Photoeffect from the L Shell*

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The differential cross section for photoeffect from an atomic shell is shown to be almost independent of principal quantum number, apart from normalization, for energies well above threshold. The high-energy limits of the total cross sections for the three L subshells are calculated exactly with methods previously applied to the K shell, and extrapolations are made to cover the entire high-energy region. A procedure is indicated to account for the effects of electron screening. It is found that the contribution from the p subshells is not negligible in heavy elements. Agreement with experiment is good.

I. INTRODUCTION

In a recent paper[1] methods were developed to obtain the high-energy limit of the total cross section for photoelectric emission from an atomic shell, neglecting screening effects of the electron cloud on the nuclear charge Z. For the K shell the result, which is expressed as a double integral, was obtained both numerically and as a power series in the parameter $a\equiv Ze^2$.[2] This information was combined with the results of Gavrila[3] on the energy dependence of the cross section to provide an extrapolation formula representing the K shell total cross section in the entire high-energy region (photon energies above 1 Mev).

The main objective of the present paper is to obtain analogous results for photoeffect from the L shells, for which information on the total cross sections at high energies is now becoming available. It is soon discovered, however, that there are simple relations among the differential cross sections for photoeffect from any shell, at all energies well above threshold. Thus the differential cross section $d\sigma$ for a shell of orbital angular momentum l is $O(a^{5+2l})$.[4] Further, $d\sigma$ for photoeffect from the (n,j,l,m) shell does not depend on the principal quantum number n when terms of relative order a^2 are neglected, except for a normalizing factor.[5] The n dependence of the normalizing factor is easily found, and consequently when the cross sections for the $2s$ and $2p$ states are known, a prediction can be made for the $3s$ and $3p$ states, etc. Another application of these results is to the high-frequency limit of bremsstrahlung, which McVoy and Fano[6] have shown to be closely connected to the photoeffect. This application will form the subject of a subsequent paper.

Section II will be devoted to establishing these relations. In Sec. III the high-energy limits of the total cross sections for photoeffect from the three L subshells are calculated, first in power series in a through relative order a, and then numerically. In Sec. IV the results are summarized, previous theoretical work is noted, and energy extrapolations are discussed. Procedures are indicated to take account of electron screening effects, which are important for these higher shells. Comparisons are made with experiment, and the agreement is found quite satisfactory.

In the following the notation of I is generally used.[7] The main parameters introduced are $a\equiv Ze^2$ (≈ 0.6 for Pb), the *total* energy ϵ of the bound electron, and δ, occurring in the exponential of bound state radial functions: $e^{-\delta r}$. It is convenient to note that $\delta^2+\epsilon^2=1$. The parameter $\lambda=\cos^{-1}\delta$ also appears.

II. GENERAL RELATIONS

Let us consider the differential cross section $d\sigma$ for photoeffect from an atomic shell specified by the quantum numbers (n,j,l,m). We shall show that, for all photon energies of order 1 or greater in comparison to a^2, $d\sigma$ does not depend on n (except for a normalizing factor) when contributions of relative order a^2 are neglected. The proof proceeds in three stages. (1) We establish what order in a is contributed to the matrix element by each term of the bound-state wave function. This gives the order in a of the cross section and specifies which terms of the wave function contribute to that order. (2) We show that these terms do not depend on n except for normalization. (3) We extend the arguments to include the terms of relative order a. For greater clarity, each part of the work will be prefaced with the corresponding nonrelativistic statements.

The photoeffect matrix element is

$$M=-e(2\pi)^{\frac{1}{2}}k^{-\frac{1}{2}}\int d^3x\,\psi_p{}^*\boldsymbol{\alpha}\cdot\mathbf{e}e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{bd}, \qquad (1)$$

with the notation of I; in the nonrelativistic (NR) case $\boldsymbol{\alpha}$ is replaced by $\mathbf{p}$. For energies well above threshold

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[1] R. H. Pratt, Phys. Rev. **117**, 1017 (1960); hereafter referred to as I.

[2] We use unrationalized units and set $\hbar=c=m_e=1$.

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

[4] $O(x)$ shall mean "of order x," $y=O(x)$ shall mean "y is of order x."

[5] This is not trivial since (contrary to a statement often made) the photoeffect even at high energies does *not* depend only on the value of the bound-state electron wave function at the origin.

[6] K. W. McVoy and U. Fano, Phys. Rev. **116**, 1168 (1959).

[7] See also H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Academic Press, Inc., New York, 1957).

ψ_p to lowest order in a is independent of a and is simply the free electron wave function $e^{i\mathbf{p}\cdot\mathbf{r}}u_p$. ψ_{bd} always contains the normalization factor $a^{\frac{3}{2}}$. Otherwise, the NR radial function is the product of $e^{-\delta r}$ and a finite polynomial in δr,[8] which begins with $(\delta r)^l$:

$$\psi_{bd}\sim a^{\frac{3}{2}}a^l Y_{lm} r^l e^{-\delta r}\sum c_s a^s r^s. \qquad (2)$$

We wish to establish whether each term in this series contributes the order $a^{\frac{3}{2}+l+s}$ to M. For this purpose it is sufficient to take ψ_p only to lowest order in a, and so to consider the integrals

$$\int d^3x\, e^{i\Delta\cdot\mathbf{r}}e^{-\delta r}Y_{lm}r^{l+s} = (-1)^s\frac{d^s}{d\delta^s}\int d^3x\, e^{i\Delta\cdot\mathbf{r}}e^{-\delta r}Y_{lm}r^l. \qquad (3)$$

Choosing an axis along $\mathbf{\Delta}=\mathbf{k}-\mathbf{p}$, only $m=0$ gives a contribution. It is not difficult to show that for small $b\equiv\delta/\Delta$ the last integral is given by an odd series in b, beginning with order b. For energies well above threshold $b=O(a)$ and can be represented by an odd series in a: the minimum momentum transfer $\Delta_{\min}$ is $O(1)$ and $\delta=O(a)$. Thus, from the derivatives, the integrals (3) will be $O(a)$ or $O(1)$ according as s is even or odd. The $s=0$ term in (2) will only contribute to M in order $a^{\frac{3}{2}+l+1}$, and the $s=1$ term will contribute in the same order. The cross section for the photoeffect is hence of order a^{5+2l}, giving a^5 for s states, a^7 for p states, etc. The first two terms of the bound-state radial function both contribute in this order. Evidently in actual calculation it is also not sufficient just to take the leading order in ψ_p (the plane wave), for the next term in a can contribute to M in the same order.

