Atomic Photoelectric Effect at High Energies*†

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Total cross sections are obtained for the photoelectric effect from the K shell of an atom of arbitrary charge, in the limit of high energies. An approximate analytic formula then is deduced to cover the entire high-energy region. For heavy elements and very high energies the differences from previous predictions are large. It is noted that these results also apply to other processes, including the one photon annihilation of fast positrons.

I. INTRODUCTION

THEORETICAL predictions of cross sections for the atomic photoelectric effect at high energies are difficult to obtain, and results have been of uncertain validity. In the present paper the use of an approximate Coulomb wave function, valid for the photoeffect at high energies, permits a simple derivation of the high energy limit of the total cross section. Approximate expressions may then be developed to describe the entire high-energy region.

The photoeffect is a vertex process in an external field in which the initial electron state is discrete (bound) and the final electron state belongs to the continuum (unbound). Neglecting radiative corrections, the matrix element is[1]

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

where $\mathbf{k}$ is the momentum and $\mathbf{e}$ the polarization vector of the incoming photon, ψ_B is the electron wave function for the bound state, and $\psi_{\mathbf{p}}$ the electron wave function for the continuum state of momentum $\mathbf{p}$. The differential cross section is obtained as

$$d\sigma=(2\pi)^{-2}|M|^2\delta(E)d^3p, \tag{2}$$

where the conservation of energy is expressed by

$$E\equiv(p^2+1)^{\frac{1}{2}}-k-\epsilon=0, \tag{3}$$

with ϵ, of order one [$\epsilon=O(1)$],[2] the total energy, including rest mass, of the bound state. Calculations are, in principle, straightforward once the wave functions are specified.

For ψ_B it is customary to assume a hydrogen-like wave function, thus neglecting electronic interactions and the finite size of the nucleus. Similarly $\psi_{\mathbf{p}}$ is taken as an appropriate solution of the Dirac equation in a pure Coulomb field. Although the methods developed here have greater applicability, these approximations will again be made in the explicit calculations.

The central difficulty in the treatment of the relativistic photoeffect arises from the wave function $\psi_{\mathbf{p}}$ of the outgoing electron. The continuum solutions of the Dirac equation are only available as an expansion in partial waves, and for high energy processes a large number of terms contribute to the matrix element. Numerical calculations of the K shell have been performed by Hulme *et al.*[3] for three elements and two energies (0.35 and 1.1 Mev); for higher energies the procedure becomes very arduous, although more feasible with modern electronic computers. It is possible to sum the series in the two limiting cases of small charge Z or high energy k. Sauter[4] thus obtained the energy dependence of the K-shell cross section in the limit of small Z, and Hall[5] obtained the charge dependence in the limit of large k. Combination of these results gives an extrapolation formula which fits smoothly to Hulme's numerical values. However, Hall's result, a double integral for which he was only able to give a rough estimate, has long been questioned. Prange and Pratt[6] and later Erber[7] have verified the double integral, but it has now been shown by several authors[8–12] that Hall's subsequent approximation is incorrect.

An alternative procedure is to establish $\psi_{\mathbf{p}}$ in successive Born approximations and obtain the cross

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[1] W. Heitler, *Quantum Theory of Radiation* (Oxford University Press, New York, 1954), 3rd ed. The notation of this book has in general been followed: in the use of unrationalized units for charge, free electrons normalized to plane waves, $p\equiv|\mathbf{p}|$, conventional Dirac matrices, etc. However the units $\hbar=c=m_e=1$ are used throughout.

[2] In general $x=O(y)$ shall mean x is of order y.

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[5] H. Hall, Revs. Modern Phys. **8**, 358 (1936); also H. Hall, Phys. Rev. **84**, 167 (1951).

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[7] T. Erber, Ann. Phys. **6**, 319 (1959); also T. Erber and R. H. Pratt, Bull. Am. Phys. Soc. **3**, 368 (1958), and T. Erber (to be published).

[8] F. G. Nagasaka, Ph.D. thesis, University of Notre Dame, 1955 (unpublished), also F. G. Nagasaka and E. Guth, Bull. Am. Phys. Soc. **4**, 13 (1959).

[9] M. Gavrila, Phys. Rev. **113**, 514 (1959); also Nuovo cimento **9**, 327 (1958).

[10] R. H. Boyer, Ph.D. thesis, University of Oxford, 1957 (unpublished), also Phys. Rev. **117**, 475 (1960).

[11] H. Banerjee, Nuovo cimento **10**, 863 (1958), **11**, 220 (1959).

[12] R. H. Pratt and T. Erber, Bull. Am. Phys. Soc. **3**, 368 (1958).

section as a power series in the parameter $a=Ze^2$, where Z is the charge of the nucleus. The use of a plane wave was attempted by Hall and Oppenheimer.[13] The difficulty is that the bound state wave functions depend on a and, in fact, only terms of relative order a survive in the matrix element. Terms of this magnitude will also come from the second term in a of the continuum wave function, which may be obtained by iterating the plane wave.[9–11] Sauter's results have been rederived in this way by Fano, McVoy, and Albers.[14] Gavrila[9] has iterated twice and so also obtained the second term in an expansion of the cross section in a, and its energy dependence. This new information on the energy dependence of the cross section is important in establishing an extrapolation formula based on the correct a-dependence of the high-energy limit.

A third approach is to introduce for ψ_p an appropriate approximate Coulomb wave function, valid for high energies in regions which contribute significantly to the matrix element. The best known such function is the so-called Sommerfeld-Maue (SM) wave function,[15,16,17] which is expected to be valid neglecting terms of order a^2/k. From the preceding remarks it is evident that such a function should give the complete charge dependence of the cross section in the high-energy limit, as well as the energy dependence of the lowest order term in $a=Ze^2$ (Sauter term). The first two terms of an expansion in a were computed by Nagasaka[8] and Banerjee.[11] Boyer[10] expressed the total cross section in the high-energy limit as a triple integral, which he evaluated numerically for one case (Pb), confirming the disagreement with Hall's estimate.

For the high-energy limit of the total cross section even simpler approximate wave functions—"modified plane waves"—suffice. The derivation of the Hall integral can be given in a few lines, the answers are expressed in a simple form, and the physical significance of each part of the result is apparent. These features make it possible to treat fairly easily not only photoeffect from the K shell but also from the L shell (to be reported separately).

The present paper begins with a discussion of approximate Coulomb wave functions (II), followed by a general derivation of the high-energy limit of photoeffect cross sections (III). Specializing to the K shell, the first three terms of a power series in a for the total cross section are obtained (IV). More important, the total cross section is then evaluated numerically for all a (V). Since there is considerable disagreement in the published literature, these calculations are given in some detail. The results are then reported and a new energy-extrapolation formula established (VI).

It should be noted that the photoeffect is one of four closely related vertex processes (the photoeffect, the one photon annihilation of positrons, and their inverses). In an appendix it is shown that at high energies the total cross sections for all four processes are essentially identical. In a second appendix previous work on the photoeffect is discussed.

II. MATRIX ELEMENTS AND WAVE FUNCTIONS

We begin by determining the regions in r space which contribute to the photoeffect matrix element at high energies. For this qualitative purpose, it is sufficient to replace ψ_B by $e^{-\delta r}$, where $1/\delta=O(1)$ is the bound state radius,[18,19] and ψ_p by the plane wave $e^{i\mathbf{p}\cdot\mathbf{r}}$. Then the matrix element is characterized by the integral

$$N\equiv\int d^3r\,\exp(-i\boldsymbol{\Delta}\cdot\mathbf{r}-\delta r)=\frac{8\pi\delta}{(\delta^2+\Delta^2)^2}, \qquad (4)$$

where the momentum transfer $\boldsymbol{\Delta}\equiv\mathbf{p}-\mathbf{k}$ is introduced. It is clear from (3) that in the high-energy limit $\Delta\gtrsim\epsilon$. Hence, if the matrix element is not to be negligible, $\Delta=O(1)$. The relation of $\mathbf{k}$, $\mathbf{p}$, and $\boldsymbol{\Delta}$ at high energies is shown in Fig. 1. Taking a coordinate axis along $\mathbf{k}$, $p_\perp(=\Delta_\perp)$, the component perpendicular to $\mathbf{k}$, is $O(1)$: at high energies electrons are mainly emitted very close to the forward direction. Also $\Delta_\parallel$, the component of $\boldsymbol{\Delta}$ parallel to $\mathbf{k}$, equals ϵ. These results will also be needed for the derivation of total cross sections.

