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Analytic calculation of screened photoeffect cross sections*

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Using the results of an analytic perturbation theory for screened Coulomb wave functions, closed-form expressions are given for screened K- and L-shell photoeffect total cross sections in the nonrelativistic dipole approximation. The analytic results agree very well with numerical dipole calculations for the same potential. These nonrelativistic dipole results are then compared with the full relativistic (including retardation) screened calculations of Scofield. Because of strong cancellations between relativistic and multipole effects, the nonrelativistic dipole results can be shown to yield accurate predictions for the photoeffect for photon energies ranging from threshold to nearly 100 keV.

I. INTRODUCTION

An analytic perturbation theory has been developed recently to obtain nonrelativistic radial wave functions in a screened Coulomb potential.[1,2] The method is based on the expansion of the potential inside an atom as a series in λr having the form

$$V(r) = (-a/r)[1 + V_1\lambda r + V_2(\lambda r)^2 + V_3(\lambda r)^2 + \cdots]. \qquad (1)$$

In Eq. (1), $a = \alpha Z$, where α is the fine-structure constant and Z is the nuclear charge. λ is a small ($\simeq \alpha Z^{1/3}$) parameter characterizing the screening, and the coefficients V_k are of order unity. We note that these coefficients are not fitted to the potential shape at small distances but, rather, over the entire interior of the atom for realistic potentials. In general, the V_k alternate in sign and decrease with increasing k so that form (1) converges rapidly in this region ($\lambda r < 1$).

With expansion (1), wave-function shapes for both bound and continuum states can be simply expressed as series in λ and are likewise accurate in the interior region. For inner-shell bound states and continuum states of not too low energy, the wave functions will reach their asymptotic forms within the region of validity of these expansions. Hence, in these circumstances, bound and continuum normalizations are also obtained as series in λ as well as bound-state energy eigenvalues.[3] The results thus obtained for nonrelativistic screened Coulomb radial wave functions are in good agreement with exact numerical calculations. Further work is now in progress on an extension to the relativistic case[4] as well as on improving the basic technique.

In order to demonstrate the power of the theory in its present form, it seems appropriate at this time to apply it to specific calculations. This will also serve to provide guidance for further improvements. Accordingly, in the present work we use the wave functions of this perturbation theory to obtain analytic expressions for screened K- and L-shell photoeffect total cross sections in nonrelativistic dipole approximation. We find that our results are very good in the energy range in which the major contribution to the dipole photoeffect matrix element arises within the interior of the atom. This implies that our perturbation theory should be useful for any process; e.g., internal conversion, threshold pair production, and tip bremsstrahlung, for which the matrix element is determined largely in the interior region.

We note that our approach is complementary to other analytic methods used in photoeffect; for example, the quantum-defect theory[5] and its generalizations. In the quantum-defect theory one uses the fact that at large distances the potential seen by an electron is essentially Coulombic. The effect of inner-electron screening, then, is only to change the normalization and phase of the exterior Coulomb wave function. Moreover, at low energies the phase shift can be determined semiempirically by analytically continuing the quantum-defect parameter to positive energies. In this way one obtains analytic expressions for screened photoeffect cross sections which are valid for transitions of outer electrons at photon energies near threshold.[6] In a related approach, McGuire[7] introduces a modified Coulomb potential for which analytic solutions of the Schrödinger equation can be found. Although in general numerical methods are required, he is able to give an analytic expression for the dipole photoeffect cross section in two cases. By neglecting the interior region in the dipole matrix element integral and considering transitions of outer electrons he obtains an expression which is similar to that obtained from quantum-defect theory and which valid over a somewhat wider range of energies. In the other case, the outer region is neglected. However, because of the inadequacy of the potential model employed, the resulting expression can only be used for transitions in which the angular momentum quantum numbers are large. In any case, these methods are not appropriate for the discussion of inner (K- and L-) shell transitions or for photon energies significantly above threshold (keV region). On the other hand, because of our expansion (1) of the potential, we can construct analytic screened wave functions which are accurate in the interior region. In this way we can adequately determine screening effects in atomic photoeffect inner-shell transitions.

In Sec. II we briefly discuss the particular bound and continuum screened wave functions which are needed. The integrals which define the dipole matrix elements are then evaluated analytically and we obtain closed-form expressions for the total cross sections. In Sec. III we compare these analytic expressions for cross sections with numerical evaluations of nonrelativistic dipole cross sections using the Herman-Skillman potential.[8] In general, the agreement is excellent, for all but very low Z, over the entire range of photon energies excluding a small region near threshold. We then compare these results with the full relativistic (single-electron) screened calculations of Scofield.[9] Both the analytic and numerical evaluations of the nonrelativistic dipole total cross sections for photoeffect agree very well with the full relativistic screened results. This agreement is found not only at low energies, but also for photon energies approaching 100 keV. Since this is well beyond the expected range of validity of the nonrelativistic dipole approximation, the agreement indicates a strong cancellation between relativistic and higher multipole contributions. Hence, our analytic expressions for screened photoeffect cross sections should be of considerable utility over a wide range of energy.

