High-energy atomic photoelectric effect and bremsstrahlung

R. Y. Yin,* O. V. Gabriel,† and R. H. Pratt
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
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The relativistic photoionization cross sections from $ns_{1/2}, np_{1/2}, np_{3/2}$ subshells, in the high-energy limit, have been analytically obtained. The main effects of screening enter through their effects on bound-state normalizations and energy levels. To estimate further effects, the screened potential at small distances is analytically described by a power-series expansion in the small distance r. For this high-energy-limit situation, both bound and continuum wave functions are expanded in power series for small r. The bound-free transition cross sections are then calculated analytically. Our results show that, beyond the known screening effect described by normalization factors, the screening effect enters the cross sections primarily through the change in bound-state energy and is otherwise not too sensitive to the expansion coefficients of the potential. The formulas contain no explicit n dependence. Comparisons with existing finite-energy numerical results indicate that ratios, though not absolute values, of cross sections attain their high-energy limits relatively early. Using Poincaré's theorem, all the photoionization results may be analytically continued to the high-frequency region of the spectrum of electron bremsstrahlung. Screening is dominated by the "extra" screening (namely, the screening which is not described by the known "normalization screening") except in the very tip region (a few eV above threshold), where normalization screening is much more important. The extension to positron bremsstrahlung is also discussed.

I. INTRODUCTION

In this paper we present analytic relativistic expressions for screened atomic photoeffect cross sections in the high-energy limit, for the ns and np subshells of all elements. The same expressions also characterize the high-frequency (hard-photon end point) region of the bremsstrahlung spectrum in the high-energy limit of incident electron (or positron) energy. Preliminary results of this approach for the ns and $2p$ cases have been reported by Gabriel.[1] Analytic results for the high-energy limit are desirable, since they give some physical insight into the diverse aspects of the photoelectric process and they complement numerical predictions which are available for finite photon energy. Furthermore, such high-energy predictions become of greater practical interest with the extension of current experiments to higher energies[2] and developments in the theoretical calculation of radiative corrections.[3]

Analytic results for photoelectric effect in the high-energy limit have been obtained previously,[4,5] but without taking into account atomic electron screening of the nuclear charge, i.e., the atomic electron ejected as a photoelectron was described both in the initial and final state as moving in a point Coulomb potential. Later Pratt and Tseng[6] identified the screening effect on high-energy inner-shell photoeffect cross sections as primarily associated with the screened bound-state normalization constants. Many features of the photoeffect process can be understood with the realization that for energies sufficiently far above threshold, the important regions in configuration space for the determination of the matrix element are small, ultimately (in a full relativistic multipole theory) of the order of an electron Compton wavelength ($r \sim 1$ in the system of units adopted here) and not where the bound-electron wave function is large except for the K shell of very-high-Z elements).

In the nonrelativistic dipole case this dominant region would continue to contract toward the origin with increasing energies. Now, at small distances, the screened potential has a point Coulomb character, and the inner-shell wave functions are hydrogenic in shape and differ from point Coulomb wave functions only in their normalization. Consequently we can get approximate predictions for the total photoelectric cross sections in a screened potential simply by multiplying the point Coulomb results by the square of the ratio of screened to point Coulomb bound-state normalizations. This also implies that at high energy the angular distribution shapes and polarization correlations are independent of screening. Further, because small-distance wave-function shapes are independent of principal quantum number n, one predicts for the same reason that results for different subshells of the same angular momentum are similarly related: Angular distribution shapes and correlations are independent of principal quantum member n, cross sections are dependent on n only through bound-state normalization.[4]