It is easy to establish that regions $r=O(k^n)$, $n\neq0$, do not contribute to (4) at high energies, i.e., the important regions are $r=O(1)$. Similarly, a small angular interval of extent k^{-n}, $n>0$, will give a vanishing contribution unless it is in a direction such that $\boldsymbol{\Delta}\cdot\mathbf{r}=0$. From Fig. 1 and the previous discussion it may be determined that

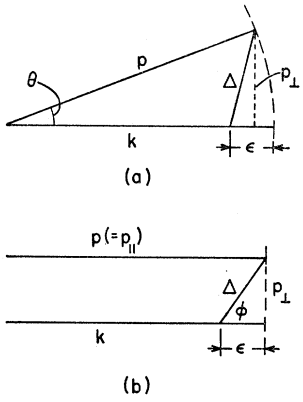

FIG. 1. Relation of photon momentum $\mathbf{k}$, electron momentum $\mathbf{p}$, and momentum transfer $\boldsymbol{\Delta}$, imposed by the requirement of energy conservation. (a) very high energies, (b) the limit of high energies. Dimensions are exaggerated.

[13] H. Hall and J. Oppenheimer, Phys. Rev. **38**, 71 (1931).
[14] U. Fano, K. W. McVoy, and J. R. Albers, Phys. Rev. **116**, 1147 (1959).
[15] A. Sommerfeld and A. W. Maue, Ann. Physik. **22**, 629 (1935); W. H. Furry, Phys. Rev. **46**, 391 (1934).
[16] H. A. Bethe and L. C. Maximon, Phys. Rev. **93**, 768 (1954).
[17] H. Olsen, L. C. Maximon, and H. Wergeland, Phys. Rev. **106**, 27 (1957).

[18] Here all parameters are considered of order of magnitude one in comparison to the energy k. This also implies that the limit of high energies would be taken before the limit of small Z.
[19] For a treatment of relativistic bound state wave functions in the Coulomb field, see H. Bethe and E. Salpeter, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1957), Vol. 35, Part I.

for no Δ of interest can this direction coincide with k [$\phi=90°$ implies $\Delta=O(k)$]. Thus, if cylindrical coordinates ρ, ζ, z are introduced with z axis along $\mathbf{k}$, the important contributions to the matrix element come from $\rho=O(1)$, $z=O(1)$. An approximate Coulomb wave function must be valid in these regions.

To obtain such a wave function we begin with the Dirac equation

$$(\epsilon_p-V-\beta+i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})\psi_{\mathbf{p}}=0 \tag{5}$$

for an electron of energy ϵ_p in the Coulomb potential V. Multiplication on the left with the operator $(\epsilon_p-V+\beta-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla})$ gives the iterated equation

$$[\nabla^2+p^2-2\epsilon_pV+V^2+i\boldsymbol{\alpha}\cdot(\boldsymbol{\nabla}V)]\psi_{\mathbf{p}}=0. \tag{6}$$

Following now with the substitution $\psi_{\mathbf{p}}=e^{i\mathbf{p}\cdot\mathbf{r}}Fu$, where u is taken as a free-field spinor, yields

$$[2ip\cdot\boldsymbol{\nabla}+\nabla^2-2\epsilon_pV+V^2+i\boldsymbol{\alpha}\cdot(\boldsymbol{\nabla}V)]Fu=0. \tag{7}$$

When ϵ_pr is large F may be chosen as a solution of the differential equation

$$[2i\mathbf{p}\cdot\boldsymbol{\nabla}+\nabla^2-2\epsilon_pV]F=0. \tag{8}$$

This choice leads to the SM wave function.[16,17,20]

For some high-energy problems an even simpler function suffices. This is obtained by solving (8) without the factor ∇^2:

$$(i\mathbf{p}\cdot\boldsymbol{\nabla}-\epsilon_pV)F=0. \tag{9}$$

Writing $F=e^{i\chi}$, the solutions for χ at high energies are

$$\chi_+=-\int_{-\infty}^{z}V(\rho,z')dz', \tag{10a}$$

$$\chi_-=+\int_{z}^{\infty}V(\rho,z')dz', \tag{10b}$$

which are chosen to satisfy the boundary conditions incoming (outgoing) plane waves at $\mp\infty$, respectively.[17] (The requirement of plane waves also specifies the normalization.) χ_- is the solution needed for the photoeffect, χ_+ for the inverse photoeffect. An inspection of the argument indicates that to obtain the similar positron wave functions the sign of the potential is to be reversed and the free electron spinor u is to be replaced by the free positron spinor v^*.

For a pure Coulomb field $V=-a/r$ the integrals (10) diverge at $\pm\infty$, corresponding to the well-known fact that for such a field it is not correct to impose plane waves as a boundary condition.[21] Instead, the incoming (outgoing) electron near $\mp\infty$ should be described by the distorted plane wave

$$e^{i\mathbf{p}\cdot\mathbf{r}\mp ia\ln(pr\mp\mathbf{p}\cdot\mathbf{r})}. \tag{11}$$

The general solution for χ is $a\ln(z+r)$, to which arbitrary constants (which may be functions of ρ, p, etc.) may be added. By adding $\pm a\ln p$, $-a\ln\rho^2$, etc., precisely the results (11) are obtained. In other words, for a Coulomb field the desired solutions are

$$\chi_\pm=\mp a\ln(pr\mp\mathbf{p}\cdot\mathbf{r}). \tag{12}$$

Computing ∇^2F/ϵ_pVF at high energies, the additional condition for the validity of these wave functions is found to be $pr\pm\mathbf{p}\cdot\mathbf{r}$ large. Indeed, (12) may be obtained as the limit of the confluent hypergeometric functions of the SM solution for $pr\pm\mathbf{p}\cdot\mathbf{r}$ large.[6] For the photoeffect at large energies we have shown that we need a wave function valid in the region for which both $z=O(1)$, $\rho=O(1)$. The modified plane wave (12) is accurate in these regions.[22] For the Coulomb field the approximate wave function is essentially the asymptotic form of the exact wave function. But more relevant, for $r=O(1)$, it is the high-energy limit of the exact wave function.

III. DERIVATION OF PHOTOEFFECT CROSS SECTIONS

In view of the preceding discussion we take for the wave function $\psi_{\mathbf{p}}$ of the outgoing electron

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

We also now introduce the notation

$$\psi_B\equiv(2\delta)^{\gamma+\frac{1}{2}}r^{\gamma-1}e^{-\delta r}\psi_N, \tag{14}$$

for the bound state wave function,[19] where $\gamma=(\kappa^2-a^2)^{\frac{1}{2}}$ ($\kappa=j+\frac{1}{2}$, j the total angular momentum of the state), and $\delta=(1-\epsilon^2)^{\frac{1}{2}}$ (ϵ, as before, the total energy of the bound state). The spinor ψ_N consists of spherical harmonics and polynomials in r; it is finite for $r=0$. With these substitutions the matrix element may be rewritten

$$M=-e(2\pi)^{\frac{1}{2}}k^{-\frac{1}{2}}(2\delta)^{\gamma+\frac{1}{2}}\times\int d^3r\,\exp(-i\boldsymbol{\Delta}\cdot\mathbf{r}-i\chi_-)e^{-\delta r}r^{\gamma-1}S(r), \tag{15}$$

$$S(r)=u^*(\mathbf{p})\boldsymbol{\alpha}\cdot\mathbf{e}\psi_N,$$

where again $\boldsymbol{\Delta}=\mathbf{p}-\mathbf{k}$ is the momentum transfer.

Introducing cylindrical coordinates for $\mathbf{p}$ with axis in the $\mathbf{k}$ direction, the total cross section for the photoeffect is

$$\begin{aligned}\sigma&=(2\pi)^{-2}\int d^2p_\perp dp_{11}\,\langle|M|^2\rangle_{\mathrm{Av}}\delta(E)\\&=(2\pi)^{-2}\int d^2p_\perp dE\,(dp_{11}/dE)\langle|M|^2\rangle_{\mathrm{Av}}\delta(E)\\&=(2\pi)^{-2}\int_0^{2\pi}d\theta\int_0^{p}p_\perp dp_\perp\frac{p}{p_{11}}\langle|M|^2\rangle_{\mathrm{Av}}\Big|_{E=0},\end{aligned} \tag{16}$$

[20] The SM function actually also includes a spinor term of the next order in energy, which is not needed for the high-energy limit of the photoeffect.