II. CALCULATION OF ANALYTIC CROSS SECTIONS

The differential cross section for photoeffect in nonrelativistic dipole approximation can be written in the form (we choose units such that $\hbar = c = m_e = 1$)

$$\frac{d\sigma}{d\Omega} = (2\pi)^2 \alpha\omega |M_{fi}|^2, \tag{2}$$

where ω is the incident photon energy and the matrix element M_{fi} is given by[10]

$$M_{fi} = \int \psi_f^* \vec{r} \cdot \vec{\epsilon} \psi_i \, d\tau. \tag{3}$$

In Eq. (3), ψ_i is the initial bound-state wave function normalized such that $\int |\psi_i|^2 d\tau = 1$, and ψ_f is the final continuum electron wave function corresponding to an incoming spherical plus outgoing plane wave normalized on the energy scale so that

$$\int \psi_{E'}^* \psi_E \, d\tau = \delta(E - E')\delta(\hat{k} - \hat{k}').$$

$\vec{\epsilon}_j$ is the photon polarization vector, where $j = 1, 2$, corresponding to the two possible photon polarizations.

If the bound-state wave function is written in the form

$$\psi_i = R_{nl}(r) Y_{lm}(\theta, \phi), \tag{4}$$

and the continuum wave function is expanded in a partial wave series

$$\psi_f = \sum_{l'} (2l' + 1) i^{l'} e^{-i\delta_{l'}} R_{l'}(kr) P_{l'}(\hat{k} \cdot \hat{r}), \tag{5}$$

then the total photoeffect cross section for the subshell labeled n and l, σ_{nl}, is given by

$$\begin{aligned} \sigma_{nl} &= (2\pi)^2 \alpha\omega \int \sum_{j,m} |M_{fi}|^2 d\Omega \\ &= (2\pi)^2 \alpha\omega \tfrac{2}{3}(4\pi)^2 [(l+1) |\langle k, l+1 | r | n, l\rangle|^2 \\ &\qquad + l |\langle k, l-1 | r | n, l\rangle|^2], \end{aligned} \tag{6}$$

where the radial matrix elements for $l' = l \pm 1$ are defined by

$$\langle k, l' | r | n, l\rangle = \int_0^\infty r^2 \, dr R_{l'}^*(kr) r R_{nl}(r). \tag{7}$$

Thus, in order to evaluate the dipole photoeffect total cross section we need only calculate the screened radial matrix elements $\langle k, l\pm 1 | r | n, l\rangle$.

The radial wave functions which we need for the evaluation of the matrix elements, (7), are discussed in Refs. 1 and 2. First, we consider the bound state. We write

$$R_{nl}(r) = N_{nl} r^l e^{-ar/n} s_{nl}(r), \tag{8}$$

where the radial function $s_{nl}(r)$, to any finite order in λ, is a polynomial in r. For the $1S$, $2S$, and $2P$ states, in particular, we have, through third order in λ,

$$\begin{aligned} s_{10}(r) &= 1 + \tfrac{1}{2}\Lambda_2 (ar)^2 + \Lambda_3 (ar)^2 (1 + \tfrac{1}{3} ar), \\ s_{20}(r) &= 1 - \tfrac{1}{2} ar + 2\Lambda_2 (ar)^2 (1 - \tfrac{1}{4} ar) \\ &\qquad + 2\Lambda_3 (ar)^2 (7 - \tfrac{7}{6} ar - \tfrac{1}{6}(ar)^2), \\ s_{21}(r) &= 1 + \Lambda_2 (ar)^2 + 2\Lambda_3 (ar)^2 (3 + \tfrac{1}{3} ar), \end{aligned} \tag{9}$$

where $\Lambda_k = V_k (\lambda/a)^k \equiv V_k (1.13 Z^{-2/3})^k$. We note that the zero-order terms in (9) are precisely the point Coulomb radial functions $s_{nl}^c(r)$. The corresponding normalizations N_{nl} and energy eigenvalues T_{nl} are given by

$$N_{10}=N_{10}^c(1-\tfrac{3}{2}\Lambda_2-\tfrac{11}{2}\Delta_3),$$
$$N_{20}=N_{20}^c(1-24\Lambda_2-328\Lambda_3), \qquad (10)$$
$$N_{21}=N_{21}^c(1-30\Lambda_2-320\Lambda_3),$$

where

$$N_{nl}^c=\left(\frac{2a}{n}\right)^{l+3/2}\frac{1}{(2l+1)!}\left(\frac{(n+l)!}{2n(n-l-1)!}\right)^{1/2} \qquad (11)$$

is the point Coulomb normalization, and

$$T_{10}=-\tfrac{1}{2}a^2(1+2\Lambda_1+3\Lambda_2+6\Lambda_3),$$
$$T_{20}=-\tfrac{1}{8}a^2(1+8\Lambda_1+48\Lambda_2+336\Lambda_3), \qquad (12)$$
$$T_{21}=-\tfrac{1}{8}a^2(1+8\Lambda_1+40\Lambda_2+240\Lambda_3),$$

where the point Coulomb energy is just $T_{nl}^c=-a^2/2n^2$.

