(\epsilon_x+i\epsilon_y),\quad \epsilon_0=\epsilon_z,\quad \epsilon_{-1}=(1/\sqrt{2})(\epsilon_x-i\epsilon_y),$$

and similarly,

$$\sigma_1=(-1/\sqrt{2})(\sigma_x+i\sigma_y),\quad \sigma_0=\sigma_z,\quad \sigma_{-1}=(1/\sqrt{2})(\sigma_x-i\sigma_y).$$

[29] The angular-momentum coupling coefficients and the spherical harmonics used are those as defined in M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

[30] H. R. Hulme, Proc. Roy. Soc. (London) **A133**, 381 (1931).

Integrating over the solid angle $d\Omega_r$ and using the Wigner-Eckart theorem[31] gives

$$A_{x_1m_1lm-x_2m_2}=(3[l_2'][l]/4\pi[l_1])^{1/2}C(l_2'll_1)\sum_{u_2} C(\tfrac{1}{2}1\tfrac{1}{2};u_2,m_1-m-m_2)C(l_1\tfrac{1}{2}j_1;m+m_2-u_2,m_1-m-m_2+u_2)$$
$$\times C(l_2'\tfrac{1}{2}j_2;m_2-u_2,u_2)C(l_2'll_1;m_2-u_2,m)\,,$$

$$A_{-x_1m_1lmx_2m_2}=A_{x_1m_1lm-x_2m_2}(l_1\to l_1',\,l_2'\to l_2)\,,$$

where $[a]=2a+1$ and $C(l_al_bl_c)=C(l_al_bl_c;00)$. The sum over final electron spins gives

$$\sum_S P_{\bar{x}_1\bar{m}_1}(\hat{p},S)P_{x_1m_1}{}^\dagger(\hat{p},S)=\Omega_{\bar{x}_1\bar{m}_1}{}^\dagger(\hat{p})\Omega_{x_1m_1}(\hat{p})\,. \tag{7}$$

For the sum over polarizations we use

$$\sum_\epsilon \epsilon_\lambda{}^*\epsilon_{\bar\lambda}=\delta_{\lambda\bar\lambda}-(4\pi/3)Y_{1,\lambda}{}^*(\hat{k})Y_{1,\bar\lambda}(\hat{k})=\delta_{\lambda\bar\lambda}-(-)^\lambda\sum_{L=0}^{2}(4\pi/[L])^{1/2}C(11L)C(11L;-\lambda\bar\lambda)Y_{L,\bar\lambda-\lambda}(\hat{k})\,,$$

employing the coupling rule for spherical harmonics.[32] We wish to carry out the sums over the projection numbers m_2, m_1, $\bar{m}_1$, m, $\bar{m}$. This task is simplified considerably if we choose $\hat{k}=\hat{Z}$. Then

$$Y_{l,m}{}^*(\hat{k})=([l]/4\pi)^{1/2}\delta_{m0}\quad Y_{\bar{l},\bar{m}}(\hat{k})=([\bar{l}]/4\pi)^{1/2}\delta_{\bar{m}0}\,,$$

where δ_{ij} is the Kronecker symbol, and two of the sums are eliminated. With m and $\bar{m}$ both zero, a third sum is eliminated by virtue of the sum over polarizations,

$$\sum_\epsilon \epsilon_{m_1-m-m_2}{}^*\epsilon_{\bar{m}_1-\bar{m}-m_2}=\sum_\epsilon \epsilon_{m_1-m_2}{}^*\epsilon_{\bar{m}_1-m_2}=\delta_{m_1\bar{m}_1}\{1-(-)^{m_1-m_2}\sum_L C(11L)C(11L;m_2-m_1,m_1-m_2)\}\,, \tag{8}$$

leaving only sums over m_2 and m_1. This still appears to be a sizeable problem since, for example, $A_{x_1m_1l-x_2m_2}$ contains four C coefficients which depend on m_2, so that a total of eight are implied in the square of the matrix element. This number can be reduced by using the relations between C and Racah coefficients,[33] and the symmetry relations for C coefficients.[34] For $m=0$, $A_{x_1m_1l-x_2m_2}$ has the form

$$A_{x_1m_1l-x_2m_2}=(3[l][l_2']/4\pi[l_1])^{1/2}C(l_2'll_1)\sum_{u_2} C(\tfrac{1}{2}1\tfrac{1}{2};u_2,m_1-m_2)C(l_1\tfrac{1}{2}j_1;m_2-u_2,m_1-m_2+u_2)$$
$$\times C(l_2'\tfrac{1}{2}j_2;m_2-u_2,u_2)C(l_2'll_1;m_2-u_2,0)\,.$$

The relations between Racah and C coefficients allow us to write

$$C(l_2'll_1;m_2-u_2,0)C(l_1\tfrac{1}{2}j_1;m_2-u_2,m_1-m_2+u_2)=\sum_f([l_1][f])^{1/2}W(ll_2'j_1\tfrac{1}{2};l_1f)$$
$$\times C(lfj_1;0m_1)C(l_2'\tfrac{1}{2}f;m_2-u_2,m_1-m_2+u_2)\,,$$

where $W(abcd;ef)$ is the Racah coefficient. The resultant sum over u_2 involves a product of three C coefficients and can be done. Applying the symmetry relation

$$C(l_1l_2l_3;m_1m_2)=(-)^{l_1+l_2-l_3}C(l_2l_1l_3;m_2m_1)$$

to all three, the product can be summed directly to give

$$A_{x_1m_1l-x_2m_2}=\{(3/2\pi)[l][l_2'][j_2]\}^{1/2}C(l_2'll_1)\sum_f([f])^{1/2}W(ll_2'j_1\tfrac{1}{2};l_1f)W(1\tfrac{1}{2}fl_2';\tfrac{1}{2}j_2)$$
$$\times C(lfj_1;0m_1)C(j_21f;m_2,m_1-m_2)\,. \tag{9}$$

If we define

$$a_f(x_1,l,-x_2)=([l_2'])^{1/2}C(l_2'll_1)W(ll_2'j_1\tfrac{1}{2};l_1f)W(1\tfrac{1}{2}fl_2';\tfrac{1}{2}j_2)$$
$$a_f(-x_1,l,x_2)=a_f(x_1,l,-x_2)\big|_{l_1\to l_1'}^{l_2'\to l_2}$$

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[31] Reference 29, p. 85.
[32] Reference 29, p. 61.
[33] Reference 29, p. 110.
[34] Reference 29, pp. 38–39.