[21] Later it will be shown that for present purposes only the *difference* $\chi(z,\rho)-\chi(z'\rho)$ is needed, and consequently it is not actually necessary to impose the boundary conditions.

[22] The wave function is also valid for the region $\rho=O(\epsilon_p)$ and $z=O(\epsilon_p)$, important in bremsstrahlung.[17]

using Eq. (3) for E. The matrix element is to be summed and averaged over spins and polarizations, depending on the experimental situation. In Sec. II it was shown that M is large only if $p_\perp = O(1)$. This justifies the replacements $p/p_{11} \to 1$, $\int_0^p \to \int_0^\infty$, leading to

$$\sigma = (2\pi)^{-2} \int d^2p_\perp \langle |M|^2 \rangle_{Av} \Big|_{E=0}. \tag{17}$$

Substituting (15) for M and using the result of Sec. II (see Fig. 1) that, when cylindrical coordinates are introduced in r space with z axis along $\mathbf{k}$,

$$\mathbf{\Delta}\cdot\mathbf{r} = \mathbf{p}_\perp\cdot\boldsymbol{\varrho} + \epsilon z, \tag{18}$$

the cross section becomes[23]

$$\sigma = \frac{e^2}{2\pi k}(2\delta)^{2\gamma+1} \int d^3r d^3r' \times \int d^2p_\perp \exp[i\mathbf{p}_\perp\cdot(\boldsymbol{\varrho}-\boldsymbol{\varrho}') + i\epsilon(z-z')] \times e^{i[\chi_-(r)-\chi_-(r')]} e^{-\delta(r+r')}(rr')^{\gamma-1}F(r,r'), \tag{19}$$

$$F(r,r') = \langle S(\mathbf{r}')S^*(\mathbf{r})\rangle_{Av},$$

where orders of integration have been interchanged. The $p_\perp$ integration gives $(2\pi)^2\delta(\boldsymbol{\varrho}-\boldsymbol{\varrho}')$; with this requirement it can be shown that F is a function of z, z', and ρ, but not of the direction $\boldsymbol{\varrho}/\rho$. Thus the expression (19) reduces to the triple integral

$$\sigma = \frac{(2\pi e)^2}{k}(2\delta)^{2\gamma+1} \int dz dz' \rho d\rho\, e^{i\epsilon(z-z')} \times \left(\frac{r+z}{r'+z'}\right)^{ia} e^{-\delta(r+r')}(rr')^{\gamma-1}F(r,r'), \tag{20}$$

where $r^2 = \rho^2+z^2$, $r'^2 = \rho^2+z'^2$, and (13) has been inserted for χ_-. Summing over final electron spins and averaging over initial photon polarizations, for high energies

$$F(r,r') = \sum \psi_N^*(r) \frac{\epsilon_p - \beta - \alpha_z p_z}{2\epsilon_p} \psi_N(r') \underset{p\to\infty}{\to} \sum_i \psi_N^*(r)[(1-\alpha_z)/2]\psi_N(r'), \tag{21}$$

where the z axis is taken along $\mathbf{p}$ (or $\mathbf{k}$). The remaining sum (or average) is over initial electron states. For the K shell $\delta = a$, $\gamma = \epsilon = (1-a^2)^{\frac{1}{2}}$, and

$$F = \frac{1+\epsilon}{8\pi\Gamma(2\gamma+1)}\left[1 + \frac{1-\epsilon}{1+\epsilon}(\cos\theta'\cos\theta + \sin\theta'\sin\theta) + i\left(\frac{1-\epsilon}{1+\epsilon}\right)^{\frac{1}{2}}(\cos\theta - \cos\theta')\right]. \tag{22}$$

[23] The notation here has been taken to conform to that of reference 6, which however contains several misprints.

The cross section (20) is easily reduced to a double integral by performing the integration over ρ.[24] A further integration can be expressed with incomplete beta functions; a final integration apparently leads to generalized hypergeometric functions.[7,10] As such functions are not tabulated, two alternative procedures may be investigated: (a) expansion of the integrand as a power series in its parameters, leading to simpler integrals and an answer in the form of a power series, or (b) direct numerical evaluation of the integral. Both these methods have been used, and the results for the K shell will be reported in succeeding sections. Since the choice of an expansion parameter is not unique, various analytic forms can be obtained. A satisfactory discussion of their convergence does not appear possible, and it is necessary to use the numerical work as a guide in determining the suitability of alternative forms. For this reason, while the power series work is instructive, the numerical work must be considered more reliable. In practice the two methods will complement each other, for the numerical calculations become increasingly difficult as a approaches zero.

For numerical purposes it was desired to make one of the integrations as simple as possible. This may be done by introducing the substitutions

$$x = \frac{z'-z}{r'+r}, \quad y = \frac{z'+z}{r'+r}. \tag{23}$$

For convenience also rewrite (21) as

$$F(r,r') \equiv \sum_{n=0} \rho^n F_n(\theta,\theta'), \tag{24}$$

where the F_n defined by (24) are polynomials in $\cos\theta = z/r$, $\sin\theta = \rho/r$, etc., but do not depend on ρ or r separately (they are also functions of the parameters a, δ, ϵ, etc.). This finite series in ρ arises from the polynomials in r of the bound state wave function. Then, performing the ρ integral,

$$\sigma = \frac{(2\pi e)^2}{k}(\delta)^{2\gamma+1}\Gamma(2\gamma+2) \int_{-1}^{+1}\int_{-1}^{+1} dxdy \times \left(\frac{1-x}{1+x}\right)^{ia} (\delta+i\epsilon x)^{-(2\gamma+2)}(1-x^2y^2)^\gamma \times \sum_{n=0} \frac{\Gamma(2\gamma+2+n)}{\Gamma(2\gamma+2)} 2^{-n}(\delta+i\epsilon x)^{-n} \times [(1-x^2)(1-y^2)]^{n/2}F_n(x,y). \tag{25}$$

The y integrals are comparatively simple and may be recognized as incomplete beta functions. Numerical methods may then be applied to the x integration (Sec. IV).[25]

[24] This would not be true for a screened potential.

[25] An alternative procedure, recently used by Boyer[10] for one choice of parameters, is to numerically obtain M in (15) as a

If the integrand is to be expanded as a power series in its parameters, several approaches are possible, depending on which parameters are expanded. Since δ, γ, ϵ are all functions of a, an obvious method is to attempt to expand the integrand in powers of a and perform the resulting integrals. This is essentially the method which has been followed here.[26] It is, however, not straightforward to expand the integrand of (25) in powers of a. Setting $a=0$ gives a term x^{-4} and so a divergent integral, although in fact (for the K shell) the integral must be of order a^2. The leading term can be extracted from (25) with a more careful analysis, but to obtain higher terms of the power series in this way is very tedious. Looking back at the triple integral (20), it becomes evident that setting $a=0$ removes the exponential that guarantees the convergence of the integral, although the limit $a\rightarrow 0$ yields a well-defined integral. A transformation is hence desired which will explicitly display the behavior of the integral for small a. Such a form can indeed be obtained, although it is more complicated than (25).