In the continuum case, we write the screened radial wave function $R_{l'}(kr)$ in the form

$$N^{-1}(k,l')R_{l'}(kr)=r^{l'}e^{-ik_cr}s_{l'}(k_cr), \qquad (13)$$

where the radial function $s_{l'}(k_cr)$ reduces to the point Coulomb result $s_{l'}^c(k_cr)$ in the limit $\lambda\to 0$. We note, however, that the parameter k_c, which appears on the right-hand side of Eq. (13), is not necessarily equal to k, the magnitude of the asymptotic momentum for the screened wave function. Instead, we define k_c by means of the equation

$$\tfrac{1}{2}k^2-\tfrac{1}{2}k_c^2=T-T_c=\delta T, \qquad (14)$$

where, in general, δT may assume any finite value. The formalism then allows us to relate the screened radial wave function of energy T to a point Coulomb wave function of shifted energy T_c plus small correction terms. Our next consideration, then, is the choice of δT.

It has previously been noted that for a variety of physical processes one can most simply compare screened and point Coulomb results corresponding to the same photon energy.[11] In general, this implies that continuum electron (positron) energies must be shifted in order to satisfy the appropriate energy-conservation relations. One can understand this in part by noting that, at energies not too near threshold, the dominant contribution to the matrix elements of these processes is determined at relatively small distances, and that the shape of screened and point Coulomb wave functions near the origin will be closest when compared for shifted energy.[12] For a process like photoeffect it therefore seems most sensible to choose δT in Eq. (14) to accommodate this observation. In this case, comparing screened and point Coulomb results at the same photon energy implies that the energy of the ejected continuum electron must be shifted an amount

$$\delta T=\delta T_B=T_{nl}-T_{nl}^c, \qquad (15)$$

where δT_B is the shift in the bound-state energy due to screening.

In the following we will assume that for photoeffect from each subshell the continuum wavefunction energy shift is given by Eq. (15). Then, using the exact (screened) energy conservation relation with Eq. (14), we find

$$\tfrac{1}{2}k_c^2=\omega-a^2/2n^2, \qquad (16)$$

so that k_c is just the usual Stobbe parameter which appears in the nonrelativistic point Coulomb dipole cross section. In this way, we will find that our analytic expression for the screened photoeffect cross section can be written in terms of the appropriate point Coulomb result, multiplied by a screening correction which can be expressed in terms of simple elementary functions of the photon energy.

We note that according to the normalization screening theory of photoeffect[12] it is reasonable to expect that screening corrections can be given in terms of a simple factor multiplying the point Coulomb results. At energies sufficiently above threshold it is known that the only effect of atomic electron screening is due to the change in the bound state normalization. Hence, in this case, screening may be ignored except as an external multiplicative factor given by the square of the ratio of screened to point Coulomb bound-state normalizations. Even at relatively low energies this normalization factor will give a major part of the screening corrections. The energy dependence of the screened cross section will be essentially that of the point Coulomb case with only small additional correction terms so that a perturbation theory is appropriate. We will thus find that our formalism considerably simplifies the description of screening effects in atomic photoeffect.

The actual form of the screened continuum radial function $s_{l'}(k_cr)$ for arbitrary energy shift is given in Ref. 2. We have

$$s_{l'}(k_cr)=s_{l'}^c(k_cr)+\lambda^2A_2(l',k_cr)+\lambda^3A_3(l',k_cr)+\cdots, \qquad (17)$$

where

$$s_{l'}^c(k_cr)=M(l'+1+i\nu,2l'+2,2ik_cr) \qquad (18)$$

is the usual point Coulomb radial function corresponding to an electron energy $T_c=\tfrac{1}{2}k_c^2$, and

$$A_k(l',k_cr)=\sum_{s=-k}^{k}\alpha_s^k(-i\nu,l')M(l'+1+i\nu-s,2l'+2,2ik_cr)+\beta_0^k(-i\nu,l')\frac{\partial}{\partial\nu}M(l'+1+i\nu,2l'+2,2ik_cr). \qquad (19)$$

TABLE I. Coefficients $\alpha_s^k(-i\nu,l')$ and $\beta_0^k(-i\nu,l')$ which appear in our expansion of the wave function, Eq. (19). These depend on the bound state quantum numbers n and l since our choice for the energy shift [Eq. (15)] depends on the particular bound state from which the electron is ejected. Values of α_s^k for $s<0$ are determined by relation (20).

s	$\dfrac{\alpha_s^2(-i\nu,l')}{\nu^2V_2/4a^2}$	$\dfrac{\alpha_s^3(-i\nu,l')}{\nu^4V_3/4a^3}$
0	$3\nu^2(2l'+3)-4(l'+1)d_2$	$-[10\nu^2(l'+2)-\frac{1}{3}(l'+1)(8l'^2+13l'-6)-4a(l'+1)d_3/\nu^2]$
1	$(l'+1-i\nu)[2i\nu(2i\nu-1)+2d_2]$	$\frac{1}{2}(l'+1-i\nu)[15i\nu(1-i\nu)+3l'(l'+1)-6+4ad_3/\nu^2]$
2	$\frac{1}{2}i\nu(l'+2-i\nu)(l'+1-i\nu)$	$\frac{3}{2}(1-i\nu)(l'+2-i\nu)(l'+1-i\nu)$
3		$-\frac{1}{6}(l'+3-i\nu)(l'+2-i\nu)(l'+1-i\nu)$

$\beta_0^2(-i\nu,l')=4\nu(\nu^2V_2/4a^2)\{\frac{1}{2}[3\nu^2+l'(l'+1)]-d_2\}$ $\beta_0^3(-i\nu,l')=2\nu(\nu^4V_3/4a^3)\{[-5\nu^2+1-3l'(l'+1)]-2ad_3/\nu^2\}$

$d_2=\frac{1}{2}[-3n^2+l(l+1)]$, $d_3=(-n^2/2a)[5n^2+1-3l(l+1)]$, $l'=l\pm 1$

In these equations, $M(a,b,x)$ is a regular confluent hypergeometric function[13] and $\nu=a/k_c$. We note that β_0^k is real and that the coefficients α_s^k satisfy the relation

$$[\alpha_s^k(-i\nu,l')]^*=\alpha_{-s}^k(-i\nu,l'), \tag{20}$$

so that the screened radial wave function is real. The explicit forms of β_0^k and α_s^k for $k=2,3$, using the particular energy shifts (15), are given in Table I.