and use (7), (8), and (9), then

$$\tfrac{1}{2}\sum_{\epsilon,S,m_2}|M|^2=48\pi^2\sum_{\substack{x_1\bar{x}_1\\ l\bar{l}}}\sum_{\substack{f\bar{f}\\ m_1}}[j_2][l][\bar{l}]([f][\bar{f}])^{1/2}\Omega_{\bar{x}_1m_1}{}^\dagger(\hat{p})\Omega_{x_1m_1}(\hat{p})\{a_f(x_1,l,-x_2)a_f(\bar{x}_1,\bar{l},-x_2)I_{x_1lx_2}I_{\bar{x}_1\bar{l}x_2}{}^*$$

$$+a_f(-x_1,l,x_2)a_{\bar f}(-\bar{x}_1,\bar{l},x_2)J_{x_1lx_2}J_{\bar{x}_1\bar{l}x_2}{}^*-2a_f(x_1,l,-x_2)a_{\bar f}(-\bar{x}_1,\bar{l},x_2)\,\mathrm{Re}I_{x_1lx_2}J_{\bar{x}_1\bar{l}x_2}{}^*\}$$

$$\times\sum_{m_2}\{1-(-)^{m_1-m_2}\sum_L C(11L)C(11L;m_2-m_1,m_1-m_2)\}C(j_21f;m_2,m_1-m_2)$$

$$\times C(j_21\bar{f};m_2,m_1-m_2)C(lfj_1;0m_1)C(\bar{l}\bar{f}\bar{j}_1;0m_1).$$

The sum over m_2 therefore gives rise to sums over products of two and three C coefficients. The former yields just the orthogonality relation for C coefficients,[35] and the latter can be carried out in a manner similar to that for u_2.

To carry out the sum over m_1, the product (7) must be expanded using (4). Employing the orthogonality of the Pauli spinors and the coupling rule spherical harmonics, the sums in (7) can be performed to give

$$\Omega_{\bar{x}_1m_1}{}^\dagger(\hat{p})\Omega_{x_1m_1}(\hat{p})=[(-)^{m_1+1/2}/4\pi]([j_1][\bar{j}_1][l_1][\bar{l}_1])^{1/2}\sum_\lambda C(l_1\bar{l}_1\lambda)W(j_1\bar{j}_1l_1\bar{l}_1;\lambda\tfrac{1}{2})P_\lambda(\cos\theta)C(\bar{j}_1j_1\lambda;-m_1m_1),$$

where $P_\lambda(\cos\theta)$ is the Legendre polynomial of order λ. The sum over m_1 will involve products of three and four C coefficients and can be performed in a manner similar to the previous sums. If we then sum over L, we obtain the differential cross section for the atomic photoeffect for any shell,

$$d\sigma/d\Omega=(1/4\pi)\sum_{\lambda=0}^{\infty}A_\lambda P_\lambda(\cos\theta),$$

where

$$A_\lambda=\alpha(pW/k)24\pi\sum_{\substack{x_1\bar{x}_1\\ l\bar{l}}}\sum_{f\bar{f}}[j_2][j_1][\bar{j}_1][l][\bar{l}]([l_1][\bar{l}_1])^{1/2}C(l_1\bar{l}_1\lambda)W(j_1\bar{j}_1l_1\bar{l}_1;\lambda\tfrac{1}{2})\{a_f(x_1,l,-x_2)a_f(\bar{x}_1,\bar{l},-x_2)$$

$$\times I_{x_1lx_2}I_{\bar{x}_1\bar{l}x_2}{}^*+a_f(-x_1,l,x_2)a_f(-\bar{x}_1,\bar{l},x_2)J_{x_1lx_2}J_{\bar{x}_1\bar{l}x_2}{}^*-2a_f(x_1,l,-x_2)$$

$$\times a_f(-\bar{x}_1,\bar{l},x_2)\,\mathrm{Re}I_{x_1lx_2}J_{\bar{x}_1\bar{l}x_2}{}^*\}T_{x_1\bar{x}_1l\bar{l}\lambda}{}^{j_2f\bar{f}},$$

and

$$T_{x_1\bar{x}_1l\bar{l}\lambda}{}^{j_2f\bar{f}}=(-)^{(1/2)-f}[f]\{\tfrac{2}{3}\delta_{f\bar{f}}(lC\bar{l}\lambda)W(j_1\bar{j}_1l\bar{l};\lambda f)+(-)^{l+\lambda}C(112)[\bar{f}]W(fj_221;1\bar{f})\sum_t[t]W(ltj_1\bar{j}_1;\lambda f)$$

$$\times W(\bar{l}\bar{j}_12f;\bar{f}t)C(lt\lambda)C(\bar{l}t2)\}.$$

The total cross section is obtained by integrating over $d\Omega$, with the result

$$\sigma=A_0.$$

2. Radial Matrix Elements: K and L Shells

The radial parts, $I_{x_1lx_2}$ and $J_{x_1lx_2}$, of the matrix element are written in terms of unspecified radial functions for the bound and continuum states. The large and small components of the latter may be given as

$$g_{x_1}{}^{(i)}=-\left(\frac{W+m}{2W}\right)^{1/2}e^{-i\delta_{x_1}+\nu\pi/2}\frac{|\Gamma(\gamma_K-i\nu)|}{\Gamma(2\gamma_K+1)}(2pr)^{\gamma_K-1}\{\ \}_+$$

$$f_{x_1}{}^{(i)}=i\left(\frac{W-m}{2W}\right)^{1/2}e^{-i\delta_{x_1}+\nu\pi/2}\frac{|\Gamma(\gamma_K-i\nu)|}{\Gamma(2\gamma_K+1)}(2pr)^{\gamma_K-1}\{\ \}_-,$$

where

$$\{\ \}_\pm=(\gamma_K+i\nu)e^{-ipr+i\eta}F(\gamma_K+1+i\nu,2\gamma_K+1,2ipr)\pm\text{c.c.}$$

$$\delta_{x_1}=\eta-\gamma_K\pi/2+\arg\Gamma(\gamma_K-i\nu),\quad \gamma_K=(K^2-\alpha^2Z^2)^{1/2},\quad K=|x_1|,$$

$$e^{-2i\eta}=\frac{\gamma_K+i\nu}{-x_1+i\nu'}=-\frac{x_1+i\nu'}{\gamma_K-i\nu},\quad \nu=\frac{\alpha ZW}{p},\quad \nu'=\frac{m\nu}{W},$$

[35] Reference 29, p. 34.

$\Gamma(a)$ is the gamma function, and $F(a,b,Z)$ is the confluent hypergeometric function.[36] The photoeffect for any atomic shell can then be studied, by merely specifying the appropriate g_{x_2} and f_{x_2} and carrying out the evaluation of the radial integrals. We want to consider the K and L shells, and therefore we shall give the appropriate bound-state radial functions.