In the relativistic radial functions[7] the finite polynomial of (2) is replaced by the finite sum $(\delta r)^{\gamma-1}\sum c_s(\delta r)^s$. The coefficients c_s are not all of order one. The "small component" f contains the factor $(1-\epsilon)^{\frac{1}{2}}$, which is of order a. Further, whenever $\kappa>0$ the first term c_0 in the series for the "large component" g is of order a^2 rather than one. Neglecting terms of relative order a^2 we may replace γ by k. For $\kappa<0$ ($k=l+1$, $j=l+\frac{1}{2}$), the first few terms of the large and small components may be summarized:

$$\begin{aligned}&\text{large: } a^{\frac{3}{2}}a^l e^{-\delta r}Y_l r^l(1+c_1ar+c_2a^2r^2+\cdots),\\ &\text{small: } a^{\frac{3}{2}}a^{l+1}e^{-\delta r}Y_{l+1}r^l(1+c_1ar+c_2a^2r^2+\cdots).\end{aligned} \qquad (4)$$

Our previous discussion then shows that the first two terms of the large component and the first term of the small component may all be expected to contribute to the matrix element in order $a^{\frac{3}{2}+l+1}$. For $\kappa>0$ ($k=l$, $j=l-\frac{1}{2}$) we have:

$$\begin{aligned}&\text{large: } a^{\frac{3}{2}}a^{l-1}e^{-\delta r}Y_l r^{l-1}(a^2+c_1ar+c_2a^2r^2+\cdots),\\ &\text{small: } a^{\frac{3}{2}}a^l e^{-\delta r}Y_{l-1}r^{l-1}(1+c_1ar+c_2a^2r^2+\cdots).\end{aligned} \qquad (5)$$

Now the first three terms of the large component and the first two terms of the small component may be expected to contribute to M in order $a^{\frac{3}{2}+l+1}$. Thus in all cases the cross section is of order a^{5+2l}; both the large and small components contribute to the result.

The next task is to establish that the terms of ψ_{bd} which contribute to M in lowest order do not depend on the principal quantum number n, apart from a numerical factor common to all such terms. To this order the exponential $e^{-\delta r}$ of the radial functions may be replaced by $1-\delta r$.[9] For the NR case the result is then evident. Thus the $1s$ radial function $e^{-ar}\approx 1-ar$, the $2s$ function $2^{-\frac{3}{2}}e^{-\frac{1}{2}ar}(1-\frac{1}{2}ar)\approx 2^{-\frac{3}{2}}(1-ar)$, etc. On expansion, the radial function for general (n,l) to this order is[7]

$$C(n,l)(2ar)^l[1-ar/(l+1)], \qquad (6)$$

where

$$C(n,l)=\frac{1}{(2l+1)!}\left[\frac{(n+l)!}{2n(n-l-1)!}\right]^{\frac{1}{2}}(2a)^{\frac{3}{2}}n^{-(\frac{3}{2}+l)}; \qquad (7)$$

the n dependence appears only as a constant of proportionality. This result may be understood directly from the radial Schrödinger equation

$$R''+\frac{2}{r}R'+2\left(E+\frac{a}{r}\right)R-\frac{l(l+1)}{r^2}R=0, \qquad (8)$$

where, $E=\epsilon-1=O(a^2)$ is the only quantity which depends on the principal quantum number n. Expanding R in powers of a as

$$R=R_0+aR_1+a^2R_2+\cdots, \qquad (9)$$

then R_0 and R_1 will be determined from the equations

$$\begin{aligned}&R_0''+\frac{2}{r}R_0'-\frac{l(l+1)}{r^2}R_0=0,\\ &R_1''+\frac{2}{r}R_1'+\frac{2}{r}R_0-\frac{l(l+1)}{r^2}R_1=0\end{aligned} \qquad (10)$$

which are independent of E, and they can depend on E only through a common normalizing factor. The argument is equally applicable to a low-energy continuum solution.

The same conclusion is obtained for the Dirac wave functions. Direct expansion of the radial parts gives for $j=l+\frac{1}{2}$

$$\begin{pmatrix}g\\ f\end{pmatrix}=C(n,l)(2ar)^l\begin{pmatrix}1-ar/(l+1)\\ -a/2(l+1)\end{pmatrix}, \qquad (11)$$

[8] For small a, $\delta=O(a)$.

[9] The integrals can still be given a well-defined meaning. See also reference 6.

and for $j=l-\frac{1}{2}$

$$\begin{pmatrix} g \\ f \end{pmatrix} = C(n,l)(2ar)^{l-1} \times \begin{pmatrix} a^2(2l+1)/2l+2ar-2(ar)^2/(l+1) \\ a(2l+1)-2a^2r \end{pmatrix}, \quad (12)$$

where, neglecting $O(a)^2$, $C(n,l)$ is again given by (7). This property of the wave function may be demonstrated directly from the coupled differential equations for f and g; it holds also for the low-energy continuum functions. To lowest order, then, the photoeffect matrix elements need only be computed as a function of (j,l,m). The same is true for the differential cross section, for n appears in the requirement of energy conservation only in $O(a^2)$, so that to lowest order the entire n dependence of the cross section is given by $|C(n,l)|^2$.