The screened continuum normalization $N(k,l')$ can also be given as a series in λ. Explicitly, through third order, we have

$$N(k,l')=N_c(k_c,l')\big[1+\tfrac{1}{4}\Lambda_2\nu^2\{l'(l'+1)(2l'+1)-[3\nu^2+l'(l'+1)+3n^2-l(l+1)][2l'+1-\rho_{l'}]\}$$
$$-\tfrac{1}{4}\Lambda_3\nu^4(\tfrac{5}{3}l'(l'+1)(2l'+1)-\{5\nu^2-1+3l'(l'+1)-(n^2/\nu^2)[5n^2+1-3l(l+1)]\}[2l'+1-\rho_{l'}])\big], \tag{21}$$

where

$$N_c(k_c,l')=\frac{k_c^{1/2}(2k_c)^{l'}}{(2\pi)^{3/2}}\,\frac{|\Gamma(l'+1+i\nu)|}{\Gamma(2l'+2)}e^{\pi\nu/2} \tag{22}$$

is the point Coulomb normalization and

$$\rho_{l'}=\nu N_c^{-2}(k_c,l')\frac{\partial}{\partial\nu}N_c^2(k_c,l')=\rho_{l'-1}+\frac{2\nu^2}{l'^2+\nu^2},\quad \rho_0=1-\frac{2\pi\nu}{e^{2\pi\nu}-1}. \tag{23}$$

Our expression (21) for the continuum normalization, like that for the shape, depends on the bound state quantum numbers n and l since our choice for the energy shift (15) depends on the particular bound state from which the electron is ejected.

Using these analytic expressions for the screened wave functions the matrix elements $\langle k,l'|r|n,l\rangle$ can be evaluated immediately in terms of the basic integral

$$I(\nu;n,l;m,s)=\int_0^\infty dr\, r^{2l'+1+m}e^{-ar/n-ik_cr}M(l'+1+i\nu-s,2l'+2,2ik_cr)$$
$$=\Gamma(2l'+2+m)\left(\frac{a}{n}+ik_c\right)^{-l'-1+i\nu-s}\left(\frac{a}{n}-ik_c\right)^{-m-l'-1-i\nu+s}F\left(-m,l'+1+i\nu-s,2l'+2;\frac{2ik_c}{a/n+ik_c}\right), \tag{24}$$

where $l'=l\pm1$, m is an integer ≥ 0, and $F(a,b;c;z)$ is a Gaussian hypergeometric function. We note that $I(m,s)$ can be written in terms of elementary functions since, for integer m, the series which defines $F(-m,b;c;z)$ terminates. Moreover,

$$I^*(m,s)=I(m,-s), \tag{25}$$

so that the radial matrix elements will be real. The necessary algebra is straightforward but rather tedious and we simply present below the final results for the screened K- and L-shell photoeffect cross sections.

For the K shell, only one radial matrix element contributes. From Eq. (6), we have

$$\sigma_{10}=(2\pi)^2\alpha\omega\tfrac{2}{3}(4\pi)^2|\langle k,1|r|1,0\rangle|^2, \qquad (26)$$

where the square of this matrix element for the screened potential can be written in the form

$$|\langle k,1|r|1,0\rangle|^2=|\langle k_c,1|r|1,0\rangle_c|^2\chi_{10}^{+}(\nu). \qquad (27)$$

In Eq. (27),

$$|\langle k_c,1|r|1,0\rangle_c|^2=\left(\frac{2}{\pi\omega}\right)^2\left(\frac{\nu^2}{1+\nu^2}\right)^3\frac{e^{-4\nu\tan^{-1}1/\nu}}{1-e^{-2\pi\nu}} \qquad (28)$$

is the point Coulomb result[14] (Stobbe formula) and $\chi_{10}^{+}(\nu)$ is given, through third order in λ, by

$$\chi_{10}^{+}(\nu)=\left(\frac{N_{10}}{N_{10}^c}\right)^2\left[1+\Lambda_2\left(Q_{10}^{+}(3\nu^2+5)-\frac{8\nu^2}{1+\nu^2}(2+\nu^2)+3\nu^2\right)\right.$$
$$\left.-\Lambda_3\left(Q_{10}^{+}[5\nu^2(1+\nu^2)-6]+\frac{4}{3}\frac{\nu^2}{(1+\nu^2)^2}(6+7\nu^2-21\nu^4-10\nu^6)+5\nu^4\right)\right], \qquad (29)$$

where

$$Q_{10}^{+}=\nu^2\left(\frac{3+2\nu^2}{1+\nu^2}-2\nu\tan^{-1}\frac{1}{\nu}-\frac{\pi\nu}{e^{2\pi\nu}-1}\right). \qquad (30)$$

The Stobbe parameter, k_c, in this case has the value, $k_c=(2\omega-a^2)^{1/2}$ and, we recall, $\nu=a/k_c$. In Eq. (29) we have written explicitly the factor (N_{10}/N_{10}^c), which gives the screening corrections to the Stobbe formula due to the change in the bound state normalization. This factor, for the K shell, can be obtained directly from our analytic expression (10) and, for a wide range of energies, represents the major part of the screening corrections to K-shell photoeffect.