In (20) make the substitutions

$$z=\rho\sinh w, \quad z'=\rho\sinh w', \tag{26}$$

and introduce a new parameter λ defined by $\cos\lambda\equiv\delta$, obtaining

$$\sigma=\frac{(2\pi e)^2}{k}(2\delta)^{2\gamma+1}\int_0^\infty d\rho\,\rho^{2\gamma+1}\int_{-\infty}^\infty dw\int_{-\infty}^\infty dw' \times e^{ia(w-w')-\rho[\cosh(w-i\lambda)+\cosh(w'+i\lambda)]} \times(\cosh w\cosh w')^{\gamma-\kappa}\sum_{n=0}\rho^n F_n(w,w') \times(\cosh w\cosh w')^{\kappa}, \tag{27}$$

where κ, as before, is related to the total angular momentum by $\kappa=j+\frac{1}{2}$. Now make the transformation

$$x=w-i\lambda, \quad y=w'+i\lambda, \tag{28}$$

and, verifying (for finite a) that there are no intervening poles or branch cuts, return the contours to the real axis. Using the relations

$$\cosh w=(\cosh^2 x-\sin^2\lambda)^{\frac{1}{2}} \times\exp[+\tan^{-1}(\tan\lambda\tanh x)]$$

$$\cosh w'=(\cosh^2 y-\sin^2\lambda)^{\frac{1}{2}} \times\exp[-\tan^{-1}(\tan\lambda\tanh y)], \tag{29}$$

defining

$$\theta(x)\equiv ax+(\gamma-\kappa)\tan^{-1}(\tan\lambda\tanh x), \tag{30}$$

and performing the ρ integral, one obtains for the cross section

$$\sigma=\frac{(2\pi e)^2}{k}(2\delta)^{2\gamma+1}\Gamma(2\gamma+2)e^{-2a\lambda} \times\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\,e^{i[\theta(x)-\theta(y)]} \times\frac{[(\cosh^2 x-\sin^2\lambda)(\cosh^2 y-\sin^2\lambda)]^{(\gamma-\kappa)/2}}{(\cosh x+\cosh y)^{2\gamma+2}}, \times\sum_n\frac{\Gamma(2\gamma+2+n)}{\Gamma(2\gamma+2)}\frac{[\cosh(x+i\lambda)\cosh(y-i\lambda)]^{\kappa}}{(\cosh x+\cosh y)^n} \times F_n(x,y). \tag{31}$$

The integrals are now well defined for $a=0$; however, they appear of order one rather than order a^2. The final step is to expand the remaining exponent, obtaining a real integral which can be explicitly factored into parts even and odd in x and y. Then terms which are not even in both x and y will vanish; the terms which survive are of order a^2. This will be demonstrated for the K shell in the next section. The limits of integration may then be taken from 0 to ∞.

The factor $\exp(-2a\lambda)=\exp(-2a\cos^{-1}\delta)$ of (31) should particularly be noted. It appeared in a natural manner during the attempt to obtain a power series; if it were expanded in powers of a the resulting series would converge only slowly. It is tempting to argue that this is a characteristic factor, and should not be expanded. For the K shell, at least, the numerical results indeed justify this. It may be noted[9] that this factor is closely connected with the so-called Stobbe factor[1] of the nonrelativistic photoeffect. Indeed, it is easy to see that in the integral (31) for the total cross section only two differences result from the use of correct wave functions rather than a plane wave—this factor and the oscillatory factor $\exp i[\theta(x)-\theta(y)]$.[27]

IV. DEVELOPMENT IN POWER SERIES

If the procedures (26)–(31) are applied, using the form (22) for F, the total cross section for the K shell is obtained as a double integral, in a form suitable for development as a power series in the parameter a. However, to permit direct comparison with previous work, we first make the further transformation

$$u=\sinh^2(\tfrac{1}{2}x), \quad v=\sinh^2(\tfrac{1}{2}y), \tag{32}$$

function of Δ and then integrate $|M|^2$ over Δ. This has the advantage of giving the distribution in momentum transfer as an intermediate step in the calculation. However it requires at least two integrals (the real and imaginary part of M) and in Boyer's case actually six integrals, for each of many values of Δ. The present method requires only one, somewhat more complicated, integral.

[26] Alternatively, one could seek to make the "minimum expansion" in parameters needed to obtain tractable integrals. This method has been followed by Erber,[7] who hoped thereby to obtain a more rapidly converging expansion. However the resulting integrals are not completely tractable, and the analytic forms obtained are complicated and difficult to interpret. Also, as discussed in the Appendix, it appears unlikely that the convergence of the procedure is any better.

[27] In the form (25), however, the difference is entirely represented by the oscillatory factor $[(1-x)/(1+x)]^{ia}$.

and finally obtain

$$\sigma=\sigma_0 H(a)I(a), \tag{33}$$

where σ_0 is the high-energy limit of Sauter's result for small a:

$$\sigma_0=4\pi e^2a^5/k. \tag{34}$$

The factor $H(a)$ is[28]

$$H(a)=\tfrac{2}{3}(1+2\gamma)(1+\gamma)^{-1}(2a)^{2(\gamma-1)} \times\exp(-2a\cos^{-1}a), \tag{35}$$

and the integral $I(a)$ is given by

$$I(a)=\tfrac{3}{8}\int_0^\infty\int_0^\infty dudv\,\frac{A(u)A(v)}{(1+u+v)^{2+2\gamma}} \times\frac{\cos\theta(u)\cos\theta(v)+B(u)B(v)}{[u(1+u)]^{\frac{1}{2}}[v(1+v)]^{\frac{1}{2}}}, \tag{36}$$

in which

$$A(u)=\{[u+\cos^2(\tfrac{1}{2}\eta)][u+\sin^2(\tfrac{1}{2}\eta)]\}^{\frac{1}{2}(\gamma-1)},$$

$$B(u)=(1+2u)\cos\theta(u)-2[u(1+u)]^{\frac{1}{2}}\cot(\tfrac{1}{2}\eta)\sin\theta(u),$$

$$\theta(u)=a\ln\frac{(1+u)^{\frac{1}{2}}+u^{\frac{1}{2}}}{(1+u)^{\frac{1}{2}}-u^{\frac{1}{2}}} +(\gamma-1)\tan^{-1}\left[\frac{2(1-a^2)^{\frac{1}{2}}[u(1+u)]^{\frac{1}{2}}}{a(1+2u)}\right], \tag{37}$$

and $\sin\eta=a$. This is precisely Hall's result.[5] The Hall formula is then obtained by setting $I(a)=(a/2)^{2(\gamma-1)}$.

It is now desired to expand the integrand of (36) as a power series in a to order a^2. It is unlikely that (36) can be represented by a Taylor series; if an expansion was desired to order a^3, terms of the type $a^3\ln a$ would probably also have to be included. Indeed, the known factor $H(a)$ cannot be expanded to order a^2 without including log terms, but for $I(a)$ we will find that this is possible.

With this understanding, the expansion of components of (36) is as follows:

$$A(u)\sim 1-\tfrac{1}{2}a^2\ln[u(1+u)]^{\frac{1}{2}},$$

$$\frac{1}{(1+u+v)^{2+2\gamma}}\sim\frac{1+a^2\ln(1+u+v)}{(1+u+v)^4},$$

$$B(u)\sim\{(1+2u)-4[u(1+u)]^{\frac{1}{2}}P(u)\} +2a[u(1+u)]^{\frac{1}{2}}R(u,a) -a^2\{\tfrac{1}{2}P^2(u)(1+2u)-2[u(1+u)]^{\frac{1}{2}} \times[\tfrac{1}{3}P^3(u)+\tfrac{1}{2}P(u)]\}, \tag{38}$$

where

$$P(u)=\ln\frac{(1+u)^{\frac{1}{2}}+u^{\frac{1}{2}}}{(1+u)^{\frac{1}{2}}-u^{\frac{1}{2}}},$$

$$R(u,a)=\tan^{-1}\left(\frac{2(1-a^2)^{\frac{1}{2}}[u(1+u)]^{\frac{1}{2}}}{a(1+2u)}\right). \tag{39}$$

To this order, all the integrals over u and v are convergent. However, expansion to order a^4 would lead to integrals divergent at u or $v=0$. The factor $R(u,a)$ requires careful treatment, even in order a^2. To this order (but not in the order a^4, where it also occurs) R appears only multiplying functions which are finite at $u=0$. This is sufficient to permit the replacement

$$R(u,a)\to\frac{\pi}{2}-\frac{a}{2}\frac{(1+2u)}{[u(1+u)]^{\frac{1}{2}}}, \tag{40}$$

valid to order a. In (40) order a^2 is not required, since R appears in (38) multiplied by a, and indeed R can probably not be obtained as a simple power series.