It is now easy to extend the results to include terms of relative order a. Any such terms which arise from the portions of ψ_{bd} already discussed will have the n dependence $C(n,l)$, so that only the higher order terms of ψ_{bd} need be examined. However, from our previous results, the next terms in the expansion of (6), (11), and (12) in ar, which do have a different n dependence, will only contribute to M in relative order a^2. For the NR case this completes the proof. For the relativistic radial functions it must be remembered that we also approximated r^γ by r^k. Thus, to the order with which we are concerned, it is necessary to multiply by $1-(a^2/2k)\ln r$. This is independent of n and so does not affect the argument. The final conclusion is that, for photon energies of order one or greater, the complete n dependence of the differential cross section for the photoeffect is given by $|C(n,l)|^2$, neglecting only terms of relative order a^2.

III. CALCULATIONS

The high-energy limit of photoeffect total cross sections can be obtained with the methods developed in I for the K-shell cross section. In this limit the wave function ψ_p of the outgoing electron may be taken as the modified plane wave

$$\psi_p = ue^{i\mathbf{p}\cdot\mathbf{r}+i\chi_-}, \quad \chi_- = a\ln(pr+\mathbf{p}\cdot\mathbf{r}), \quad (13)$$

where u is a free electron spinor. Interchanging orders of integration, the total cross section is easily written as a triple integral, which is a function of the parameters a, δ, and ϵ. Changes of variables are then made which facilitate evaluation of the integral either (1) by expansion in powers of a or (2) by numerical methods on an electronic computer. For further details see I.

In this section we will obtain the high-energy limits of the L-shell total cross sections as a function of a. The three cross sections represent a sum over the eight electrons of the L shell: $2s_{\frac{1}{2}}$(2 electrons), $2p_{\frac{1}{2}}$(2 electrons), and $2p_{\frac{3}{2}}$(4 electrons). Initial photon polarization is averaged and final electron spin is summed. The first two terms of a power series in a will be established, and for large a the cross section will be computed numerically. Results, which will be discussed in the following section, will generally be expressed in units of σ_0, where,

$$\sigma_0 = 4\pi e^2 a^5/k \quad (14)$$

is the high-energy small-a limit of the K-shell total cross section. Let us introduce the notation

$$\sigma(2s_{\frac{1}{2}})\equiv\sigma(+), \quad \sigma(2p_{\frac{1}{2}})\equiv\sigma(-), \quad \sigma(2p_{\frac{3}{2}})\equiv\sigma(0), \quad (15)$$

and let $\sigma(n)$, where n ranges through $(0,\pm)$, be factored as

$$\sigma(n)=\sigma_0 H(n)I(n). \quad (16)$$

Defining

$$\begin{aligned} H(\pm) &= (2\delta)^{2(\gamma-1)}\epsilon^{-3}(2\gamma+1)^2[\pm 32\epsilon(\pm 2\epsilon+1)]^{-1}, \\ H(0) &= (2\delta)^{2(\gamma-1)}4(1-\epsilon)(2\gamma+1), \end{aligned} \quad (17)$$

then, from Eq. (20) of I, $I(n)$ is given by the triple integrals

$$I(n)=a^{-2}[\Gamma(2\gamma+2)]^{-1}\int_0^\infty \rho d\rho \int_{-\infty}^\infty \int_{-\infty}^\infty dzdz' \left(\frac{z+r}{z'+r'}\right)^{ia} \times \exp[i(z-z')\epsilon - \delta(r+r')](rr')^{\gamma-1}\sum_{i=1}^3 A_i(n). \quad (18)$$

Here

$$\begin{aligned} A_1(\pm) &= 4(1\pm\epsilon)[\epsilon^2+(1-\epsilon^2)B+i\delta\epsilon C], \\ A_2(\pm) &= 4\delta^2 rr' D^2[(1\pm\epsilon)+(1\mp\epsilon)B\pm i\delta C], \\ A_3(\pm) &= -2\delta(r+r')D[\pm 2\epsilon(1\pm\epsilon)+2(1-\epsilon^2)B \\ &\quad +2i\epsilon\delta C]\mp[4i\delta^2 D(r'\cos\theta - r\cos\theta')], \end{aligned} \quad (19)$$

and

$$\begin{aligned} A_1(0) &= E^2 B, \quad A_2(0)=\tfrac{3}{2}B^2-\tfrac{1}{2}, \\ A_3(0) &= iEC(\tfrac{3}{2}B+\tfrac{1}{2}), \end{aligned} \quad (20)$$

where

$$\begin{aligned} B &= \cos\theta\cos\theta'+\sin\theta\sin\theta', \quad C=\cos\theta-\cos\theta', \\ D &= (\pm 2\epsilon+1)/(2\gamma+1), \quad E=[(1+\epsilon)/(1-\epsilon)]^{\frac{1}{2}}, \end{aligned} \quad (21)$$

and the variables r and θ are related to ρ and z by

$$r=(\rho^2+z^2)^{\frac{1}{2}}, \quad r'=(\rho^2+z'^2)^{\frac{1}{2}}, \quad \cos\theta = z/r, \quad \sin\theta=\rho/r, \text{ etc.} \quad (22)$$

The simple connection of the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ cross sections arises from a similar relation between the large components of one bound-state wave function and the small components of the other, for pairs of states such that $\kappa=\pm k$.