At high energy ($\nu\ll 1$), the screened cross section (26) becomes simply

$$\sigma_{10}=\sigma_{10}^c(N_{10}/N_{10}^c)^2[1+O(\nu^2\Lambda_2)], \qquad (31)$$

where σ_{10}^c is the point Coulomb cross section. The screening corrections due to wave function shape and continuum normalization contributions vanish for large ω, so that the only effect of screening in this limit is due to the change in the bound-state normalization. This is precisely the conclusion obtained from the normalization screening theory of photoeffect[12] and has been verified independently over a wide range of photon energies and atomic numbers.

For very low energy ($\nu\gg 1$), the screening corrections (29), although at first sight divergent, are actually finite due to cancellation between divergent terms.[15] In this limit the screened cross section can be written in the form

$$\sigma_{10}=\sigma_{10}^c\left(\frac{N_{10}}{N_{10}^c}\right)^2\left[1-\Lambda_2\left(\frac{58}{15}-\frac{34}{7}\frac{1}{\nu^2}+\frac{110}{21}\frac{1}{\nu^4}\right)\right.$$
$$\left.-\Lambda_3\left(\frac{310}{21}-\frac{10274}{315}\frac{1}{\nu^2}+\frac{34246}{693}\frac{1}{\nu^4}\right)\right], \qquad (32)$$

where we have neglected correction terms of the form $e^{-2\pi\nu}$ and higher orders in $1/\nu^2$. We see from (32) that at low energies the shape and continuum normalization corrections are of the same magnitude as the bound-state normalization contribution so that screening effects are more than twice that predicted by normalization screening theory. This expression (32) can also be used for photon energies below the point Coulomb threshold ($\nu^2<0$) provided the proper analytic continuation of σ_{10}^c is employed.[16]

In a relativistic calculation including spin, the L shell comprises three subshells L_{I}, L_{II}, and L_{III}. In an entirely nonrelativistic calculation, however, only the $L_{\text{I}}(2S)$ and $L_{\text{II}}+L_{\text{III}}(2P)$ subshells are distinguished. For the $2S$ subshell, as for the $1S$, only one matrix element contributes. From Eq. (6),

$$\sigma_{20}=(2\pi)^2\alpha\omega\tfrac{2}{3}(4\pi)^2|\langle k,1|r|2,0\rangle|^2, \qquad (33)$$

where

$$|\langle k,1|r|2,0\rangle|^2=|\langle k_c,1|r|2,0\rangle_c|^2\chi_{20}^{+}(\nu). \qquad (34)$$

In Eq. (34),

$$|\langle k_c,1|r|2,0\rangle_c|^2=\left(\frac{2}{\pi\omega}\right)^2\frac{1+\nu^2}{(1+\frac{1}{4}\nu^2)^4}\left(\frac{\nu^2}{2}\right)^3\frac{e^{-4\nu\tan^{-1}2/\nu}}{1-e^{-2\pi\nu}} \qquad (35)$$

is the point Coulomb result and $\chi_{20}^{+}(\nu)$ is given by

$$\chi_{20}^{+}=\left(\frac{N_{20}}{N_{20}^{c}}\right)^{2}\left\{1+\Lambda_{2}\left(Q_{20}^{+}(3\nu^{2}+14)-\frac{4\nu^{2}}{1+\frac{1}{4}\nu^{2}}(7+\nu^{2})+3\nu^{2}\right)\right.$$
$$\left.-\Lambda_{3}\left[Q_{20}^{+}[5\nu^{2}(1+\nu^{2})-84]+\frac{2\nu^{2}}{(1+\frac{1}{4}\nu^{2})^{2}}\left(56+\frac{40}{3}\nu^{2}-\frac{11}{2}\nu^{4}-\frac{5}{6}\nu^{6}\right)+5\nu^{4}\right]\right\}, \quad (36)$$

where

$$Q_{20}^{+}=\nu^{2}\left(\frac{3+4\nu^{2}}{1+\nu^{2}}-2\nu\tan^{-1}\frac{2}{\nu}-\frac{\pi\nu}{e^{2\pi\nu}-1}\right). \quad (37)$$

For the L shell, $k_c=(2\omega-\frac{1}{4}a^2)^{1/2}$. Again, we have factored out the bound-state normalization screening corrections $(N_{20}/N_{20}^c)^2$. For sufficiently high Z, this ratio can be taken from the results of our perturbation theory, Eq. (10). For low Z, however, this ratio is quite far from unity and the series in λ for N_{20}/N_{20}^c does not converge rapidly, even though the remainder of the screening corrections, which include all of the energy dependence, are well represented by the term in curly brackets in (36). In this case, then, one may insert[17] a numerical evaluation of the (energy-independent) ratio of screened to point Coulomb bound-state normalizations in Eq. (36).