The integral $I(a)$, its integrand now written as a power series in a, to order a^2 becomes

$$I(a)=\sum_{i=1}^{6}I_i=\tfrac{3}{8}\int_0^\infty\int_0^\infty dudv\,\frac{1}{(1+u+v)^4} \times\frac{1}{[u(1+u)]^{\frac{1}{2}}[v(1+v)]^{\frac{1}{2}}}\sum_{i=1}^{6}J_i, \tag{41}$$

where, defining

$$T(u)=(1+2u)-4[u(1+u)]^{\frac{1}{2}}P(u), \tag{42}$$

then

$$\begin{aligned}
J_1&=1+T(u)T(v),\\
J_2&=\pi a\{[u(1+u)]^{\frac{1}{2}}T(v)+[v(1+v)]^{\frac{1}{2}}T(u)\},\\
J_3&=\pi^2a^2[u(1+u)]^{\frac{1}{2}}[v(1+v)]^{\frac{1}{2}},\\
J_4&=-a^2\{\tfrac{1}{2}[P^2(u)+P^2(v)]\\
&\quad+T(u)[(1+2v)(\tfrac{1}{2}P^2(v)+1)\\
&\quad-2[v(1+v)]^{\frac{1}{2}}(\tfrac{1}{3}P^3(v)+\tfrac{1}{2}P(v))]\\
&\quad+T(v)[(1+2u)(\tfrac{1}{2}P^2(v)+1)\\
&\quad-2[u(1+u)]^{\frac{1}{2}}(\tfrac{1}{3}P^3(u)+\tfrac{1}{2}P(u))]\},\\
J_5&=-\tfrac{1}{2}a^2[1+T(u)T(v)]\ln[u(1+u)]^{\frac{1}{2}}[v(1+v)]^{\frac{1}{2}},\\
J_6&=a^2[1+T(u)T(v)]\ln(1+u+v).
\end{aligned} \tag{43}$$

Now integrate by parts to remove odd powers of $P(u)$ and $P(v)$, noting that $P'(u)=[u(1+u)]^{-\frac{1}{2}}$. (In I_5, which is the most difficult term, the odd powers cannot be completely removed.) I_2 and I_3 are then simply integrated. For the remaining terms it is more convenient to use the transformations (32), returning to the x, y variables, and extending the limits of integration to $\pm\infty$. Introducing new variables

$$\tau=\tfrac{1}{2}(y+x),\quad \sigma=\tfrac{1}{2}(y-x), \tag{44}$$

[28] The definition differs from that of reference 6 by transfer of the factor $2^{2(\gamma-1)}$ from $I(a)$ to $H(a)$. In that paper, too, γ was defined as $-1+(1+a^2)^{\frac{1}{2}}$, rather than $(1-a^2)^{\frac{1}{2}}$, which has been used here to conform to standard notation.[19]

now separates the double integrals into products of single integrals for all cases except I_5. The final results are

$$I_1=1, \quad I_4=-\tfrac{1}{6}a^2(\pi^2-4),$$
$$I_2=-4\pi a/15, \quad I_5=a^2[2\ln 2-(11/12)-4\pi^2/45], \quad (45)$$
$$I_3=(\pi^2/16)a^2, \quad I_6=a^2[(17/6)-2\ln 2].$$

The total cross section for the K shell is then given as

$$\sigma=\sigma_0 H(a)\{1-(4\pi/15)a+a^2[(2+\tfrac{5}{6}-\tfrac{1}{4})-\pi^2((4/45)+\tfrac{1}{6}-\tfrac{1}{16})]\}$$
$$\approx\sigma_0 H(a)[1-0.837a+0.678a^2]. \quad (46)$$

It is evident that the approximation $I(a)\sim 1$ (Hall) is poor. The term of order a was first found by Nagasaka,[8] and has since been given also by Gavrila,[9] Banerjee,[11] and Erber.[7] Further discussion will be deferred to Sec. VI, after the numerical results have been presented.

V. NUMERICAL METHODS

The transformations (23) lead to a particularly simple expression for the K shell total cross section:

$$\sigma=\sigma_0\{[(-2\xi+3)/2\xi]a^{2\xi}\}I, \quad (47)$$

where σ_0, as previously defined, is the small-a high-energy limit of the cross section, the notation $\xi\equiv-1+\gamma\equiv-1+(1-a^2)^{\frac{1}{2}}$ is introduced, and the integral I (which must be proportional to a^2 for small a) is given by

$$I=\tfrac{1}{4}\int_{-1}^{+1}dx\int_{-1}^{+1}dy\left(\frac{1-x}{1+x}\right)^{ia}[a+i(1-a^2)^{\frac{1}{2}}x]^{-(4+2\xi)}$$
$$\times\{(1-x^2y^2)^{\xi+1}[1+(\xi/a)^2]+2(1-y^2)$$
$$\times(1-x^2y^2)^{\xi}[(i\xi/a)x-(\xi/a)^2x^2]\}. \quad (48)$$

Though the integrand is complex, consideration of the substitution $x\rightarrow -x$ shows that the integral is indeed real. In this form the physical significance of the various factors is easily traced. Thus, it has already been noted that the oscillatory factor $[(1-x)/(1+x)]^{ia}$ is the only consequence of the use of correct outgoing electron wave functions rather than plane waves; here a reflects the strength of the Coulomb potential acting on the outgoing electron. In $[a+i(1-a^2)^{\frac{1}{2}}x]^{-(4+2\xi)}$ the a arises from the bound state radius and $(1-a^2)^{\frac{1}{2}}$ from the total energy of the bound electron [compare (20) and (25)]. The power 2ξ of this factor originates in the characteristic radial dependence of the relativistic bound state wave function $r^{\gamma-1}\equiv r^{\xi}$, as does the power ξ in $(1-x^2y^2)^{\xi}$. The factors (ξ/a) arise from the "small" components of the bound state wave function.

The form (48) is also advantageous for numerical purposes, since the y integration leads to easily computable functions, leaving only the x integration to be performed numerically. For this purpose it is necessary to write (48) explicitly in real form. Using the symmetries of the integrand to reduce the limits to 0 to 1, the integral to be computed is then

$$I=\int_0^1 dx[a^2+(1-a^2)x^2]^{-(2+\xi)}\{[(1+\xi^2/a^2)A(a,x^2)-2(\xi/a)^2x^2B(a,x^2)]\cos C(a,x)$$
$$-(2\xi/a)xB(a,x^2)\sin C(a,x)\}, \quad (49)$$

where

$$C(a,x)=a\ln\frac{1-x}{1+x}-(4+2\xi)\tan^{-1}\frac{(1-a^2)^{\frac{1}{2}}}{a}x. \quad (50)$$

The incomplete beta functions $A(a,x^2)$ and $B(a,x^2)$ which result from the y integration can be calculated from their power series expansions:

$$A(a,x^2)=\int_0^1 dy\,(1-x^2y^2)^{\xi+1}$$
$$=1-(1+\xi)\sum_{r=0}c_r(-\xi)\frac{x^{2r+2}}{(2r+3)(r+1)},$$
$$B(a,x^2)=\int_0^1 dy\,(1-y^2)(1-x^2y^2)^{\xi} \quad (51)$$
$$=A(a,x^2)-[A(a,x^2)-(1-x^2)^{\xi+1}]\times(1-x^2)/2x^2(\xi+1),$$

where $c_r(n)=(n+r-1)!/(n-1)!r!$.

The Coulomb factor $\ln[(1-x)/(1+x)]$ of (50) causes the integrand (49) to undergo an infinite number of oscillations of slowly-varying amplitude in the region near $x=1$. For this reason, numerical integration was performed from $x=0$ to $1-\Delta$, for Δ small, yielding a value I^0. The remaining integral from $x=1-\Delta$ to 1 was obtained analytically as a power series in Δ, through order Δ^2. Again, this is not a true power series, for careful analysis shows that in addition to terms of order Δ^3, there are also terms of order $\Delta^{3+\xi}$. For values of a of physical interest, ξ is small and such terms are also expected to be small.[29]

The integral (49) from 0 to $1-\Delta$ was programmed on the UNIVAC I of the Operations Research Laboratory of the University of Chicago, and I^0 was obtained for sixteen values of a. In addition, several values were computed using the plane wave approximation [i.e., omitting the log term of (50)]. The contributions from the oscillatory region were evaluated by hand and added to I^0 to obtain the complete result. These contributions are large, especially for small a, as will shortly be discussed further. The machine integration was carried out with Simpson's rule. Thirty terms were kept in the power series expansions of the beta func-

[29] However, for $a=1$, $\xi=-1$, and the terms will be of the same order. Thus also there is no contradiction in the fact that the coefficient for Δ^2 separately diverges for $\xi=-1$. For a near 1, I^0 is much larger than the term in Δ, and it is not necessary to compute higher terms.

tions. Sufficient freedom was left in the program so that the region from 0 to $1-\Delta$ could be divided into three intervals of arbitrary length, each with its own arbitrary mesh. This permitted a reasonable matching to the characteristics of the integrand in the various regions of integration. For each point of the mesh was obtained (a) the value of the integrand, (b) total value of the integral to date, (c) fourth-differences estimate of error since preceding point, and (d) sum of estimated errors to date. Thus (a) displayed the function being integrated and (b) showed the relative importance of various regions and how cancellation occurred. By fitting the numerical values to the analytic corrections for various choices of Δ both the equations and the method of integration were checked. Finally, (c) and (d) provided estimates of the Simpson's rule error of the final result and also provided the information from which appropriate mesh sizes and ranges could be determined.