K shell:

$$g_{x_2}=\left(\frac{1+\gamma_1}{2}\right)^{1/2}C_K(2\lambda r)^{\gamma_1-1}e^{-\lambda r},\quad f_{x_2}=\left(\frac{1-\gamma_1}{2}\right)^{1/2}C_K(2\lambda r)^{\gamma_1-1}e^{-\lambda r},$$

$$C_K=[(2\lambda)^3/\Gamma(2\gamma_1+1)]^{1/2},\quad \lambda=m\alpha Z,\quad \gamma_1=(1-\alpha^2Z^2)^{1/2}.$$

LI shell:

$$g_{x_2}=(1+N_2/2)^{1/2}C_{LI}e^{-\lambda_2 r}(2\lambda_2 r)^{\gamma_1-1}\left\{N_2-\frac{2\lambda_2 r}{N_2-1}\right\},\quad f_{x_2}=(1-N_2/2)^{1/2}C_{LI}e^{-\lambda_2 r}(2\lambda_2 r)^{\gamma_1-1}\left\{N_2+2-\frac{2\lambda_2 r}{N_2-1}\right\},$$

$$N_2=(2+2\gamma_1)^{1/2},\quad C_{LI}=[2\lambda_2^3(N_2-1)/N_2\Gamma(2\gamma_1+1)]^{1/2},\quad \lambda_2=\lambda/N_2.$$

LII shell:

$$g_{x_2}=(1+N_2/2)^{1/2}C_{LII}e^{-\lambda_2 r}(2\lambda_2 r)^{\gamma_1-1}\left\{N_2-2-\frac{2\lambda_2 r}{N_2+1}\right\},\quad f_{x_2}=(1-N_2/2)^{1/2}C_{LII}e^{-\lambda_2 r}(2\lambda_2 r)^{\gamma_1-1}\left\{N_2-\frac{2\lambda_2 r}{N_2+1}\right\},$$

$$C_{LII}=[(N_2+1)/(N_2-1)]^{1/2}C_{LI}.$$

LIII shell:

$$g_{x_2}=(1+\gamma_2/2)^{1/2}C_{LIII}e^{-\lambda r/2}(\lambda r)^{\gamma_2-1},\quad f_{x_2}=(1-\gamma_2/2)^{1/2}C_{LIII}e^{-\lambda r/2}(\lambda r)^{\gamma_2-1}$$

$$\gamma_2=(4-\alpha^2Z^2)^{1/2},\quad C_{LIII}=[\lambda^3/2\Gamma(2\gamma_2+1)]^{1/2}.$$

These discrete radial functions have the same r structure, i.e., $r^\delta e^{-cr}$ (δ, c arbitrary), so that the resulting radial integrals may be written in terms of one general integral. If we set

$$N_I=[(W+m)/2W]^{1/2}e^{-i(\gamma_K-l+i\nu)\pi/2}\Gamma(\gamma_K-i\nu)/\Gamma(2\gamma_K+1),$$

$$N_J=i\left[\frac{(W-m)}{(W+m)}\right]^{1/2}N_I,\quad a_1=\gamma_K+1+i\nu,\quad a_2=\gamma_K+i\nu,$$

we have

$$I_{x_1lx_2}(K)=-[(1-\gamma_1)/2]^{1/2}C_KN_I\{(-x_1+i\nu')K(\lambda,a_1,\gamma_1,1)+(\gamma_K-i\nu)K(\lambda,a_2,\gamma_1,1)\}$$

$$J_{x_1lx_2}(K)=[(1+\gamma_1)/2]^{1/2}C_KN_J\{(-x_1+i\nu')K(\lambda,a_1,\gamma_1,1)-(\gamma_K-i\nu)K(\lambda,a_2,\gamma_1,1)\},$$

$$I_{x_1lx_2}(L\text{I})=-\left(1-\frac{N_2}{2}\right)^{1/2}C_{LI}N_I\Big\{(N_2+2)[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,1)+(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,1)]$$
$$-\frac{1}{N_2-1}[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,0)+(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,0)]\Big\}$$

$$J_{x_1lx_2}(L\text{I})=\left(1+\frac{N_2}{2}\right)^{1/2}C_{LI}N_J\Big\{N_2[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,1)-(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,1)]$$
$$-\frac{1}{N_2-1}[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,0)-(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,0)]\Big\}$$

$$I_{x_1lx_2}(L\text{II})=-\left(1-\frac{N_2}{2}\right)^{1/2}C_{LII}N_I\Big\{N_2[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,1)+(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,1)]$$
$$-\frac{1}{N_2+1}[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,0)+(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,0)]\Big\}$$

$$J_{x_1lx_2}(L\text{II})=\left(1+\frac{N_2}{2}\right)^{1/2}C_{LII}N_J\Big\{(N_2-2)[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,1)-(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,1)]$$
$$-\frac{1}{N_2+1}[(-x_1+i\nu')K(\lambda_2,a_1,\gamma_1,0)-(\gamma_K-i\nu)K(\lambda_2,a_2,\gamma_1,0)]\Big\}$$

[36] See, for example, *Higher Transcendental Functions, Bateman Manuscript Project,* edited by A. Erdelyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, Chaps. I and VI.

$$I_{x_1lx_2}(L\text{III})=-\left(1-\frac{\gamma_2}{2}\right)^{1/2}C_{LIII}N_I\{(-x_1+i\nu')K(\lambda/2,a_1,\gamma_2,1)+(\gamma_K-i\nu)K(\lambda/2,a_2,\gamma_2,1)\}$$

$$J_{x_1lx_2}(L\text{III})=\left(1+\frac{\gamma_2}{2}\right)^{1/2}C_{LIII}N_J\{(-x_1+i\nu')K(\lambda/2,a_1,\gamma_2,1)-(\gamma_K-i\nu)K(\lambda/2,a_2,\gamma_2,1)\}.$$

The general integral, in terms of which these are written, is

$$K(\xi,a,\gamma,\eta)=\int_0^\infty r^2dr\; j_l(kr)e^{-(\xi+ip)r}(2pr)^{\gamma_K-1}(2\xi r)^{\gamma-\eta}F(a,b,2ipr),$$

where $b=2\gamma_K+1$. To integrate this, we use the exact asymptotic representation for $j_l(kr)$[37]

$$j_l(kr)=i^{l+1}e^{-ikr}\sum_{m=0}^{l}\frac{(-l,\,m)(1+l,\,m)}{(1,m)}\frac{i^m}{(2kr)^{m+1}}+\text{c.c.},$$

where $(\delta,m)=\delta(\delta+1)\cdots(\delta+m-1)$, and $(\delta,0)\equiv1$. In addition, we replace the confluent hypergeometric function with the integral representation[38]

$$F(a,b,2ipr)=\frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)}\int_0^1 u^{a-1}(1-u)^{b-a-1}e^{2ipru}du.$$

If we substitute this and the expression for $j_l(kr)$ into K, we have

$$K=\frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)}\sum_{m=0}^{l}\frac{(-l,\,m)(1+l,\,m)}{(1,m)}i^m\left\{i^{l+1}\int_0^\infty r^2dr(2pr)^{\gamma_K-1}(2\xi r)^{\gamma-\eta}(2kr)^{-m-1}e^{-(\xi+ip+ik)r}\right.$$
$$\times\int_0^1 u^{a-1}(1-u)^{b-a-1}e^{2ipru}du-i^{-l-1}\int_0^\infty r^2dr(2pr)^{\gamma_K-1}(2\xi r)^{\gamma-\eta}(-2kr)^{-m-1}e^{-(\xi+ip-ik)r}$$
$$\left.\times\int_0^1 u^{a-1}(1-u)^{b-a-1}e^{2ipru}du\right\}.$$