At high energy the screened cross section (33) approaches the limit expected from normalization screening theory

$$\sigma_{20}=\sigma_{20}^{c}(N_{20}/N_{20}^{c})^{2}[1+O(\nu^{2}\Lambda_{2})]. \quad (38)$$

For very low energy ($\nu\gg1$), neglecting higher orders in $1/\nu^2$,

$$\sigma_{20}=\sigma_{20}^{c}\left(\frac{N_{20}}{N_{20}^{c}}\right)^{2}\left[1-\Lambda_{2}\left(\frac{341}{15}-\frac{4673}{35}\frac{1}{\nu^{2}}+\frac{1825}{3}\frac{1}{\nu^{4}}\right)-\Lambda_{3}\left(\frac{6500}{21}-\frac{830\,812}{315}\frac{1}{\nu^{2}}+\frac{151\,788}{99}\frac{1}{\nu^{4}}\right)\right]. \quad (39)$$

In this region the shape and continuum normalization screening corrections are about half the bound-state normalization corrections. Thus, for low Z especially, the screening corrections will be large at low energy and our $L_{\rm I}$ perturbation series does not converge rapidly. For nearly all Z, however, at photon energies on the order of the Coulomb L-shell binding energy above threshold and higher, the corrections due to screening for the 2S case are very well represented by an analytic expression (36).

For the 2P subshell we have from Eq. (6),

$$\sigma_{21}=(2\pi)^{2}\alpha\omega\tfrac{2}{3}(4\pi)^{2}[2\,|\langle k,2|r|2,1\rangle|^{2}+|\langle k,0|r|2,1\rangle|^{2}], \quad (40)$$

where

$$|\langle k,1\pm1|r|2,1\rangle|^{2}=|\langle k_c,1\pm1|r|2,1\rangle_c|^{2}\chi_{21}^{\pm}(\nu). \quad (41)$$

In Eq. (41),

$$|\langle k_c,l'|r|2,1\rangle_c|^{2}=\frac{1}{3}\left(\frac{2}{\pi\omega}\right)^{2}\frac{(\frac{1}{2}\nu^{2})^{4}e^{-4\nu\tan^{-1}2/\nu}}{(1+\frac{1}{4}\nu^{2})^{5}(1-e^{-2\pi\nu})}\times\begin{cases}2(1+\nu^{2}) & \text{for } l'=2\\ \frac{1}{8}(4+\nu^{2}) & \text{for } l'=0\end{cases} \quad (42)$$

are the point Coulomb results and the $\chi_{21}^{\pm}(\nu)$ are given by

$$\chi_{21}^{+}(\nu)=\left(\frac{N_{21}}{N_{21}^{c}}\right)^{2}\left[1+\Lambda_{2}\left(Q_{21}^{+}(3\nu^{2}+16)-\frac{2\nu^{2}}{1+\frac{1}{4}\nu^{2}}(5\nu^{2}+28)+15\nu^{2}\right)\right.$$
$$\left.-\Lambda_{3}\left(Q_{21}^{+}[\nu^{2}(5\nu^{2}+17)-60]-\frac{1}{6}\frac{\nu^{2}}{(1+\frac{1}{4}\nu^{2})^{2}}(25\nu^{6}+210\nu^{4}+200\nu^{2}-432)+25\nu^{4}\right)\right] \quad (43a)$$

and

$$\chi_{21}^{-}(\nu)=\left(\frac{N_{21}}{N_{21}^{c}}\right)^{2}\left[1+\Lambda_{2}\left(Q_{21}^{-}(3\nu^{2}+10)-\frac{1}{2}\frac{\nu^{2}}{1+\frac{1}{4}\nu^{2}}(8\nu^{2}+40)\right)\right.$$
$$\left.-\Lambda_{3}\left(Q_{21}^{-}[\nu^{2}(5\nu^{2}-1)-60]-\frac{1}{3}\frac{\nu^{2}}{(1+\frac{1}{4}\nu^{2})^{2}}(5\nu^{2}+27\nu^{4}-128\nu^{2}-432)\right)\right], \quad (43b)$$

where

$$Q_{21}^{+} = \nu^2\left(\frac{16+23\nu^2+4\nu^4}{(4+\nu^2)(1+\nu^2)} - 2\nu\tan^{-1}\frac{2}{\nu} - \frac{\pi\nu}{e^{2\pi\nu}-1}\right) \tag{44a}$$

and

$$Q_{21}^{-} = \nu^2\left(4 - 2\nu\tan^{-1}\frac{2}{\nu} - \frac{\pi\nu}{e^{2\pi\nu}-1}\right). \tag{44b}$$