The general behavior of the integrand (49) is fairly easily understood. The magnitude is mainly determined by the factor $[a^2+(1-a^2)x^2]^{-(2+\xi)}$ and hence is largest near $x=0$, decreasing to $O(1)$ near $x=1$. For x near 0, the magnitude is increasingly large as $a\to 0$. This is compensated by the phase factor $(4+2\xi)\tan^{-1}(1-a^2)^{\frac{1}{2}}x/a$ which causes a complete oscillation between $x=0$ and $x\sim 2a$. The Coulomb factor $a\ln[(1-x)/(1+x)]$ produces further oscillations which decrease the integral from the plane wave result. As previously noted, near $x=1$ there is an infinity of oscillations, but even for $a=0.6$ the sharp oscillations do not begin until x exceeds 0.997, and for smaller a they are confined to an extremely small region. However, since there is appreciable cancellation, especially for small a, the contribution from regions near $x=1$ is not negligible; the difference between Coulomb wave functions and plane waves is large even for small a, although (for the total cross section) it does vanish in the limit $a\to 0$.

In the numerical evaluation four sources of error must be considered: (a) round-off, (b) series expansions of the incomplete beta functions, (c) power series for the oscillatory region, (d) Simpson's rule and mesh size. It was desired to reduce the error from each of these to less than 0.1%. The difficulties in achieving this arise from the oscillatory nature of the integrand which, for small a, causes severe cancellation. The UNIVAC carries eleven places, and the errors in its function routines are known. After investigation it was concluded that round-off errors would be entirely insignificant, except for small a, where, for example, the estimated error was 0.02% for $a=0.10$ and 0.6% for $a=0.05$.

It is easily established that the error in ending the series for the incomplete beta functions after n terms is bounded by

$$[(1+\xi)/2n]x^{2n+4}c_{n+1}(-\xi). \tag{52}$$

This is proportional to both ξ and $1+\xi$, and so the error introduced, which is negligible except for x near 1, becomes important only for a near 0.8. With 30 terms kept, even for $a=0.8$ the total error is less than 0.01%.

The accuracy of the analytic expressions for the regions near $x=1$ is estimated by assuming the error is of order $\Delta^{\xi+3}$, as already discussed. For ξ near -1, where this error is of the same order as the Δ^2 terms, the contribution of the whole oscillatory region is small in comparison to I^0. For the smaller a's, the use of $\Delta=0.01$ leads to an error of 4×10^{-6}, which is sufficiently small in comparison to the value of the integral to limit the error to 0.1% for $a\geqslant 0.15$, while $\Delta=0.005$ suffices for $a\geqslant 0.05$.

The remaining question is simply to choose mesh sizes sufficient so that 4th-derivative contributions are small. Both because of the increasing degree of cancellation and the extremely sharp initial oscillation, it is for small a that larger numbers of points are required to represent the function accurately. Practical considerations set an upper limit of 300 points for an integral; this permitted accuracy to within 0.1% at $a=0.15$ and 1% at $a=0.10$. No attempt was made to compute the integral for $a=0.05$. These considerations then determined the values which could be obtained, and their accuracy.

The program itself was checked by evaluating the special (nonphysical) case $a=1$, for which the integrals may be obtained in closed form.[30] The numerical result agreed well with the value of Prange and Pratt.[6]

VI. RESULTS AND EXTRAPOLATION TO LOWER ENERGIES

The high-energy limit of the total cross section for photoeffect from the K shell may be characterized by a function $F(a)$, where

$$\sigma=\sigma_0 F(a)=(4\pi e^2a^5/k)F(a). \tag{53}$$

Values for $F(a)$ obtained numerically with the methods of the preceding section are summarized in Table I and compared with previous predictions. For small a the numerical results agree well with the power series expression (46). A smooth curve may then be drawn for $F(a)$, as in Fig. 2, and the comparison again made with previous work. Disagreement with the Hall formula[5] is large, even for small a; for large a (the only case of experimental interest in the high-energy region) the Nagasaka formula[8] is not much closer. The one value obtained numerically by Boyer[10] agrees fairly well. This previous work is discussed in Appendix B.

A simple analytic expression may be extracted from (46) which provides a reasonable representation of $F(a)$ for all a. Equation (46) may be expected to be valid neglecting terms of order a^3 (including $a^3\ln a$, etc.). If the factor $\frac{2}{3}(1+2\gamma)(1+\gamma)^{-1}2^{2\xi}$ of $H(a)$ is expanded in

[30] In fact $a=0.99$ was computed, since to obtain $a\equiv 1$ would have required inserting into the program a definition of the value of (51) for $\xi=-1$, which to the machine would otherwise appear as 0/0. Such a definition was indeed used in the same expression for $x=0$, but the case $a\equiv 1$ was not so provided for. Indeed, more of the program is checked by *not* taking $a\equiv 1$.

powers of a and folded into $I(a)$, the power series becomes $[1-(4\pi a/15)-0.098a^2]$. In this form the term of order a^2 is negligible except for a so large that a^3 terms (which are not known) may be expected to dominate it, and consequently this a^2 term may be neglected whenever a is small enough for (46) to be applicable. This leads to the simple form

$$\sigma=\sigma_0 a^{2\xi}\exp(-2a\cos^{-1}a)[1-(4\pi/15)a],$$
$$\xi=-1+(1-a^2)^{\frac{1}{2}}\approx-a^2/2, \quad (54)$$

for which some values are listed in Table I. Even for $a=0.6$ (Pb) this differs from the exact values by only 10%. Equation (54) is very similar to the formulas of Hall and Nagasaka (especially with the approximation $2\xi\approx-a^2$ valid except near $a=1$) and may be viewed as a proposed replacement. However it provides only a convenient approximation, justified primarily by its accord with the numerical results presented in Table I and Fig. 2.

The foregoing account of the high-energy limit of the K shell photoeffect total cross section is the main result of this paper. For practical purposes, however, it is necessary to make some statement as to how rapidly the limiting values are approached, i.e., to make some further estimate of the energy dependence of the cross section. The procedure adopted here is to combine present results on the charge dependence of the cross section with the work of Sauter[4] and Gavrila[9] on the energy dependence. Predictions may be compared with Hulme's[3] numerical work at 1.1 Mev and indeed very good agreement is obtained. However similar conclusions were obtained in turn by Hall[5] and Nagasaka,[8]

TABLE I. Total cross section for the K-shell photoeffect in the high-energy limit. $\sigma/\sigma_0=F(a)$ is given for various a, according to (I) the present numerical work, (II) Hall, (III) Nagasaka, (IV) the simple numerical form (54), and (V) other work. The numerical values (I) are accurate to about 0.1% except for $a=0.10$, which is accurate to 1%.

a	I Present work	II Hall	III Nagasaka	IV Eq. (54)	V Others
0.00		1.000	1.000	1.000	
0.05		0.872	0.834		
0.10	0.6964	0.781	0.712	0.6987	
0.15	0.5957	0.711	0.619	0.5960	
0.20	0.5138	0.658	0.550	0.5137	
0.25	0.4475	0.616	0.498		
0.30	0.3942	0.580	0.461	0.3913	
0.35	0.3504	0.552	0.431		
0.40	0.3145	0.526	0.409	0.3065	
0.45	0.2846	0.504	0.397		
0.50	0.2599	0.485	0.389	0.2455	
0.55	0.2396	0.468	0.386		
0.60	0.2224	0.452	0.387	0.2005	0.235[b]
0.65	0.2082	0.436			
0.70	0.1963	0.420		0.1665	
0.80					
0.87[a]	0.1698			0.158	
0.99	0.1601				
1.00				0.163	0.159[c]

[a] $(3)^{1/2}/2$.
[b] R. H. Boyer, reference 10.
[c] R. E. Prange and R. H. Pratt, reference 6.