The r integrand goes to zero at the upper limit if $\text{Im}u>-\xi/2p$. At the lower limit, the integral is obviously convergent for all but one of the values which it assumes for each shell. For this one value, a term can be added and subtracted from the integrand to give rise to two valid representations of the gamma function. Therefore, we can interchange orders of integration and obtain, by transforming the r integrals,

$$K=\frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)}\sum_{m=0}^{l}\frac{(-l,\,m)(1+l,\,m)}{(1,m)}i^m\int_0^1 du u^{a-1}(1-u)^{b-a-1}\left\{\frac{i^{l+1}(2p)^{\gamma_K-1}(2\xi)^{\gamma-\eta}(2k)^{-m-1}}{(\xi+ip+ik-2ipu)^{\gamma_K+\gamma+1-\eta-m}}\right.$$
$$\left.-\frac{i^{-l-1}(2p)^{\gamma_K-1}(2\xi)^{\gamma-\eta}(-2k)^{-m-1}}{(\xi+ip-ik-2ipu)^{\gamma_K+\gamma+1-\eta-m}}\right\}\int_0^\infty dt t^{\gamma_K+\gamma-\eta-m}e^{-t}.$$

The t integral gives just the gamma function, and after some reworking we can write

$$K=\frac{\Gamma(b)\Gamma(\gamma+\gamma_K+1-\eta)}{\Gamma(a)\Gamma(b-a)}e^{i\pi(l+\eta-\gamma-\gamma_K)}\sum_{m=0}^{l}\frac{(-l,\,m)(1+l,\,m)}{(1,m)(\eta-\gamma-\gamma_K,\,m)}\frac{1}{8pk^2}\int_0^1 du u^{a-1}(1-u)^{b-a-1}$$
$$\times\{x^{\gamma_K}z^{\gamma-\eta}y^{1-m}(1-xu)^{-(\gamma+\gamma_K-\eta-m)-1}-x_1^{\gamma_K}y_1^{1-m}z_1^{\gamma-\eta}e^{-i\pi(l+m)}(1-x_1u)^{-(\gamma+\gamma_K-\eta-m)-1}\},$$

where

$$x=2p/(p+k-i\xi),\quad y=kx/p,\quad z=\xi x/p,\quad x_1=x(-k),\quad y_1=y(-k),\quad z_1=z(-k).$$

[37] P. M. Moorse and H. Feshback, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part II, p. 1465.

[38] W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), p. 88.

The integrals over du are just integral representations for the hypergeometric function.[39] Therefore K becomes

$$K=\frac{\Gamma(\gamma+\gamma_K+1-\eta)}{8pk^2}e^{i(\pi/2)(l+\eta-\gamma-\gamma_K)}\sum_{m=0}^{l}\frac{(-l,m)(1+l,m)}{(1,m)(\eta-\gamma-\gamma_K,m)}\{x^{\gamma_K}z^{\gamma-\eta}y^{1-m}F(\gamma+\gamma_K+1-\eta-m,a,b,x)$$
$$-x_1^{\gamma_K}z_1^{\gamma-\eta}y_1^{1-m}e^{-i\pi(l+m)}F(\gamma+\gamma_K+1-\eta-m,a,b,x_1)\}.$$

We can analytically continue the second hypergeometric function[40] to obtain finally

$$K(\xi,a,\gamma,\eta)=x^{\gamma_K}yz^{\gamma-\eta}\frac{\Gamma(\gamma+\gamma_K+1-\eta)}{8pk^2}e^{i(\pi/2)(l+\eta-\gamma-\gamma_K)}\sum_{m=0}^{l}\frac{(-l,m)(1+l,m)}{(1,m)(\eta-\gamma-\gamma_K,m)}\frac{1}{y^m}\Bigg\{F(\gamma+\gamma_K+1-\eta-m,a,b,x)$$
$$+e^{i\pi(\gamma+\gamma_K-l-\eta)}\left(\frac{p+k-i\xi}{p+k+i\xi}\right)^{\gamma+\gamma_K+1-\eta-m}F(\gamma+\gamma_K+1-\eta-m,b-a,b,x^*)\Bigg\}.$$

IV. RESULTS AND DISCUSSION

1. Presentation and Comparison

A program was written for Notre Dame's UNIVAC-1107 computer, to evaluate $d\sigma/d\Omega$ for an arbitrary target and photon energy, for the K and L shells. Explicit numerical evaluation was done for uranium and lead targets and for incident-photon energies of 0.081, 0.103, 0.279, 0.354, 0.412, 0.662, and 1.332 MeV. At the first two energies, the cross sections could only be evaluated for the L subshells, as these energies are below the K-shell threshold. The energies were chosen primarily to coincide with the experimental values of Hultberg[26] and of Sujkowski[27] for which raw angular distributions were obtained for the L shell. Some of the corresponding K-shell angular distributions could also be checked against the numerical work of Pratt *et al.*[15]

The number of partial waves (x_1 values) included was determined by the relative size of the radial matrix elements. The partial-wave sum was usually terminated when this relative size was down by four orders of magnitude. Thus, for example, 11 partial waves were used for 0.412 MeV, 16 for 0.612 MeV, and 22 for 1.332 MeV. Once the x_1 values were chosen, all the other sums were determined by the triangular relations. The radial matrix elements were evaluated with double precision. Any error in this evaluation was found to be in the second word, for all cases. The first word of the radial integrals was used for combining with the vector-addition coefficients, and this was always exact. The programs for determining Racah and C coefficients were checked against tables[41] and found to be good in the first word. Therefore, the main source of error is truncation and rounding, incurred in the combination of radial matrix elements with vector-coupling coefficients.

The total cross sections obtained for the K shell can be compared with experimental and previous theoretical results, as a rough verification of the present calculation. This comparison is given in Table I for a number of photon energies and a uranium target. The present results are seen to be in good agreement with the others. Additionally for a lead target and a photon energy of 0.354 MeV, the total cross section obtained was $\sigma_k=54.95$ b, which compares well with the value of 54.4 taken from the curve of Hulme *et al.*[4] We shall give a discussion of the accuracy of the calculations and the checks which have been applied, following presentation and comparison of results.

Exact total cross sections for the L shell, or the L subshells, have not been calculated or measured directly. Thus the cross sections for the L subshells, given in Table II, cannot be compared explicitly with other values. Hultberg,[26] however, has measured the ratio

TABLE I. K-shell total cross sections in barns for uranium: (1) present work, (2) HNO (Ref. 15), (3) Pratt *et al.* (Ref. 15), (4) Colgate's absorption measurements (Ref. 19).