However, as we shall demonstrate, additional screening effects do persist in the high energy limit for the relativistic case, reflecting the fact that the dominant region does not continue to contract and even at electron Compton wavelength distances there are deviations from the point Coulomb shape. It is possible to calculate these additional relativistic screening effects by combining the formalism developed for the point Coulomb high-energy-limit cross sections[4] (requiring a modified plane wave, i.e., a three-dimensional eikonal wave function for the continuum state) with an analytic description of the screened bound and continuum wave functions. More precisely speaking, other than normalization, the dominant screening effects

on the shape of the bound wave function at small distances can be described by its "energy shift" (from the point Coulomb energy), consistent with the previous finding of Oh in a nonrelativistic calculation.[7] The remaining screening effects on the bound state and the screening effects on the continuum state can be estimated by using an analytic perturbation theory, which we call briefly APT, developed for the analytic description of screening effects on atomic processes characterized by distances well in the interior of the atom.[8] The theory expands a screened wave function of specified energy, at small distances, with reference to a Coulomb wave function of (perhaps different) specified energy. Here we extend this approach, determining analytic screening corrections in the eikonal factor of the modified plane wave, characterizing the high energy limit of a continuum state of definite momentum. More precisely, we determine screening modifications to the difference of two such eikonal factors. (In the high energy limit only the phase, not the amplitude, is modified at finite—Compton wavelength—distance.)

High-energy-limit results for photoeffect subshell cross sections for given (n,l,j) can be expressed in terms of a double expansion in $a \equiv \alpha Z$, with Z the atomic number and α the fine-structure constant, screened binding energies (which can be calculated numerically, for inner shells from APT, by WKB methods, etc.), and screening parameters Λ_1, Λ_2, characterizing the relativistic screened atomic potential at Compton wavelength distances. We neglect terms of relative order a^4 and higher and we retain only the leading term in k^{-1}, where k is the energy of the incident photon. It is known that APT gives a poorer description of screening in low-Z elements. But since screening becomes less important at high energy in low-Z elements (unlike in low-energy photoeffect), adequate results can still be obtained in all cases and the main analytic approximation, as already indicated, is that Coulomb terms have not been calculated to all orders.

The results for photoionization can also be extended, by analytic continuation, to give predictions for the high-frequency region of the bremsstrahlung spectrum in the high-energy limit of incident electron (or positron) kinetic energy. In this situation the high-energy incident electron loses almost all of its kinetic energy and the wave function of the low-energy outgoing electron at small distances has the same shape as for a bound state. As exploited by Fano, Koch, and Motz,[9] this process is an analytic continuation of inverse atomic photoelectric effect, i.e., of direct radiative recombination. Following the analysis and procedures previously given by Pratt[10] and Jabbur and Pratt,[11] we can obtain the analytic formulas for high-energy tip-region electron and positron bremsstrahlung from our work, providing an extension of their results from the Coulombic to the screened case.

We outline the general assumptions and formalism which underlie our calculations in Sec. II. The expressions for ns and np subshell photoelectric cross sections, as well as a discussion of these results, are presented in Sec. III. Corresponding results for the high-frequency region of the bremsstrahlung spectrum of high-energy electrons and positrons are given in Sec. IV.

II. GENERAL FORMALISM

The formalism used in this work was developed by Pratt[4,5] and has been subsequently extended by Jabbur and Pratt[11] in their study of the high-frequency region of the bremsstrahlung spectrum.

A. Assumptions leading to the single-electron transition matrix element

The following assumptions discussed in the review article of Pratt *et al.*[6] will be adopted in this work.

(1) The target is a single isolated neutral atom in its ground state.

(2) Bound and continuum electrons in the field of the target atom can be described as solutions of the Dirac equation for a single electron interacting with a central potential which is Coulombic at small distances.

(3) The photoelectric process can be treated as a first-order radiation field interaction transition of a single electron between bound and continuum states in the same central potential.