To make a series expansion in a it is convenient to introduce the variables x and y by

$$z=\rho\sinh(x+i\lambda), \quad z'=\rho\sinh(y-i\lambda), \quad \cos\lambda=\delta, \quad (23)$$

and return the contours to the real axis. Performing the ρ integration and then explicitly writing the result as a real double integral,

$$I(n)=a^{-2}e^{-2a\lambda}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\partial x\partial y \times\frac{[(\cosh^2x-\sin^2\lambda)(\cosh^2y-\sin^2\lambda)]^{\frac{1}{2}(\gamma-k)}}{(\cosh x+\cosh y)^{2\gamma+2}} \times\sum_{i=1}^{3}K_i(n), \quad (24)$$

where $k=j+\frac{1}{2}$, j is the total angular momentum of the bound state, and the functions $K_i(n)$ are given in the Appendix. To this point the treatment is exact. If now the integrand is expanded in powers of a, keeping the first two nonvanishing powers, then

$$I(n)\approx e^{-2a\lambda}\sum_{i=1}^{3}I_i(n) =e^{-2a\lambda}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dxdy(\cosh x+\cosh y)^{-2(1+k)} \times\sum_{i=1}^{3}J_i(n). \quad (25)$$

With the abbreviations

$$R=(\cosh x+\cosh y),\quad S=\cosh x\cosh y,\quad T=\sinh x\sinh y,\quad P_x=\sinh x\cosh y,\quad P_y=\sinh y\cosh x, \quad (26)$$

the J's are given to lowest order as

$$\begin{aligned}
&J_1(+)=2(1+4xyT),\quad J_2(+)=40R^{-2}T^2,\\
&J_3(+)=-16R^{-1}T(x\sinh y+y\sinh x),\\
&J_1(-)=\tfrac{1}{8}a^2(1+4xyT),\\
&J_2(-)=(5/18)a^2R^{-2}[1+10S+9S^2\\
&\qquad -3R^2+16xyT(1+S)-4T(xP_y+yP_x)\\
&\qquad -8(1+S)(xP_x+yP_y)],\\
&J_3(-)=\tfrac{1}{12}a^2R^{-1}[4R-16xyRT+8R(xP_x+yP_y)\\
&\qquad -8(1+S)(x\sinh x+y\sinh y)\\
&\qquad +4T(x\sinh y+y\sinh x)],\\
&J_1(0)=7+16S+9S^2-(15/2)R^2,\\
&J_2(0)=16xyT(1+S),\\
&J_3(0)=-(2+12S)(xP_x+yP_y)\\
&\qquad +10(x\sinh x\cosh x+y\sinh y\cosh y).
\end{aligned} \quad (27)$$

The terms of relative order a are obtained with the substitutions for x and y (where they appear linearly, not in the hyperbolic functions)

$$x\to x-2^{-(1+k)}\pi a\epsilon_x,\quad y\to y-2^{-(1+k)}\pi a\epsilon_y \quad (28)$$

where ϵ_x is the usual step function: ±1 according as $x>0$ or $x<0$. Evaluation of the integrals is routine, and one finds

$$\begin{aligned}
&I_1(+)=(28/9)-(8/9)\pi a,\quad I_2(+)=8/9,\\
&I_3(+)=-(8/3)+(8/15)\pi a,\\
&I_1(-)=a^2[(7/36)-(1/18)\pi a],\\
&I_2(-)=a^2[(5/54)-(1/45)\pi a],\\
&I_3(-)=a^2[-(11/54)+(31/270)\pi a],\\
&I_1(0)=16/45,\quad I_2(0)+I_3(0)\\
&\qquad =(8/45)-(22/175)\pi a.
\end{aligned} \quad (29)$$

It was found in I that if the exponential $e^{-2a\lambda}$ of $I(n)$ and the factor $\delta^{2(\gamma-1)}$ of H were not expanded, then the remaining terms of relative order a^2 were very small, and indeed the expression so obtained was in good agreement with the numerical results for all a. The same appears to be true for the L-shell cross sections. When terms of $O(a^2)$ are treated in this fashion the results for the cross sections may be written

$$\begin{aligned}
&\sigma(2s_{\frac{1}{2}})=(1/8)\delta^{2(\gamma-1)}e^{-2a\lambda}[1-(4/15)\pi a]\sigma_0,\\
&\sigma(2p_{\frac{1}{2}})=(3/32)\delta^{2\gamma}e^{-2a\lambda}[1+(4/9)\pi a]\sigma_0,\\
&\sigma(2p_{\frac{3}{2}})=(1/3)\sigma^{2(\gamma-1)}e^{-2a\lambda}[1-(33/140)\pi a]\sigma_0.
\end{aligned} \quad (30)$$

Further discussion will be deferred to the next section.

For a numerical evaluation of $I(n)$ in Eq. (18) it is useful to introduce the variables x and y by

$$x=\frac{z'-z}{r'+r},\quad y=\frac{z'+z}{r'+r}. \quad (31)$$

Then, after performing the ρ integration,

$$I(n)=a^{-2}2^{-(2\gamma+2)}\int_{-1}^{+1}\int_{-1}^{+1}dxdy\left(\frac{1-x}{1+x}\right)^{ia} \times(\delta+i\epsilon x)^{-(2\gamma+2)}(1-x^2y^2)^{\gamma}\sum_{i=1}^{3}A_i'(n). \quad (32)$$

Here

$$\begin{aligned}
&A_1'(\pm)=4(1\pm\epsilon)[\epsilon^2+(1-\epsilon^2)B'+i\delta\epsilon C'],\\
&A_2'(\pm)=\delta^2(2\gamma+3)(2\gamma+2)D'^2(1-x^2y^2)\\
&\qquad\times[(1\pm\epsilon)+(1\mp\epsilon)B'\pm i\delta C'],\\
&A_3'(\pm)=-2\delta(2\gamma+2)D'[\pm2\epsilon(1\pm\epsilon)+2(1-\epsilon^2)B'\\
&\qquad +2i\epsilon\delta C']\mp[4i\delta^2(2\gamma+2)D'(x+C')],
\end{aligned} \quad (33)$$

and

$$A_1'(0)=E^2B',\quad A_2'(0)=\tfrac{3}{2}B'^2-\tfrac{1}{2},\quad A_3'(0)=iEC'(\tfrac{3}{2}B'+\tfrac{1}{2}), \quad (34)$$

where now

$$\begin{aligned}
&B'=\frac{2(1-x^2)}{1-x^2y^2}-1,\quad C'=-\frac{2x(1-y^2)}{1-x^2y^2},\\
&D'=(\delta+i\epsilon x)^{-1}(\pm2\epsilon+1)/(2\gamma+1),\\
&E=[(1+\epsilon)/(1-\epsilon)]^{\frac{1}{2}}.
\end{aligned} \quad (35)$$

TABLE I. Tests of the machine program for values of a which can be computed analytically. Values of σ/σ_0 obtained by the two methods are compared.