	Theoretical			Experimental
K (MeV)	(1)	(2)	(3)	(4)
0.279	154.3	154	155	
0.412	59.47	59.5	59.9	58.6±0.2
0.662	20.21	20.2	20.4	19.9±0.1
1.332	4.928		4.93	4.7±0.1

TABLE II. Total cross sections for the L subshells in barns.

Z	k (MeV)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
82	0.081	275.2	166.2	170.0
	0.103	153.9	81.23	78.29
	0.279	12.75	4.367	3.294
	0.354	7.086	2.250	1.614
92	0.081	382.4	322.6	297.6
	0.103	219.0	162.6	139.4
	0.279	19.86	9.710	6.213
	0.354	11.26	5.102	3.070
	0.412	7.891	3.422	1.98
	0.662	2.727	1.055	0.555
	1.332	0.6649	0.2365	0.111

[39] Reference 38, p. 8.
[40] Reference 36, p. 105.
[41] A. Simon, J. H. Vandersluis, L. C. Biedenharn, Oak Ridge National Laboratory Report No. 1679, 1954 (unpublished).

TABLE III. $d\sigma/d\Omega$ in b/sr for (1) present work, and (2) Pratt *et al.*, for a uranium target.

θ(°)	$k=0.662$ MeV (1)	$k=0.662$ MeV (2)	$k=1.332$ MeV (1)	$k=1.332$ MeV (2)
0	1.559	1.55	2.734	2.50
5	3.421	3.40	4.784	4.32
10	7.339	7.29	6.715	6.58
15	10.34	10.3	5.675	5.86
20	11.07	11.0	3.857	3.86
25	10.08	10.0	2.474	2.43
30	8.340	8.60	1.569	1.56
35	6.533	6.51	1.025	1.01
40	4.969	4.95	0.688	0.685
45	3.732	3.72	0.477	0.492
50	2.793	2.79	0.346	0.344
55	2.093	2.09	0.256	0.247
60	1.578	1.58	0.192	0.192
65	1.202	1.2	0.150	0.155
70	0.925	0.92	0.119	0.119
75	0.716	0.72	0.094	0.091
80	0.560	0.57	0.077	0.076
85	0.445	0.45	0.064	0.066
90	0.359	0.36	0.052	0.052
95	0.291	0.29	0.043	
100	0.239	0.24	0.037	
105	0.199	0.20	0.031	
110	0.170	0.17		
115	0.146	0.15		
120	0.127	0.13		
125	0.112	0.11		

σ_k/σ_L for uranium, and he finds it to be essentially independent of energy and equal to 5.3 ± 0.2. Using the results calculated here, we have

k (MeV):	0.279	0.354	0.412	0.662	1.332
σ_k/σ_L:	4.31	4.41	4.47	4.66	4.87

for uranium. This ratio changes with energy, but slowly. It is also interesting to note the results, for uranium,

k (MeV):	0.279	0.354	0.412	0.682	1.332
σ_k/σ_L:	7.77	7.61	7.54	7.41	7.41.

These ratios are surprisingly close to the value of 8

TABLE IV. Differential cross sections in b/sr for the $L_{\rm I}$, $L_{\rm II}$, $L_{\rm III}$ subshells at $k=0.662$ MeV and $Z=92$.

θ(°)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.219	1.742	0.226
5	0.430	1.704	0.339
10	0.894	1.543	0.531
15	1.290	1.233	0.583
20	1.430	0.868	0.476
25	1.338	0.562	0.325
30	1.128	0.351	0.206
35	0.895	0.219	0.131
40	0.686	0.138	0.085
45	0.518	0.088	0.057
50	0.388	0.057	0.039
55	0.292	0.037	0.028
60	0.220	0.026	0.021
65	0.168	0.019	0.016
70	0.129	0.014	0.013
75	0.100	0.010	0.011
80	0.078	0.008	0.009
85	0.062	0.007	0.008
90	0.050	0.006	
95	0.041	0.005	
100	0.033	0.004	
105	0.028	0.004	
110	0.024	0.003	
115	0.020	0.003	
120	0.018		
125	0.016		

TABLE V. Differential cross sections in b/sr for the $L_{\rm I}$, $L_{\rm II}$, $L_{\rm III}$ subshells at $k=1.332$ MeV and $Z=92$.

θ(°)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.406	1.289	0.097
5	0.610	1.126	0.199
10	0.824	0.712	0.264
15	0.731	0.329	0.173
20	0.518	0.136	0.085
25	0.340	0.060	0.043
30	0.219	0.030	0.024
35	0.144	0.015	0.014
40	0.098	0.0076	0.0087
45	0.068	0.0048	0.0059
50	0.049	0.0033	0.0042
55	0.036	0.0019	0.0031
60	0.028	0.0014	0.0024
65	0.022	0.0012	0.0019
70	0.017	0.0008	0.0015
75	0.014	0.0006	0.0012
80	0.011		
85	0.0091		
90	0.0075		
95	0.0062		
100	0.0053		
105	0.0045		

TABLE VI. $d\sigma/d\Omega$ in b/sr for the L subshells, for 0.081-MeV photons on uranium.

θ(°)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.969	27.02	15.84
5	1.634	27.83	17.22
10	3.559	30.13	21.12
15	6.552	33.59	26.89
20	10.35	37.72	33.58
25	14.69	41.96	40.20
30	19.33	45.76	45.86
35	24.05	48.69	49.94
40	28.70	50.45	52.11
45	33.12	50.92	52.37
50	37.14	50.13	50.91
55	40.62	48.24	48.11
60	43.42	45.45	44.38
65	45.43	42.05	40.10
70	46.58	38.27	35.63
75	46.88	34.36	31.24
80	46.35	30.47	27.09
85	45.09	27.77	23.31
90	43.18	23.33	19.94
95	40.76	20.23	17.00
100	37.94	17.47	14.47
105	34.83	15.08	12.33
110	31.56	13.03	10.52
115	28.21	11.30	9.019
120	24.88	9.858	7.774
125	21.64	8.675	6.750
130	18.55	7.714	5.912
135	15.66	6.941	5.229
140	13.01	6.328	4.674
145	10.62	5.848	4.226
150	8.512	5.479	3.866
155	6.709	5.200	3.580
160	5.221	4.994	3.359
165	4.056	4.847	3.194
170	3.222	4.750	3.080
175	2.719	4.694	3.014
180	2.552	4.676	2.992

TABLE VII. $d\sigma/d\Omega$ in b/sr for the L subshells, for 0.103-MeV photons on uranium.