These assumptions imply the neglect of extended structure in the target, molecular, and solid-state effects, temperature and pressure effects, electronic correlations, nonlocal exchange, higher-order quantum electrodynamic effects, etc. The photoeffect matrix element deduced from first-order relativistic external field quantum electrodynamics is given by

$$M = -(2\pi\alpha/k)^{1/2} \int \psi_p^* \boldsymbol{\alpha}\cdot\mathbf{e} e^{i\mathbf{k}\cdot\mathbf{r}} \psi_b d^3r \ , \tag{1}$$

where $\mathbf{k}$ is the photon momentum. $\mathbf{p}$ is the momentum of the ejected electron, α are the Dirac matrices, and $\mathbf{e}$ is the photon polarization vector.[4] ψ_p and ψ_b are solutions (continuum and bound wave functions) of the Dirac equation:

$$[-i\boldsymbol{\alpha}\cdot\nabla + \beta + V(r)]\psi_{\kappa m} = \varepsilon\psi_{\kappa m} \ , \tag{2}$$

where $V(r)$ is the potential. Natural units ($\hbar = c = m_c = 1$) are used throughout this chapter. This single-particle matrix element is used to find the differential cross section

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

where $W = (P^2+1)^{1/2} - k - \varepsilon$ is the energy transfer and ε is the energy of the bound electron (which includes rest mass energy). Integration over final electron energy, with the δ-function of energy conservation, leads to the differential cross section for the photoelectron angular distribution.

It has been argued by Pratt[4] that in the high-energy limit the matrix element (1) is decided at electron Compton wavelength distances. The argument can be briefly summarized as follows: The integrand in (1) contains the factor $\exp[-i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}]$, where $\mid \mathbf{p}-\mathbf{k} \mid \simeq \mid \mathbf{p} \mid - \mid \mathbf{k} \mid \to 1$ for most transitions, as $\varepsilon \to \infty$, from energy conservation. This means important contributions to the integral occur when r is of the order of 1 (in the unit of electron Compton wavelength), since for larger distances the integrand oscillates rapidly. This fact underlies the present work.

B. Assumptions leading to the high-energy-limit matrix element expressed in terms of integrals over eikonal wave functions

For ψ_b, relativistic APT bound-state wave functions[8] are already available, although we give a more direct calculation of the needed small-distance behavior in Sec. II C. The central difficulty in relativistic photoeffect calculations arise from ψ_p. The full continuum solutions of the Dirac equation in a potential (even a point Coulomb potential) have been available only in a partial-wave expansion, and at high energies an increasingly large number of terms in this expansion contribute to the matrix element. Consequently, even by the MeV range, a direct calculation of the cross section becomes an arduous task. For the high-energy limit of photoeffect, use of an approximate continuum wave function was justified by Pratt.[4] This distorted plane wave is a solution of the three-dimensional eikonal equation (obtained from the Sommerfeld-Maue equation by dropping the ∇^2 term),

$$(i\mathbf{p}\cdot\nabla-\varepsilon_p V)\psi_p=0 \ , \tag{4}$$

where ε_p is the energy of the ejected electron. Specifying the boundary conditions appropriate for the outgoing photoelectron, the desired solution is

$$\psi_p=ue^{i(\mathbf{p}\cdot\mathbf{r}+\chi_-)} \ , \tag{5}$$

where u is the field-free electron spinor and the distortion function χ is given by

$$\chi_\pm(\mathbf{r})=\chi_\pm(\rho,z)=+\int_{-\infty}^{-z} V(\rho,z')dz' \ , \tag{6}$$

where χ_- is the solution needed for the photoeffect and χ_+ is the solution needed for the inverse photoeffect. These solutions χ_+ and χ_- are chosen to satisfy the boundary condition for a plane wave (at $\pm\infty$) with outgoing or incoming spherical waves, respectively. In Eq. (6), V is taken as the same screened central potential seen by the initial bound electron. (If the potential has a long-range Coulombic tail, the χ's must be modified to include logarithmic phase factors, but these changes will not contribute to the *difference* in χ's needed for this paper.)