Shell	Machine	Analytic result
$2s_{\frac{1}{2}}$	0.0194 at $a=0.99$	0.0193 at $a\equiv 1$
$2p_{\frac{1}{2}}$	0.0820 at $a=0.99$	0.1096 at $a\equiv 1$
	0.1073 at $a=0.9999$	
$2p_{\frac{3}{2}}$	0.0043 at $a=1.732$	0.0043 at $a\equiv\sqrt{3}$

The y integrals are quite simple and may be expressed in terms of one incomplete beta function, to be obtained from a rapidly converging power series. After the remaining x integration is written in real form, the problem is suitable for machine calculation on an electronic computer. One complication remains: owing to the factor $[(1-x)/(1+x)]^{ia}$ the integrand goes through an infinite number of oscillations near $x=\pm 1$. For this reason the numerical integration is performed for the region $0\leq |x|\leq 1-\Delta$, where Δ is a small number, and the integral over the remaining region is obtained analytically as a power series in Δ. For further details of these procedures see I.

Two tests were made of the correctness of the machine programs. (1) For $a=\frac{1}{2}\sqrt{3}(n=\pm)$ or $a=\frac{1}{2}\sqrt{7}(n=0)$ the integrand is easily computed and was found in agreement with the machine values up to the accuracy of the hand calculation (five places). Evaluations of the various functions, including the incomplete beta functions, were also available from the machine data and could be compared with their exact values. (2) For $a=1(n=\pm)$ or $a=\sqrt{3}(n=0)$ the integral itself can be evaluated analytically and compared with the machine result. In practice, the programs used were not well-defined for these values of the parameters (see footnote 30 of I), but values sufficiently close to them may be used. The results of these tests are shown in Table I. The agreement is quite satisfactory.[10]

In the numerical computation of the K-shell cross section the attempt was made to keep errors within 0.1%. It was found that the main limitation on accuracy came simply from the finite size of the mesh used to represent the integrand, for which an upper limit of 300 points was set by practical considerations. As a is taken smaller, the absolute magnitude of the integrand increases, but owing to increasingly severe cancellation the value of the integral becomes much smaller; hence a larger mesh is required to represent the integrand with sufficient accuracy. For the K shell the smallest a which could be obtained with the desired accuracy was $a=0.15$.

It was desired to obtain the L-shell cross sections with an error limited to less than 1%. Since this allows more leeway, only the leading term in the analytic Δ series was used, and as compensation the values of Δ were taken smaller. Difficulties, however, again arise in representing the integrand. The L-shell integrands are more oscillatory than those for the K shell, and the values of the integrals are smaller. Indeed, for a given value of a, larger meshes had to be used to obtain L-shell cross sections within 1% than had been used to obtain the K-shell cross section within 0.1%. For the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ cross sections the smallest values which could be computed were, respectively, $a=0.3$ and $a=0.4$, and for the $2p_{\frac{3}{2}}$ case the smallest was $a=0.5$. Hence, even more so than for the K shell, the numerical results must be supplemented by the power series expansions of Eq. (30). Of course it is the large a values which are of greatest interest at high energies.

TABLE II. High-energy limit of L-shell total cross sections (unscreened). For each subshell σ/σ_0 is given as a function of a, (1) as determined from Eq. (30), and (2) as found with the electronic computer. The K-shell results of I are also given. Values from the computer are accurate to 1%.

a	$1s$	$2s_{\frac{1}{2}}$ (1)	$2s_{\frac{1}{2}}$ (2)	$2p_{\frac{1}{2}}$ (1)	$2p_{\frac{1}{2}}$ (2)	$2p_{\frac{3}{2}}$ (1)	$2p_{\frac{3}{2}}$ (2)
0.10	0.6987	0.0873	...	0.00020	...	0.00058	...
0.20	0.5138	0.0641	...	0.00075	...	0.00165	...
0.30	0.3942	0.0486	0.0491	0.00159	...	0.00271	...
0.40	0.3145	0.0379	0.0392	0.00278	0.00310	0.00357	...
0.50	0.2599	0.0301	0.0329	0.00441	0.00520	0.00419	0.00388
0.60	0.2224	0.0252	0.0286	0.00678	0.0084	0.00455	0.00418
0.70	0.1963	0.0201	0.0256	0.0103	0.0134	0.00470	0.00434
0.87	0.1698	0.0149	0.0221	0.0225	0.0309	0.00446	0.00440

IV. RESULTS

The results obtained for L-shell cross sections may now be summarized. From Sec. II, the differential cross section for the $2s_{\frac{1}{2}}$ shell is closely related to the K-shell cross section. Neglecting terms of $O(a^2)$,

$$d\sigma(2s_{\frac{1}{2}})=\tfrac{1}{8}d\sigma(1s), \tag{36}$$

so that the angular distributions and polarization correlations are identical. The total cross section is $\frac{1}{8}$ of that for the K shell and can be obtained from the expression of reference 1 in the entire high-energy region. The only general statement obtained for the $2p_{\frac{1}{2}}$ and $2p_{\frac{3}{2}}$ differential cross sections is that for small a they are of order a^7, i.e., $O(a^2)$ relative to the $2s_{\frac{1}{2}}$ and K shell cross sections.

Section III has provided detailed information on the high-energy limit of total cross sections for the L shell. The numerical results obtained and the predictions of Eq. (30) are shown in Tables II and III, in which for reference the corresponding K-shell cross sections are also listed.[11] The $2s_{\frac{1}{2}}$ shell is very nearly one-eighth of the K shell for all a, while the $2p$ shells become im-

[10] It will be noted that the $2p_{\frac{1}{2}}$ cross section is rapidly rising near $a=1$, as for example would result from a $(1+2\gamma)^{-1}$ dependence.