θ(°)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.421	18.24	9.52
5	0.908	18.78	10.44
10	2.318	20.29	13.02
15	4.520	22.48	16.68
20	7.324	24.91	20.68
25	10.52	27.16	24.29
30	13.90	28.86	26.94
35	17.26	29.77	28.32
40	20.43	29.78	28.40
45	23.24	28.95	27.36
50	25.55	27.40	25.46
55	27.26	25.34	23.03
60	28.32	22.96	20.36
65	28.71	20.45	17.67
70	28.48	17.96	15.12
75	27.71	15.58	12.82
80	26.50	13.40	10.79
85	24.94	11.45	9.061
90	23.15	9.739	7.602
95	21.22	8.272	6.392
100	19.21	7.034	5.398
105	17.19	6.004	4.590
110	15.22	5.159	3.935
115	13.33	4.474	3.407
120	11.56	3.924	2.982
125	9.915	3.488	2.640
130	8.414	3.145	2.366
135	7.063	2.878	2.147
140	5.862	2.672	1.972
145	4.810	2.516	1.832
150	3.906	2.399	1.720
155	3.148	2.314	1.631
160	2.533	2.253	1.560
165	2.059	2.211	1.505
170	1.723	2.185	1.467
175	1.522	2.170	1.443
180	1.456	2.166	1.435

TABLE VIII. $d\sigma/d\Omega$ in b/sr for the L subshells, for 0.081-MeV photons on lead.

θ(°)	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.387	17.24	11.93
5	0.994	17.75	12.81
10	2.764	19.20	15.27
15	5.553	21.30	18.83
20	9.145	23.70	22.83
25	13.28	25.97	26.59
30	17.66	27.77	29.55
35	22.03	28.86	31.36
40	26.11	29.12	31.91
45	29.69	28.57	31.28
50	32.59	27.31	29.68
55	34.70	25.50	27.41
60	35.97	23.33	24.73
65	36.41	20.98	21.90
70	36.08	18.59	19.10
75	35.08	16.27	16.48
80	33.51	14.11	14.10
85	31.52	12.16	12.00
90	29.23	10.43	10.20
95	26.75	8.931	8.671
100	24.17	7.659	7.394
105	21.58	6.594	6.340
110	19.03	5.716	5.476
115	16.59	5.000	4.774
120	14.29	4.424	4.206
125	12.14	3.966	3.748
130	10.18	3.605	3.379
135	8.416	3.324	3.084
140	6.839	3.108	2.850
145	5.458	2.943	2.664
150	4.269	2.820	2.519
155	3.271	2.730	2.405
160	2.461	2.666	2.316
165	1.836	2.622	2.248
170	1.391	2.593	2.199
175	1.126	2.577	2.169
180	1.038	2.572	2.159

predicted by Moroi and Mullin,[6] who have neglected relative order $\alpha^2 Z^2$, which is not small for uranium.

Stobbe[42] has calculated nonrelativistic total cross sections for the K and L shells, and he gives the ratio

$$R_s(\sigma_{L_{\rm II}}+\sigma_{L_{\rm III}})/\sigma_{L_{\rm I}}=I_B(3+8I_B/k)/(k+3I_B)\,,$$

where I_B is the mean ionization energy of the L shell.

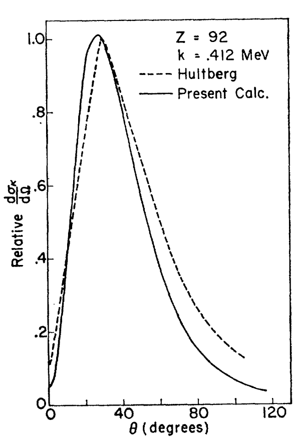

FIG. 1. Relative K-shell differential cross sections for 0.412-MeV photons on uranium. The present results are compared with Hultberg's experimental values, and both are normalized to a maximum value of one.

If we compare R_s for the energies we have considered with the values (R) we have calculated here, for uranium, we have

k (MeV)	0.081	0.103	0.279	0.354	0.412	0.662	1.332
R_s	1.005	0.794	0.302	0.239	0.206	0.129	0.064
R	1.622	1.38	0.802	0.726	0.685	0.590	0.523.

The discrepancy is quite large and increases with increasing energy, as would be expected. The large difference at energies less than the electron rest energy

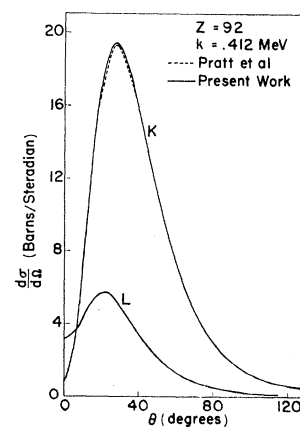

FIG. 2. K-shell angular distributions in b/sr for 0.412-MeV photons on uranium. Present results are compared with those of Pratt *et al.* The total L-shell angular distribution is also given.

[42] M. Stobbe, Ann. Physik 7, 661 (1930).

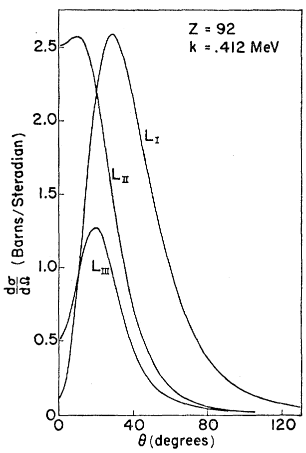

FIG. 3. Angular distributions for the three L subshells for 0.412- MeV photons on uranium.

points up the necessity for a relativistic treatment for large Z. It also illustrates the inaccuracy concomitant with using Stobbe's formulas for determining ratios of cross sections from various shells, as was done by White[22] for example, when they were essentially all that were available. Hultberg[26] gives relative differential cross sections for the K shell for 0.412, 0.662, and 1.332 MeV and for $Z=92$. We can make a comparison with his results by normalizing both his and our angular distributions to maximimum values of unity. Figure 1 has this comparison for $k=0.412$ MeV, for which it should be remembered that we have neglected everything but the pure Coulomb interaction. We can also compare the K-shell angular distributions with the numerical results obtained by Pratt *et al.*[15] In Fig. 2 we have plotted the differential cross sections obtained here and by Pratt for 0.412-MeV photons on uranium. The curves can be seen to be essentially on top of one another. The numerical results for the other energies of Hultberg's experiment, for uranium, are compared with those of Pratt *et al.* in Table III. For all three energies, the two sets of values are in agreement, within the accuracy of the present work and that stated by Pratt *et al.*

Figure 2 also contains a plot of the differential cross section for the entire L shell. The area under this curve is seen to be a non-negligible fraction of that under the K-shell curve. The shapes of the two curves differ a little. This is due to the fact that the differential cross section for the L_{II} subshell is large, relative to those for the other L subshells, in the forward direction. This is shown in Fig. 3, which illustrates the separate contri-

TABLE IX. $d\sigma/d\Omega$ in b/sr for the L subshells, for 0.103-MeV photons on lead.