Essentially the same considerations hold for the $2P$ case as for the $2S$ cross section. A major part of the screening corrections are due to the change in the bound state normalization. For all but very high Z this must be evaluated numerically. The energy dependence, however, is given by the wave-function shape and continuum normalization contributions which are well represented, for almost all energies, by our expressions[18] for $\chi_{21}^{\pm}(\nu)$, Eqs. (43). At high energy we reproduce the result of normalization screening theory

$$\sigma_{21} = \sigma_{21}^{c}(N_{21}/N_{21}^{c})^2[1+O(\nu^2\Lambda_2)], \tag{45}$$

where σ_{21}^{c} is the point Coulomb cross section of shifted energy. At low energy ($\nu \gg 1$), neglecting higher-order terms in $1/\nu^2$, the $2P$ cross section can be written in the form

$$\sigma_{21} = \sigma_{21}^{c}\left(\frac{N_{21}}{N_{21}^{c}}\right)^2\left[1 - \frac{16}{55}\Lambda_2\left(47 - \frac{86\,644}{231}\frac{1}{\nu^2} + \frac{4\,671\,664}{2541}\frac{1}{\nu^4}\right) - \frac{128}{1155}\Lambda_3\left(817 - \frac{516\,932}{33}\frac{1}{\nu^2} + \frac{38\,650\,544}{363}\frac{1}{\nu^4}\right)\right]. \tag{46}$$

Again, in this region the shape and continuum normalization corrections are about half the bound-state normalization contribution. Thus, particularly for low Z, the screening corrections will be large at low energy and our perturbation series does not converge rapidly. On the other hand, for photon energies on the order of the L-shell Coulomb binding energy above threshold and higher, our analytic expressions for $\chi_{21}^{\pm}(\nu)$, Eq. (44), give results in good agreement with exact numerical values.

III. DISCUSSION OF RESULTS

In Tables II–IV we compare our analytic predictions for screened K, $L_{\rm I}$, and $L_{\rm II}+L_{\rm III}$ nonrelativistic dipole photoeffect total cross sections with the results of exact numerical evaluations of these cross sections in the same (screened) potential. We also compare the nonrelativistic results with the full relativistic screened calculations of Scofield.[9] Three elements Ca($Z=20$), Kr($Z=36$), and Au($Z=79$), are considered which show typical results for low, medium, and high Z.

The screened potential which we have employed in this work is the Herman-Skillman self-consistent potential.[8] In Ref. 1 we have indicated how to obtain the coefficients V_k which appear in our expansion of the potential [Eq. (1)] and have also given some typical values of these potential coefficients for neutral atoms in the range $Z=6-92$.

The best results for the screened cross section are obtained for the K shell [cf. Table II]. This is due to the fact that, for the ground state, all of the wave function is included in the region in which our expansion of the potential is valid. Hence, in this case the wave function is particularly well represented by our perturbation series. We see that even for relatively low Z at low energy, our analytic expression for the K-shell photoeffect total cross section reproduces the numerical results to better than 1%. Even better agreement could be obtained if the numerical screened bound-state normalization were used. When we

TABLE II. Comparison of our analytic results for the K shell $\sigma_{\rm an}$, with exact numerical values of the K-shell nonrelativistic dipole cross section $\sigma_{\rm num}$, and with the full relativistic results of Scofield $\sigma_{\rm rel}$. T_B is the Herman-Skillman ground-state binding energy, $T_c=\frac{1}{2}a^2$ being the corresponding point Coulomb energy. All energies are in keV. Cross sections are in barns.

Z	ω	$\sigma_{\rm an}$	$\sigma_{\rm num}$	$\sigma_{\rm rel}$
20 ($T_B=3.99$)	6	2.223(4)	2.217	2.218
($T_c=5.44$)	10	5.526(3)	5.544	5.560
	20	7.511(2)	7.544	7.583
	40	9.252(1)	9.293	9.396
	60	2.619(1)	2.631	2.681
	80	1.055(0)	1.059	1.091
36 ($T_B=14.0$)	15	1.416(4)	1.394	1.383
($T_c=17.6$)	20	6.633(3)	6.571	6.609
	40	9.709(2)	9.667	9.793
	60	2.987(2)	2.979	3.044
	80	1.269(2)	1.266	1.306
	100	6.459(1)	6.448	6.728
	200	7.543(0)	7.538	8.501
79 ($T_B=73.4$)	80	2.317(3)	2.294	...
($T_c=84.9$)	90	1.695(3)	1.680	...
	100	1.277(3)	1.267	1.273
	120	7.771(2)	7.719	...
	150	4.178(2)	4.155	4.416
	200	1.843(2)	1.835	2.057

TABLE III. Comparison of our analytic results for the L_I subshell σ_{an}, with exact numerical values σ_{num}, and with the full relativistic results σ_{rel}. T_B is the exact screened 2S binding energy and $T_c = \frac{1}{8}a^2$ is the point Coulomb binding energy. Energies are in keV and cross sections are in barns.

Z	ω	σ_{an}	σ_{num}	σ_{rel}
20 (T_B=0.430)	2	2.102(4)	1.913	1.922
(T_c=1.36)	3	7.983(3)	7.844	7.898
	4	4.003(3)	4.012	4.044
	6	1.463(3)	1.484	1.498
	10	3.861(2)	3.919	3.963
	20	5.630(1)	5.697	5.781
	40	7.290(0)	7.332	7.513
	60	2.106(0)	···	2.185
36 (T_B=1.84)	5	1.300(4)	1.248	1.260
(T_c=4.41)	8	4.618(3)	4.577	4.663
	10	2.768(3)	2.758	2.819
	20	5.104(2)	5.105	5.270
	40	8.108(1)	8.118	8.467
	60	2.597(1)	2.603	2.739
	80	1.130(1)	1.133	1.204
	100	5.846(0)	5.856	6.307
79 (T_B=12.3)	25	2.845(3)	2.813	···
(T_c=21.2)	30	1.925(3)	1.910	1.993
	40	1.016(3)	1.011	1.084
	60	3.931(2)	3.920	4.363
	80	1.939(2)	1.935	2.212
	100	1.101(2)	1.099	1.286

TABLE IV. Comparison of results for the 2P case. σ_{an} is our analytic result, σ_{num} is the corresponding numerical value for the 2P nonrelativistic dipole cross section, and σ_{rel} is the result of Scofield. T_B is the 2P binding energy determined from the Herman-Skillman potential and $T_c = \frac{1}{8}a^2$. Energies are in keV and cross sections are in barns.