[11] Somewhat better agreement is obtained for very large a with the reasonable assumption that, in the a^5 factor of σ_0, a^3 comes from normalization but the remaining a^2 is really $4\delta^2$. The values for Eq. (30) given in Tables II and III have been modified in this way.

TABLE III. High-energy limit of L-shell total cross sections (unscreened). The ratios of cross sections σ_L/σ_K are given for each subshell and for the complete shell. The data are taken from Table II, for large a using the computer values and for small a using the analytic values as the basis for an extrapolation.

a	$2s_{\frac{1}{2}}/1s$	$2p_{\frac{1}{2}}/1s$	$2p_{\frac{3}{2}}/1s$	σ_L/σ_K
0.10	0.125	0.000	0.001	0.126
0.20	0.125	0.002	0.003	0.130
0.30	0.125	0.004	0.007	0.136
0.40	0.125	0.010	0.011	0.146
0.50	0.126	0.020	0.015	0.161
0.60	0.129	0.038	0.019	0.186
0.70	0.130	0.068	0.022	0.220
0.87	0.130	0.182	0.025	0.337

portant only for large a. Of course the NR prediction has the p shells vanishing faster with increasing energy and so not contributing for any a in this limit.

The only previous work on L-shell cross sections at relativistic energies appears to be that of Hall and Rarita,[12] treating the high-energy limit of the $2s_{\frac{1}{2}}$ shell in the same fashion as Hall[13] had previously treated the K-shell cross section. Hall's method has been discussed in I. The biggest error is in neglecting the terms of relative order a [the $-(4\pi a/15)$ term] but this does not affect the ratio of the two cross sections, since it is common to both. Hall and Rarita concluded that the deviation of the ratio from $\frac{1}{8}$ arises from the normalization, i.e., from the factor $\delta^{2(\gamma-1)}$ of Eq. (30). For heavy elements this increases the ratio to 0.20. However, this estimate neglects the δ dependence of λ in the "Coulomb factor" $e^{-2a\lambda}$; when both factors are considered the deviation is small. Concerning the p shells, Hall and Rarita state that a rough estimate indicates that they are inappreciable.

Gavrila[14] has now used his higher Born approximation procedure to obtain differential and total cross sections for the L shell. His result for the $2s_{\frac{1}{2}}$ differential cross section neglects terms of relative order a^2, and is identically $\frac{1}{8}$th of the K-shell cross section he had obtained in the same way.[3] The discussion of Sec. II indicates why this is so. Gavrila obtained the p-shell cross sections only to lowest order in a; the high-energy limits for his total cross sections may be written

$$\sigma(2p_{\frac{1}{2}})/\sigma(1s)=(3/128)a^2,\quad \sigma(2p_{\frac{3}{2}})/\sigma(1s)=\tfrac{1}{12}a^2,\qquad (37)$$

which agree with Eq. (30) to lowest order in a.

As in I, the high-energy limits we have obtained may be combined with Gavrila's energy dependence to yield an extrapolation formula for general energy and charge. Thus, in analogy with Eqs. (64) and (65) of I, defining $R(a)$ by

$$\sigma(2s_{\frac{1}{2}})=\tfrac{1}{8}\delta^{2(\gamma-1)}e^{-2a\lambda}[1-(4/15)\pi a+R(a)]\sigma_0,\qquad (38)$$

where R can be determined from the numerical results on the high-energy limit, the interpolation formula is

$$\sigma(2s_{\frac{1}{2}})=\tfrac{1}{8}\sigma_0\beta^3k^{-4}(1-\beta^2)^{-\frac{3}{2}}\delta^{2(\gamma-1)}M(\beta)\times\{1+\pi a[N(\beta)/M(\beta)]+R(a)\}\times\exp[-2(a/\beta)\cos^{-1}\delta],\qquad (39)$$

where $M(\beta)$ and $N(\beta)$ are defined by Gavrila or in I. Angular distributions for the K and L shells can easily be obtained in the same way. $R(a)$ is always small and β does not greatly deviate from one at high energies, so that for energies above 1 Mev Eq. (39) predicts that the ratio $\sigma(2s_{\frac{1}{2}})/\sigma(1s)$ is practically energy independent, as well as practically charge independent. Similar expressions could be written for the p shells. However, for these Gavrila has not determined the energy dependence for the terms of order a, corresponding to $N(\beta)$, and the K-shell work indicates that this is needed before the energy dependence in the 1–10-Mev region can be discussed. For comparison with experiment we will make the assumption, roughly in accord with Gavrila's results above 0.5 Mev, that the p shells have the same energy dependence as the s shells, so that all ratios are energy-independent.

Some remarks should now be made concerning screening. The results so far presented, like almost all work on the photoeffect, assumes hydrogen-like wave functions for the electrons. It has been customary to compensate for the screening effect of other electrons by assuming that the process occurs in a Coulomb field of effective charge $Z_{\text{eff}}=Z-S$. The screening parameter S measures the charge density of other electrons inside the shell under consideration; S is often taken as 0.30 for the K shell and 4.15 for the L shell.[15] It is easy to see from Sec. II that this is not a correct procedure for the photoeffect at high energies, which takes place at distances for which ar is not large. At such distances the effect of screening is to reduce a by an amount of the order of $(S/137)a^3r^3$; this will introduce a correction

TABLE IV. High-energy limits of K- and L-shell cross sections, σ/σ_0, corrected for screening. The predicted ratios of σ_K/σ_L are also given, (1) without screening, (2) corrected for screening as in the text, (3) using the effective-charge method. It has been argued that these ratios are largely independent of energy.