θ(°)	L_I	L_{II}	L_{III}
0	0.161	11.12	6.998
5	0.632	11.45	7.559
10	2.000	12.34	9.101
15	4.131	13.58	11.25
20	6.822	14.88	13.51
25	9.828	15.94	15.42
30	12.88	16.58	16.65
35	15.75	16.67	17.06
40	18.21	16.22	16.69
45	20.13	15.32	15.69
50	21.42	14.08	14.26
55	22.07	12.64	12.62
60	22.12	11.14	10.94
65	21.63	9.654	9.332
70	20.71	8.226	7.871
75	19.47	7.014	6.592
80	18.01	5.915	5.502
85	16.43	4.973	4.593
90	14.80	4.182	3.847
95	13.18	3.528	3.244
100	11.62	2.995	2.760
105	10.14	2.567	2.376
110	8.764	2.227	2.073
115	7.503	1.960	1.832
120	6.363	1.752	1.640
125	5.344	1.592	1.488
130	4.442	1.470	1.366
135	3.652	1.378	1.271
140	2.967	1.309	1.196
145	2.380	1.258	1.137
150	1.885	1.221	1.091
155	1.477	1.195	1.054
160	1.151	1.177	1.024
165	0.902	1.166	1.000
170	0.727	1.159	0.981
175	0.624	1.156	0.969
180	0.589	1.155	0.965

TABLE X. $d\sigma/d\Omega$ in b/sr for the K and L shells, for 0.279-MeV photons on uranium.

θ(°)	K	L_I	L_{II}	L_{III}
0	0.220	0.023	4.081	1.130
5	2.091	0.273	4.166	1.347
10	7.180	0.961	4.347	1.876
15	14.13	1.920	4.463	2.433
20	21.32	2.934	4.376	2.758
25	27.34	3.799	4.049	2.749
30	31.41	4.380	3.543	2.467
35	33.30	4.633	2.958	2.045
40	33.26	4.590	2.382	1.606
45	31.74	4.325	1.871	1.222
50	29.24	3.923	1.445	0.916
55	26.24	3.456	1.106	0.686
60	23.06	2.979	0.844	0.516
65	19.96	2.526	0.643	0.392
70	17.07	2.117	0.491	0.302
75	14.46	1.760	0.378	0.236
80	12.18	1.455	0.294	0.189
85	10.20	1.199	0.233	0.156
90	8.529	0.986	0.189	0.133
95	7.120	0.810	0.156	0.116
100	5.942	0.667	0.132	0.102
105	4.964	0.552	0.113	0.090
110	4.154	0.459	0.100	0.081
115	3.489	0.384	0.090	0.074
120	2.945	0.324	0.083	0.069
125	2.502	0.275	0.078	0.060
130	2.141	0.237	0.074	0.056
135	1.848	0.207	0.071	0.053
140	1.612	0.183	0.069	0.050
145	1.422	0.165	0.068	0.048
150	1.272	0.151	0.066	0.047
155	1.155	0.139	0.065	0.046
160	1.066	0.131	0.064	0.044
165	1.000	0.125		
170	0.955	0.121		
175	0.928	0.119		
180	0.920	0.118		

butions from the L subshells. The L-subshell angular distributions for 0.662- and 1.332-MeV photons on uranium are given in Tables IV and V.

A number of additional differential cross sections, for the K and L shells, are presented in Tables VI–XIII. These are given for lead and uranium targets, and for a number of photon energies. The values of 0.081, 0.103, and 0.279 MeV correspond to Sujkowski's[27] experimental energies for $Z=92$. He has measured the ratio $(\sigma_{L_{\rm I}}+\sigma_{L_{\rm II}})/\sigma_{L_{\rm III}}$ for 0.103 MeV. If we compare his value with ours we have

$$(\sigma_{L_{\rm I}}+\sigma_{L_{\rm II}})/\sigma_{L_{\rm III}}=2.74 \quad \text{present work}$$
$$=3.03\pm0.15 \quad \text{Sujkowski}$$

in fair agreement. This would seem to indicate that the effects of screening are not the same for all three subshells, at this energy. We can also compare the ratio $\sigma_{L_{\rm II}}/\sigma_{L_{\rm III}}$ for 0.081 MeV and $Z=92$. We have

$$\sigma_{L_{\rm II}}/\sigma_{L_{\rm III}}=1.08 \quad \text{present work}$$
$$=0.92\pm0.15 \quad \text{Sujkowski.}$$

This result is almost within the experimental error. In general, poorer agreement should be expected as the energy decreases, since the effects of screening on the final electron become more important.[1]

TABLE XI. $d\sigma/d\Omega$ in b/sr for the K and L shells, for 0.354-MeV photons on uranium.

θ(°)	K	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.546	0.068	3.081	0.702
5	2.403	0.299	3.122	0.876
10	7.243	0.916	3.181	1.270
15	13.29	1.715	3.124	1.615
20	18.70	2.463	2.877	1.722
25	22.27	2.983	2.474	1.581
30	23.69	3.205	2.005	1.301
35	23.26	3.159	1.555	0.996
40	21.55	2.924	1.171	0.733
45	19.16	2.585	0.866	0.530
50	16.53	2.212	0.635	0.382
55	13.95	1.849	0.464	0.277
60	11.60	1.521	0.340	0.203
65	9.544	1.238	0.250	0.152
70	7.796	1.002	0.187	0.117
75	6.343	0.806	0.142	0.094
80	5.152	0.648	0.110	0.077
85	4.184	0.522	0.087	0.064
90	3.403	0.421	0.070	0.055
95	2.775	0.341	0.058	0.048
100	2.274	0.278	0.050	0.042
105	1.879	0.228	0.044	0.038
110	1.560	0.189	0.039	0.034
115	1.310	0.159	0.035	0.031
120	1.111	0.135	0.033	0.028
125	0.954	0.117	0.031	0.026
130	0.832	0.102	0.029	0.025
135	0.736	0.091	0.028	
140	0.661	0.082	0.027	
145	0.603	0.076	0.027	
150	0.558	0.071	0.027	
155	0.525	0.068	0.026	
160	0.500	0.065	0.026	
165	0.482	0.063		
170	0.470	0.062		
175	0.462	0.061		
180	0.460	0.061		

TABLE XII. $d\sigma/d\Omega$ in b/sr for the K and L shells, for 0.279-MeV photons on lead.