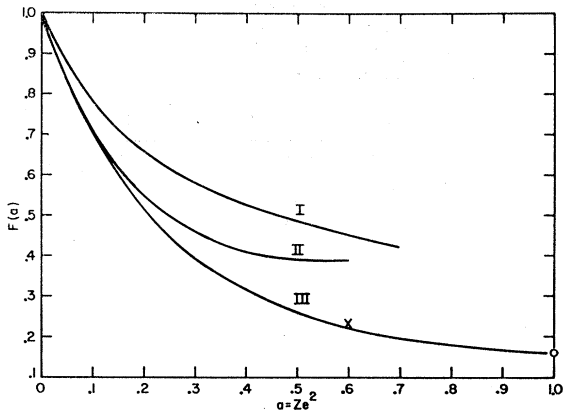

FIG. 2. Total cross section for K-shell photoeffect in high-energy limit. $\sigma/\sigma_0=F(a)$ is plotted against $a=Ze^2$ according to Hall (I), Nagasaka (II), and the present work (III). Boyer's numerical value is shown (×), as well as the limiting case obtained by Prange and Pratt (○).

and hence it is desirable to enter a note of caution. The extremely close agreement of the extrapolation at so low an energy is accidental, considering the magnitude of terms being omitted, and hence the formula must be used with caution. The expected accuracy will be discussed later.

If the high-energy limit of the cross section is written

$$\sigma=\sigma_0 F(a), \quad (55)$$

Sauter's result for the energy dependence of the cross section in the limit of small a may be written

$$\sigma=\sigma_0 S(k), \quad (56)$$

leading to the composite formula

$$\sigma=\sigma_0 S(k)F(a), \quad (57)$$

which neglects terms of order a/k. Here

$$S(k)=[\beta^3/k^4(1-\beta^2)^{\frac{1}{2}}]M(\beta), \quad (58)$$

and the electron velocity β is given by

$$\epsilon_p=(1-\beta^2)^{-\frac{1}{2}}=k+(1-a^2)^{\frac{1}{2}}, \quad (59)$$

and

$$M(\beta)=\tfrac{4}{3}+\frac{[1-2(1-\beta^2)^{\frac{1}{2}}][1-(1-\beta^2)^{\frac{1}{2}}]}{\beta^2(1-\beta^2)^{\frac{1}{2}}}\times\left[1+\frac{1-\beta^2}{2\beta}\ln\frac{1-\beta}{1+\beta}\right]. \quad (60)$$

It may be objected that to be consistent a^2 should be omitted in (59); however, for large a this has a serious effect on (58) owing to the high powers which appear, and since there is agreement as to the correct functional form[5,8] it should probably be preserved. The effect on $M(\beta)$ would be much less severe; however, according to Nagasaka, in (60) it is more correct to make the replacement

$$1-2(1-\beta^2)^{\frac{1}{2}}\rightarrow 1-[1+(1-a^2)^{\frac{1}{2}}](1-\beta^2)^{\frac{1}{2}}. \quad (61)$$

TABLE II. Energy dependence of the K-shell photoeffect total cross section, according to (65). σ/σ_0 is computed as a function of $a=Ze^2$ and the photon energy k (in Mev).

a \ k	1	2	3	5	10	∞
0.0	2.79	1.67	1.41	1.24	1.12	1.00
0.1	2.13	1.26	1.05	0.90	0.80	0.70
0.2	1.71	1.00	0.82	0.69	0.60	0.51
0.4	1.22	0.71	0.58	0.47	0.40	0.31
0.6	0.96	0.59	0.48	0.38	0.31	0.22

It is now desired to modify (57) so as to incorporate Gavrila's[9] recent further results on the energy dependence.[31] This work is a complete evaluation of the cross section to order a; the result essentially is

$$\sigma=\sigma_0\frac{\beta^3}{k^4(1-\beta^2)^{\frac{3}{2}}}\left[M(\beta)\left(1-\frac{\pi a}{\beta}\right)+\pi aN(\beta)\right], \quad (62)$$

where $M(\beta)$ was previously defined and

$$N(\beta)=\frac{1}{\beta^3}\left\{-\frac{4}{15}\frac{1}{(1-\beta^2)^{\frac{1}{2}}}+\frac{34}{15}-\frac{63}{15}(1-\beta^2)^{\frac{1}{2}}\right.$$
$$+\frac{25}{15}(1-\beta^2)+\frac{8}{15}(1-\beta^2)^{\frac{3}{2}}+(1-\beta^2)^{\frac{1}{2}}$$
$$\left.\times[1-2(1-\beta^2)^{\frac{1}{2}}][1-(1-\beta^2)^{\frac{1}{2}}]\frac{1}{2\beta}\ln\frac{1-\beta}{1+\beta}\right\}. \quad (63)$$

The term $-\pi a/\beta$ comes from expansion of the Coulomb exponential; this suggests that the energy dependence $M(\beta)$ multiplies this Coulomb factor.

To incorporate (62) with the present results, write for the high-energy limit

$$\sigma=\sigma_0F(a)$$
$$=\sigma_0a^{2\xi}[\exp(-2a\cos^{-1}a)][1-(4\pi/15)a+R(a)], \quad (64)$$

where $R(a)$ is defined by the equation. From previous discussion $R(a)$ is small for all a; this would not be true if the Coulomb factor had not first been factored out from the power series. One is hence lead to the interpolation formula

$$\sigma=\sigma_0\frac{\beta^3}{k^4(1-\beta^2)^{\frac{3}{2}}}a^{2\xi}M(\beta)\exp[-2(a/\beta)\cos^{-1}a]$$
$$\times\{1+\pi a[N(\beta)/M(\beta)]+R(a)\}, \quad (65)$$

where $\xi=-1+(1-a^2)^{\frac{1}{2}}$.

Some calculations with the formula (65) are presented in Table II, and for Lead the predictions are shown in Fig. 3. Good agreement is obtained with all three of Hulme's numerical values at 1.1 Mev. The energy dependence for the term $-4\pi a/15$ which Gavrila's work supplied is very important in determining (65). Although $N(\beta)/M(\beta)=-4/15$ for $\beta=1$, in the limit of low energies it vanishes, and even for energies in the 0.5–2.0-Mev region $\pi aN/M$ is small in comparison to one. This also means that the limiting values (55) are approached very slowly: for Lead the cross section differs by less than 10% from (55) only above 50 Mev.

The form (65) is presumably valid neglecting terms of order a^2/k, and thus should be quite useful in the high-energy region, even for heavier elements. However the extremely close agreement with Hulme, even for heavy elements, at so low an energy as 1.1 Mev is fortuitous. The following remarks demonstrate this rather strongly. The complete energy dependence of the Coulomb exponential (as distinguished from the factor $M(\beta)$ which multiplies it) is known,[8,9] and indeed nonrelativistically it becomes the Stobbe factor. Noting that $R(a)$ is very small, it is tempting to insert this Coulomb energy dependence and suppose that the main energy dependence of the cross section is thereby included. In fact this makes the result worse. From the power series work it may be seen that the smallness of $R(a)$ is the result of the cancellation of many factors. There is no reason to believe that these have the same energy dependence or that the cancellation continues to occur at lower energies. Such effects must to some extent compensate the additional energy dependence of the Coulomb factor.

Hall and Nagasaka used similar interpolation procedures. Since Hall omitted the $-4\pi a/15$ factor from his high-energy result, it is not surprising that he could get good agreement with Hulme's low-energy result, for at low energies the factor indeed becomes negligible. Likewise, the large positive a^2 term in Nagasaka's power series tends to give a high-energy result similar to Hall's, and so again it is possible for him to obtain agreement with Hulme without having the correct energy dependence of the power series. For Lead the Hall and Nagasaka interpolation formulas are also

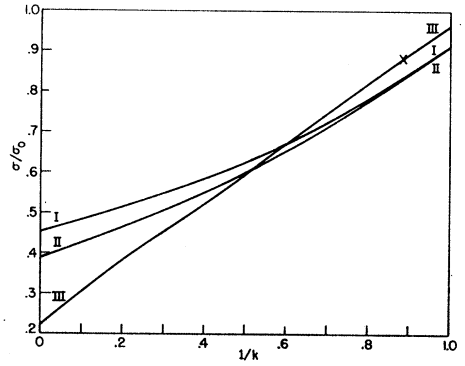

FIG. 3. Energy dependence of the K-shell photoeffect total cross section for Lead, according to Hall (I), Nagasaka (II), and the present work (III). σ/σ_0 is plotted against inverse photon energy $1/k$ in $(\text{Mev})^{-1}$. Hulme's numerical value (X) is also shown.