a	$1s$	$2s_{\frac{1}{2}}$	$2p_{\frac{1}{2}}$	$2p_{\frac{3}{2}}$	σ_K/σ_L 1	σ_K/σ_L 2	σ_K/σ_L 3
0.10	0.615	0.0480	0.0001	0.0002	8.0	12.7	39.5
0.20	0.483	0.0433	0.0004	0.0008	7.7	10.9	14.9
0.30	0.379	0.0364	0.0009	0.0014	7.4	9.8	11.6
0.40	0.305	0.0310	0.0020	0.0021	6.9	8.8	9.6
0.50	0.255	0.0275	0.0039	0.0029	6.2	7.5	8.0
0.60	0.218	0.0249	0.0069	0.0034	5.4	6.2	6.9
0.70	0.192	0.0225	0.0122	0.0038	4.6	5.0	5.7

[12] H. Hall and W. Rarita, Phys. Rev. **46**, 143 (1934).
[13] H. Hall, Revs. Modern Phys. **8**, 358 (1936).
[14] M. Gavrila (to be published).

[15] For further discussion see G. W. Grodstein, U. S. Department of Commerce, National Bureau of Standards Circular 583 (U. S. Government Printing Office, Washington, D. C., 1957).

to the cross section of relative order $(S/137)a^2$ or less, which is small even for heavy elements. Thus in the regions which contribute to the photoeffect the changes in wave function shape produced by screening are small. However, the change in the normalization of these wave functions will be important; for example, in the $a^{\frac{3}{2}+l}$ factor of Eq. (2) it would probably be appropriate to use a Z_{eff}. We conclude that angular distributions and polarization correlations may be largely independent of screening, but that screening effects will decrease the absolute magnitude of L-shell cross sections. A more precise estimate may be made taking the change of normalization of the bound-state wave function at the origin from the work of Brysk and Rose.[16] (The change in normalization of an outgoing electron of relativistic energy is assumed small.) Values of the K- and L-shell cross sections corrected in this way are listed in Table IV; the ratio of K- to L-shell cross sections is given both with and without this correction, and also using the effective-charge method consistently.

The results of Sec. II allow us to estimate M- and N-shell total cross sections by combining information from Tables II and III and Eq. (7)—we could have obtained a very good estimate of the $2s$ cross section in this way from the $1s$ cross section. Note that Eq. (7) does not give the actual ratio of wave functions at the origin, since it omits terms $O(a^2)$ in the normalization. Screening can be taken into account by using a Z_{eff} in the factor a^{3+2l}, with S as tabulated by Grodstein.[15] (This would have worked fairly well for the L shells.) Again it will be assumed that ratios are independent of energy.

Experimental results are available for three ratios of total cross sections:

$$\sigma_K/\sigma_L, \quad \sigma_L/\sigma_{M'}, \quad (\sigma_{L(\mathrm{I})}+\sigma_{L(\mathrm{II})})/\sigma_{L(\mathrm{III})}, \tag{40}$$

where M' refers to cross sections from all shells other than K and L. This work is due to Latyshev,[17] to Hultberg,[18] and to Grigor'ev and Zolotavin[19]; these papers also review other experiments.

The greatest amount of information is available on σ_K/σ_L, for which there is general agreement that in heavy elements and over a broad energy range the ratio is close to 5. For lighter elements the ratio is closer to 8. This is precisely what Table IV predicts. (Of course Hall and Rarita would have made a similar prediction, but according to the present work the increasing importance of the L shell for large Z is not due to the $2s_{\frac{1}{2}}$ subshell but to the p shells.) Table V compares theory and experiment. Agreement is best when screening is accounted for by correcting the normalization, as we have indicated. It thus appears that the behavior of the ratio σ_K/σ_L can be understood in terms of an increasing importance of p states for large Z and screening effects which are most noticeable for small Z.

TABLE V. Comparison of experimental and theoretical values for the ratio σ_K/σ_L. The theoretical results are given (1) without screening, (2) corrected for screening as in the text, (3) using the effective-charge method. Experimental values for very low energies are not shown, also those for which indicated experimental errors are more than 10%.

Element	Experimenter	Experimental value	Theoretical values (1)	(2)	(3)
Sb	Grigor'ev and Zolotavin	9.3 ± 0.3	7.0	9.1	10.1
Pt	Grigor'ev and Zolotavin	5.8 ± 0.5	5.6	6.6	7.2
Pb	Grigor'ev and Zolotavin	5.1 ± 0.3	5.4	6.2	6.9
Bi	Grigor'ev and Zolotavin	6.0 ± 0.2	5.3	6.1	6.8
Th	Grigor'ev and Zolotavin	5.2 ± 0.6	4.9	5.5	6.2
U	Hultberg	5.3 ± 0.2	4.8	5.3	6.0

Hultberg found $\sigma_L/\sigma_{M'}=2.6\pm0.15$ for U in the 1-Mev region, while Grigor'ev and Zolotavin find values of the order of 3.5 at low energies. It had previously been customary to take this ratio as 4. If the cross sections for higher shells are determined as indicated, the predicted ratio without screening is 1.8. Rather than use a Z_{eff}, one can obtain the screening correction to normalization from Cohen's[20] recent self-consistent field calculation for this atom, and the predicted ratio with screening is found to be 3.3. This includes only s and p states, neglects terms of relative order a^2, and uses the same energy dependence for p states as for s states. If it is assumed that the d states, which contribute to M' but not to L, are of the same magnitude relative to p states as the p states are to s states, then the unscreened ratio becomes 1.4 and the screened ratio about 2.7.

Grigor'ev and Zolotavin find that for Bi at 0.26 Mev the ratio $(\sigma_{L(\mathrm{I})}+\sigma_{L(\mathrm{II})})/\sigma_{L(\mathrm{III})}$ is only 5 and beginning to level off, while according to NR theory it should be 6.3 at 0.26 Mev and should become infinite as the energy increases. From Table IV we predict that the limiting value of the ratio should be 9, in reasonable accord with the trend of the data, and practically independent of screening.