θ(°)	K	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.158	0.018	2.130	0.742
5	1.918	0.249	2.172	0.860
10	6.604	0.867	2.255	1.141
15	12.73	1.683	2.288	1.424
20	18.61	2.475	2.199	1.566
25	23.00	3.067	1.979	1.521
30	25.34	3.377	1.675	1.330
35	25.73	3.413	1.350	1.076
40	24.60	3.237	1.050	0.826
45	22.49	2.928	0.797	0.617
50	19.88	2.557	0.598	0.457
55	17.15	2.176	0.445	0.340
60	14.52	1.818	0.331	0.255
65	12.13	1.498	0.246	0.194
70	10.04	1.223	0.185	1.149
75	8.246	0.992	0.141	0.117
80	6.742	0.802	0.110	0.095
85	5.498	0.646	0.088	0.079
90	4.478	0.521	0.072	0.068
95	3.649	0.420	0.060	0.060
100	2.975	0.340	0.052	0.053
105	2.430	0.276	0.046	0.047
110	1.989	0.225	0.041	0.042
115	1.635	0.185	0.038	0.039
120	1.352	0.153	0.036	0.036
125	1.126	0.128	0.034	0.034
130	0.945	0.108	0.033	
135	0.800	0.092	0.032	
140	0.684	0.080	0.031	
145	0.592	0.070	0.031	
150	0.521	0.063		
155	0.466	0.057		
160	0.425	0.053		
165	0.394	0.050		
170	0.373	0.048		
175	0.360	0.047		
180	0.356	0.046		

2. Checks and Accuracy

Two types of checks were made on the calculation. The first of these was to take a low Z value ($Z=5$), and to compare the resulting angular distributions and total cross sections with those obtained from the approximate calculations of Gavrila.[8,17] Qualitative agreement was obtained for all four shells, but the quantitative disparity was as large as 10% in some places.

A more stringent check was needed, and this was obtained by replacing the final-state wave function with the first term of the Sommerfeld-Maue wave function.[43] We shall briefly indicate the procedure. For the conjugate of this replacement we have

$$\psi_f^\dagger=N_f e^{-i\mathbf{p}\cdot\mathbf{r}}F(i\nu,1,ipr+i\mathbf{p}\cdot\mathbf{r})u^\dagger(\mathbf{p}),$$

where $N_f=\Gamma(1-i\nu)e^{\nu\pi/2}$. For the numerical program, this can be incorporated by changing the radial matrix elements. The position-dependent part of $\psi_f^\dagger$ can be

[43] A. Sommerfeld and A. W. Maue, Ann. Physik 22, 629 (1935).

TABLE XIII. $d\sigma/d\Omega$ in b/sr for the K and L shells, for 0.354-MeV photons on lead.

θ(°)	K	$L_{\rm I}$	$L_{\rm II}$	$L_{\rm III}$
0	0.332	0.042	1.566	0.453
5	1.968	0.250	1.585	0.546
10	6.127	0.783	1.604	0.752
15	11.07	1.428	1.551	0.922
20	15.09	1.968	1.393	0.954
25	17.30	2.273	1.159	0.852
30	17.66	2.328	0.905	0.684
35	16.63	2.191	0.676	0.512
40	14.80	1.943	0.491	0.370
45	12.65	1.652	0.351	0.265
50	10.52	1.364	0.249	0.189
55	8.578	1.105	0.177	0.137
60	6.909	0.883	0.126	0.100
65	5.519	0.700	0.091	0.075
70	4.387	0.553	0.068	0.058
75	3.481	0.435	0.051	0.047
80	2.762	0.343	0.040	0.039
85	2.195	0.271	0.032	0.033
90	1.748	0.215	0.026	0.028
95	1.398	0.171	0.022	0.024
100	1.123	0.137	0.020	0.022
105	0.910	0.111	0.018	0.020
110	0.742	0.090	0.016	0.018
115	0.611	0.074	0.015	0.016
120	0.508	0.062	0.014	0.014
125	0.428	0.052	0.013	0.013
130	0.366	0.045	0.013	
135	0.318	0.040	0.012	
140	0.280	0.035		
145	0.250	0.032		
150	0.228	0.029		
155	0.211	0.027		
160	0.198	0.026		
165	0.189	0.025		
170	0.183	0.024		
175	0.179			
180	0.178			

expanded in a series of Legendre polynomials as

$$e^{-i\mathbf{p}\cdot\mathbf{r}}F(i\nu,\,1,\,ipr+i\mathbf{p}\cdot\mathbf{r})=\sum_l a_l(pr)P_l(\hat{p}\cdot\hat{r})\,,$$

and the coefficients $a_l(pr)$ can be determined in the usual way. Following Gordon[44] we obtain

$$\psi_f{}^\dagger=\sum_l(2l+1)i^l\mathfrak{L}_l(pr)P_l(\hat{p}\cdot\hat{r})u^\dagger(\mathbf{p})\,,$$

where

$$\mathfrak{L}_l(pr)=e^{\nu\pi/2+il\pi}\frac{\Gamma(l+1-i\nu)}{\Gamma(2l+2)}(2pr)^l \times F(l+1-i\nu,\,2l+2,\,-2ipr)\,.$$

[44] W. Gordon, Z. Physik **48**, 187 (1928).

Expressing $P_l(\hat{p}\cdot\hat{r})$ in terms of spherical harmonics this becomes

$$\psi_f{}^\dagger=4\pi\sum_{l,m}i^l\mathfrak{L}_l(pr)Y_{l,m}(\hat{p})Y_{l,m}{}^*(\hat{r})u^\dagger(\mathbf{p})$$

$$=4\pi\sum_{\varkappa_1 m_1}C_{\varkappa_1 m_1}{}^\dagger(-ig_{\varkappa_1}{}^*\Omega_{\varkappa_1 m_1}{}^\dagger(\hat{r}),\,f_{\varkappa_1}{}^*\Omega_{-\varkappa_1 m_1}(\hat{r}))\,.$$

Using the orthogonality of the $\Omega_{\varkappa m}$'s and the relation[45]

$$\boldsymbol{\sigma}\cdot\hat{p}\Omega_{\varkappa m}(\hat{p})=-\Omega_{-\varkappa m}(\hat{p})$$

we get

$$C_{\varkappa_1 m_1}=(\Omega_{\varkappa_1 m_1}(\hat{p}),v)$$

$$g_{\varkappa_1}{}^*=i^{l_1+1}\left(\frac{W+m}{2W}\right)^{1/2}\mathfrak{L}_{l_1}(pr)$$

$$f_{\varkappa_1}{}^*=-i^{l_1'}\left(\frac{W-m}{2W}\right)^{1/2}\mathfrak{L}_{l_1'}(pr)\,.$$

By inserting $g_{\varkappa_1}{}^*$ and $f_{\varkappa_1}{}^*$ into the radial matrix elements the replacement is accomplished. In addition, to simplify the corresponding analytical calculation, we set $r^{\gamma_1-1}=1$ for the K, $L_{\rm I}$, and $L_{\rm II}$ bound-state functions and $r^{\gamma_2-1}=r$ for the $L_{\rm III}$ bound state. The radial matrix elements can be evaluated in a manner similar to the previous ones, and the analytical cross sections could be evaluated in a straightforward way. Both were evaluated for $Z=5$ and $k=0.200$ MeV. Twelve partial waves were required in the numerical part. The agreement obtained was better than 1% for the K, $L_{\rm I}$, and $L_{\rm II}$ shells, and about 1% for the $L_{\rm III}$ subshell.

ACKNOWLEDGMENT

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[45] M. E. Rose, *Relativistic Electron Theory* (John Wiley & Sons, Inc., New York, 1961), p. 28.