Z	ω	σ_{an}	σ_{num}	σ_{rel}
20 (T_B=0.356)	2	2.573(4)	2.777	2.813
(T_c=1.36)	5	1.305(3)	1.387	1.424
	10	1.144(2)	1.184	1.241
	15	2.551(1)	2.625	2.802
	20	8.536(0)	8.741	9.528
	30	1.757(0)	1.794	2.029
	40	5.587(−1)	5.603	6.682
36 (T_B=1.68)	5	2.641(4)	2.662	2.766
(T_c=4.41)	8	6.061(3)	6.136	6.488
	10	2.942(3)	2.970	3.173
	15	7.567(2)	7.604	8.313
	20	2.790(2)	2.799	3.126
	30	6.527(1)	6.544	7.617
	40	2.258(1)	2.265	2.742
	60	4.857(0)	4.887	6.377
	80	1.591(0)	1.601	2.253
79 (T_B=11.8)	25	6.251(3)	6.233	···
(T_c=21.2)	30	3.546(3)	3.537	4.545
	40	1.415(3)	1.410	1.929
	50	6.805(2)	6.787	9.793
	60	3.695(2)	3.684	5.590
	80	1.378(2)	1.374	2.287
	100	6.294(1)	6.276	11.39

compare our nonrelativistic dipole results with the full relativistic calculations for the K shell, we see that the agreement is also very good (within a few percent) for photon energies up to nearly 100 keV. This is well beyond the expected range of validity of the nonrelativistic dipole approximation. Since one can show that relativistic or multipole effects separately become important above 10 keV, these results imply an effective cancellation between relativistic and higher multipole contributions in the total cross section from S states.[19]

For the L shell, using bound-state normalizations obtained numerically, the agreement between our analytic results and exact numerical evaluations of the screened dipole cross section is very good [cf. Tables III and IV]. At intermediate and high energies, for all Z, the analytic expression is within 1% of the numerical calculation. It is only at very low photon energies, for low Z, particularly in the 2P case, that differences between analytic and numerical results become significant. This is due to the fact that the principal contribution to the dipole matrix element in this case comes from a part of configuration space nearer the edge of the atom. In this region our expansion of the potential [Eq. (1)] is not converging rapidly and our perturbation scheme breaks down. When we compare the nonrelativistic dipole results with the full relativistic calculation, we see that for the L_I cross section there is good agreement up to photon energies approaching 60 keV. Although this range is not as great as for the K shell, it is still well beyond the expected range of validity of the dipole approximation. For the 2P cross section however, there is agreement between the nonrelativistic dipole and full relativistic results only for photon energies below 10 keV. Thus, for non-S states there does not appear any cancellation between higher order relativistic and multipole contributions in the total cross section.

We conclude that our analytic perturbation theory can be used to accurately predict screened nonrelativistic dipole K- and L- shell photoeffect total cross sections over a wide range of atomic numbers and photon energies. Hence, it should also be useful for other processes in which the major contribution to the matrix element comes from the region of configuration space within the interior of the atom. Moreover, due to cancellation between relativistic and multipole corrections in total cross sections for S states, our results also reproduce the full relativistic screened results of Scofield in these cases for energies ranging up to 100 keV.

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[10]We have also used the derivative form of the dipole matrix element to check our results. The expressions obtained were the same in each case.

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[15]Since our screened wave functions are finite in the limit $\nu \to \infty$ (see Ref. 2), we may expect that σ_{nl} is also finite in this limit. This result, however, provides a convenient check on our expression for the screening corrections.

[16]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin and Academic, New York, 1957).

[17]In our comparisons with numerical results for the L shell (Sec. III), we use bound-state normalizations obtained numerically.

[18]These expressions for $\chi_{21}^{\pm}$ can also be used to determine screening corrections to the ratio of cross sections from different bound electron magnetic substates. See, for example, Sung Dahm Oh and R. H. Pratt, Phys. Rev. A 10, 1198 (1974). Also, screening effects on shell ratios can be predicted using our results for $\chi_{nl}^{\pm}$ [cf. R. H. Pratt, Akiva Ron, and H. K. Tseng, Rev. Mod. Phys. 45, 273 (1973)].

[19]This cancellation, which is not observed in the differential cross section, has been noted previously in the point Coulomb case by Akiva Ron [University of Pittsburgh preprint No. 6985207-17 (1972) (unpublished)]. In addition, V. Florescu (private communication) has been able to account quantitatively for the agreement of the nonrelativistic dipole and full relativistic total cross sections at threshold in the point Coulomb case and it has been conjectured that cancellation may occur generally for S states in any first-order QED process. A complete explanation of this phenomenon, however has not yet been given.