In closing it is appropriate to discuss the relevance of our results for the several processes which are closely related to the photoeffect. It was shown in I that in the high-energy limit the total cross section for the photoeffect, the one-photon annihilation of fast positrons, and their inverses are identical, apart from the statistics of initial and final states, for an electron of a given shell. Another closely related process is the high-frequency limit of bremsstrahlung, which Fano and

[16] H. Brysk and M. E. Rose, Revs. Modern Phys. **30**, 1169 (1958).
[17] G. D. Latyshev, Revs. Modern Phys. **19**, 132 (1947).
[18] S. Hultberg, Arkiv Fysik **15**, 307 (1959).
[19] E. P. Grigor'ev and A. V. Zolotavin, J. Exptl. Theoret. Phys. (U.S.S.R.) **36**, 393 (1959) [translation: Soviet Phys. JETP **9**, 272 (1959)].
[20] S. Cohen, Phys. Rev. **118**, 489 (1960); also University of California Radiation Laboratory Report UCRL-8633 (unpublished).

McVoy[6] have shown to have a matrix element identical to that for the inverse photoeffect to lowest order in a, apart from normalizing factors. The results of Sec. II depend only on properties of the bound state (or low-energy) electron wave function, and so are immediately applicable to all these processes. Thus we know to the same extent (neglecting order a^2) that the differential cross section for one-photon annihilation with a $2s$ electron is one-eighth of that for a $1s$ electron, and we can also draw all other analogous conclusions. The bremsstrahlung limit is more complex, as the low-energy outgoing electron wave function is given by a sum of terms, the first of which is related to photoeffect from the s states, the next two to photoeffect from the $p_{\frac{1}{2}}$ and $p_{\frac{3}{2}}$ states, etc. This will form the subject of a subsequent paper.

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APPENDIX

Using the abbreviations of Eqs. (21) and (26), and also introducing

$$\theta(x)=ax+(\gamma-k)\tan^{-1}(\tan\lambda\tanh x), \tag{41}$$

the functions $K_i(n)$ of Eq. (24) may be written

$$\begin{aligned}K_i(n)=C_i(n)[&d_{in}(x,y)\cos\theta(x)\cos\theta(y)\\&+e_{in}(x,y)\sin\theta(x)\sin\theta(y)\\&+f_{in}(x,y)\sin\theta(x)\cos\theta(y)\\&+f_{in}(y,x)\sin\theta(y)\cos\theta(x)],\end{aligned} \tag{42}$$

where

$$\begin{aligned}&C_1(\pm)=4\delta^2(1\pm\epsilon),\\&C_2(\pm)=4\delta^2(2\gamma+3)(2\gamma+2)(1\mp\epsilon)D^2R^{-2},\\&C_3(\pm)=4\delta^2(2\gamma+2)DR^{-1},\quad C_i(0)=1.\end{aligned} \tag{43}$$

Introducing the further abbreviations

$$\sigma(\pm)=\delta^{-1}(\epsilon\pm1),\quad \sigma(0)=\delta^{-1}(1+\epsilon), \tag{44}$$

then the functions d, e, and f are given as

$$\begin{aligned}&d_{1\pm}=1,\quad d_{2\pm}=\delta^2S(1+S)+\epsilon^2\delta^2T^2-\epsilon\delta\sigma(P_x^2+P_y^2),\\&d_{3\pm}=-\delta^2R,\quad e_{1\pm}=\delta^{-2}T,\quad e_{2\pm}=(\epsilon+\delta\sigma)^2ST+\epsilon^2T,\\&e_{3\pm}=(-1\mp2\epsilon)RT,\quad f_{1\pm}=0,\\&f_{2\pm}(x,y)=-\delta P_x[\epsilon+S(2\epsilon\pm1)]+(\epsilon^2\sigma+\epsilon\delta\sigma^2)TP_y,\\&f_{3\pm}(x,y)=\pm\delta\epsilon^2RT+\delta\epsilon\sinh x(1\mp\epsilon S)\\&\qquad-\epsilon\delta^{-1}(1\pm\epsilon^3)T\sinh y\pm\delta\sinh x\\&\qquad\qquad\times(\delta^2\cosh^2x-\epsilon^2\sinh^2y),\end{aligned} \tag{45}$$

and

$$\begin{aligned}d_{10}=&3\epsilon^2S+(\delta^2\sinh^2x-\epsilon^2\cosh^2x-\tfrac{1}{2})\\&\times(\delta^2\sinh^2y-\epsilon^2\cosh^2y-\tfrac{1}{2})+\tfrac{3}{4}+\sigma^2[\delta^2S(1+\epsilon^2S)\\&+\epsilon^2\delta^2T^2+\epsilon^2\delta^2(P_x^2+P_y^2)]-\sigma\epsilon\delta[(3-8\delta^2)S\\&+4\delta^2R^2-4(\delta^2-\epsilon^2)S^2-(1+2\delta^2)],\\e_{20}=&3\delta^2T+4\epsilon^2\delta^2ST+\sigma^2[(\epsilon^2-\delta^2)^2ST+\epsilon^2T]\\&+\sigma[3\epsilon\delta T-4\epsilon\delta(\delta^2-\epsilon^2)ST],\\f_{30}=&3\epsilon\delta P_x-2\epsilon\delta(\delta^2TP_y-\epsilon^2SP_x-\tfrac{1}{2})\\&-\epsilon\delta\sigma^2P_x[1+(\epsilon^2-\delta^2)S]-\sigma[\tfrac{1}{2}(\delta^2-\epsilon^2)(3S+1)\\&+SP_x(3\epsilon^2\delta^2-\epsilon^4)+TP_y(3\epsilon^2\delta^2-\delta^4)],\\d_{20}=&d_{30}=e_{10}=e_{30}=f_{10}=f_{20}=0.\end{aligned} \tag{46}$$