[31] I have been informed by Dr. Bengt Nagel that he has obtained a similar result by iterating the SM function.

shown in Fig. 3. It is seen that the errors of these estimates do not appear until quite high energies—above 3 Mev for even a 10% effect.

A definite prediction has thus been made for K-shell photoeffect total cross sections at high energies.[32] In the high-energy limit these cross sections are smaller (by a factor of two for heavy elements) then had previously been believed; however the limiting values are reached very slowly, and photons of at least several Mev are needed to demonstrate large deviations from previous theories.[33] It has also been shown that in the high-energy limit the four vertex processes of Appendix A have identical cross sections. In particular this predicts that the one photon annihilation of fast positrons is even less common than had been realized.

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APPENDIX A

Four closely related bound vertex processes are (a) the photoeffect, (b) its inverse, (c) the inverse of one photon pair annihilation of positrons, and (d) the one photon pair annihilation of positrons. The matrix elements are essentially:

$$\begin{aligned}&\text{(a)}\quad u^*e^{-i\mathbf{p}\cdot\mathbf{r}-i\chi_-}e^{i\mathbf{k}\cdot\mathbf{r}}\psi_B,\\&\text{(b)}\quad \psi_B{}^*e^{-i\mathbf{k}\cdot\mathbf{r}}e^{i\mathbf{p}\cdot\mathbf{r}+i\chi_+}u,\\&\text{(c)}\quad \psi_B{}^*e^{i\mathbf{k}\cdot\mathbf{r}}e^{-i\mathbf{p}\cdot\mathbf{r}+i\chi_+}v,\\&\text{(d)}\quad v^*e^{i\mathbf{p}\cdot\mathbf{r}-i\chi_-}e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_B,\end{aligned}\tag{66}$$

where the signs have been taken so that the χ's of (12) apply both to electrons and positrons. From (12)

$$\chi_--\chi_+=a\ln(p\rho)^2,\tag{67}$$

so that, in the square of the matrix element

$$\chi_-(r)-\chi_-(r')=\chi_+(r)-\chi_+(r')+a\ln(\rho/\rho')^2.\tag{68}$$

However it has been shown that the integrals for the total cross section vanish unless $\rho=\rho'$. Hence, for a discussion of total cross sections, no error is introduced by setting $\chi_-=\chi_+$ in the matrix elements. Then

$$M_b=M_a{}^*,\quad M_d=M_c{}^*.\tag{69}$$

In the high-energy limit the densities of states and the expression for energy conservation are pairwise the same, and hence so are the total cross sections.

M_a and M_d (and likewise M_b and M_c) are related by the substitutions

$$\mathbf{k}\leftrightarrow\mathbf{p},\quad u\leftrightarrow v.\tag{70}$$

The second of these has no effect in the high-energy limit. For (c) and (d) the energy conservation requirement

$$(p^2+1)^{\frac{1}{2}}=k+\epsilon\tag{71}$$

is replaced by

$$k=(p^2+1)^{\frac{1}{2}}+\epsilon,\tag{72}$$

which in the high-energy limit is again obtained through the substitution (70). All four total cross sections are thus the same, provided the weighting of states summed and averaged is equivalent. For the K shell, if (a) and (d) are defined as cross sections for capture by *both* K electrons, then in the high-energy limit

$$\sigma_a=\sigma_b=\sigma_c=\sigma_d.\tag{73}$$

The equality of these processes at high energies is needed in the discussion of dispersion relations for the scattering of light from a bound electron, to guarantee the convergence, at high energy, of an integral over energy of the difference of two cross sections.[7] However the main contributions to the integral come from low energies and the value of the integral is not greatly altered by introducing present predictions for the photoeffect at high energy.[34]

A recent and interesting application of photoeffect cross sections has been to connect the cross section for the inverse photoeffect and the cross section for bremsstrahlung near the high-frequency limit (the "tip").[35] For small Z, the matrix element for these processes (involving respectively a bound electron and a free electron of low energy) are shown equivalent up to a numerical factor. It is also argued that the connection of the cross sections is not restricted to small Z, and in this way Nagasaka's predictions for the photoeffect

[32] For many experimental purposes it is also necessary to know the cross sections from higher shells, as these are not distinguished from the K shell. The calculation of these will be the subject of a later paper.

[33] For surveys of theory and experiment at lower energies, see references 1, 5, 19, and also G. W. Grodstein, U. S. Department of Commerce, National Bureau of Standards Circular 583 (U. S. Government Printing Office, Washington, D. C., 1957).

[34] J. S. Levinger and M. L. Rustgi, Phys. Rev. **103**, 439 (1956); also J. S. Levinger, M. L. Rustgi, and K. Okamoto, Phys. Rev. **106**, 1191 (1957).

[35] U. Fano, H. W. Koch, and J. W. Motz, Phys. Rev. **112**, 1679 (1958). Also reference 14, U. Fano, Phys. Rev. **116**, 1156 (1959), and K. McVoy and U. Fano, *ibid.*, 1168.

have been translated into predictions for the bremsstrahlung tip. Agreement with experiment is good, except for the case of highest energy (15 Mev). It is interesting to note that, of the cases reported, this is the only one in which (according to the present extrapolation) Nagasaka's result is appreciably in error. It is uncertain, however, how seriously this can be taken as an argument in support of the present predictions for the photoeffect.

APPENDIX B

Discussion of previous results for the K-shell cross section evidently should begin with the work of Hall,[5] who originally obtained (33) and then made the approximation $I(a)=(a/2)^{2\xi}$. The nonanalytic form should be disregarded, and in estimating the accuracy of the approximation Hall essentially estimated the magnitude of the next term of a power series in a, taking the first term as 1. He concluded that the next term was small, rather than the large factor $-4\pi a/15$ which has now been established. Hall's argument, which has been checked by Gavrila,[9] rests on the assumption that the main contributions to (35) come from u and v near 0, and that in slowly varying factors u and v can be replaced by 0 (or by an "average" value, taken to be 1/7). It is, however, ambiguous which factors may be considered slowly varying, and with similar procedures Nagasaka could obtain a much larger value.[8] Presumably the integrand of (36), like that considered in Sec. V, is oscillatory, and although the magnitude may be greatest near $u=v=0$, the cancellations have the consequence that it is difficult to estimate in advance which regions of u and v contribute to the integral.

The next relevant work on the photoeffect is that of Nagasaka,[8] whose final result for the high-energy limit is essentially[36] (54), with the added term in the power series $1.476a^2$ instead of $-0.098a^2$. It is this large positive a^2 term which causes Nagasaka's cross section to rise for large a. It is believed that more confidence can be placed in the present results, where the power series (which was checked independently) and numerical computations are consistent. Nagasaka was apparently the first to realize the importance of the term of order a, as well as to point out the incorrectness of Hall's nonanalytic factor for $I(a)$.

Boyer[10] obtained for Lead the value $\sigma=0.235\sigma_0$, in contrast to the Hall value $0.451\sigma_0$ (our result is $0.222\sigma_0$). In this way the disagreement with the Hall formula for large a was established. The small difference between Boyer's number and the present result is probably due to the errors of Boyer's numerical method.[37]

Recently Gavrila[9] and Banerjee[11] have independently obtained the term $-4\pi a/15$, and Gavrila also derived it from Hall's double integral. Erber's[7] method of evaluation yields a complicated expression in which the term $-4\pi a/15$ can be identified in the limit of small a. His expansion parameter is ξ, the parameter a being otherwise treated exactly. Thus in (43) I_5 and I_6 correspond to an expansion in ξ, whereas I_3 and I_4 result from a further expansion in a. From (45) it does not appear that ξ is a more suitable expansion parameter, since all the integrals are of similar magnitude. The term Erber obtained is in moderate agreement with the present results, but no better than would be obtained simply from $-4\pi a/15$.

[36] In consequence of a minor arithmetic error, $4\pi/15$ is consistently evaluated as 0.832 instead of 0.837.

[37] R. H. Boyer (private communication).