Note that a smoothed representation of the interior region of the potential V, involving an expansion for small r, does not suffice to evaluate the distortion function χ. This can be seen clearly from the nonrelativistic expression given by Bechler and Pratt,[12] which remains valid in this relativistic case since relativity does not enter in the integral (6). Rewritten in our notation, their result is

$$\begin{aligned}\chi=&-a[\ln\lambda(r-z)-b_0]+a^2\Lambda_1 z\\&+a^3(\Lambda_3/2)[rz-\rho^2\ln\lambda(r-z)]\\&+a(\lambda\rho)^3 b_1+a^4\Lambda_3(\rho^2 z+z^3/3) \ ,\end{aligned} \tag{7}$$

where λ is defined by $1.13\alpha Z^{1/3}$, and $\Lambda_1,\Lambda_2,\Lambda_3$ are potential expansion coefficients used in APT (we will discuss APT in detail in Sec. II C). The coefficients b_0,b_1, given by their Eq. (3.27), cannot be found in terms of the small-distance expansion of the potential. In order to get these coefficients, one needs also to know the shape of the potential at intermediate and larger distances. Nevertheless, as far as the difference $[\chi(\mathbf{r}')-\chi(\mathbf{r})]$ is concerned, which we will see below is the only quantity needed in determining the total cross section, these b coefficients do not play any role; the knowledge of small-distance properties of the potential permits a full evaluation.

Substituting Eq. (5) into the matrix element Eq. (1), we have

$$M=-(2\pi\alpha/k)^{1/2}\int d^3r\, S(\mathbf{r})e^{-i[(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}+\chi(\mathbf{r})]} \ , \tag{8}$$

where $S(\mathbf{r})=u^\dagger\boldsymbol{\alpha}\cdot\mathbf{e}\psi_b$ and $\chi(\mathbf{r})$ is $\chi_-(\mathbf{r})$ defined in (6). It has been shown[4,10] that when there is almost complete transfer of momentum between a photon and a bound electron, as is true in the dominant circumstances of high-energy photoeffect, the cross section, integrated over all states of the outgoing high-energy particles, is just

$$\sigma=(4\pi^2\alpha/k)I \ , \tag{9}$$

where I is the triple integral

$$I=\int dz\int dz'\int\rho\, d\rho\, F(\mathbf{r},\mathbf{r}')e^{ig(\mathbf{r},\mathbf{r}')} \ , \tag{10}$$

$$F(\mathbf{r},\mathbf{r}')=\tfrac{1}{2}\sum_{\substack{\text{final spin}\\ \text{states}}}\psi_b^\dagger(\mathbf{r})(1-\alpha)\psi_b(\mathbf{r}') \ , \tag{11}$$

$$g(\mathbf{r},\mathbf{r}')=\varepsilon(z-z')+\chi(\mathbf{r})-\chi(\mathbf{r}') \ . \tag{12}$$

Here we use a cylindrical coordinate system with z axis along the incident photon momentum direction; ρ' is set equal to ρ. Thus (remembering that ε is the bound-state energy), we only need to determine the change in the distortion function of the three-dimensional eikonal wave function due to a shift in z coordinates $[\chi(\rho,z)-\chi(\rho,z')]$ in order to calculate the total cross section. It can be shown that F and g are functions of ρ, z, and z' only. A general expression for F is given in Ref. 11.

The main problem, then, is the evaluation of the triple integral I. The approach that we will adopt develops the integral as a power series in a. In order to accomplish this task we need small-distance expansions for the initial and final electron wave functions ψ_b and ψ_p. We will keep terms that contribute to the matrix element through relative order of a^3 (in all the $ns_{1/2}$, $np_{1/2}$, and $np_{3/2}$ cases) and drop all higher-order terms.

C. Small-distance behavior of wave functions

1. *Description of screening by shifted energy, with APT as supplement*

As we will demonstrate quantitatively below, the main screening effect on wave-function shapes at small distances can be described by using a Coulomb wave function of "shifted energy" (shifted from the point Coulomb energy value). Remaining screening effects, and also screening effects on continuum wave functions, can be estimated using APT.

The shifted energy ε' is defined as

$$\varepsilon'\equiv\varepsilon+\delta \ , \tag{13}$$

where ε is the eigenvalue of the Dirac equation, for a screened potential, and the factor δ is defined as the

difference between the potential energy of a test electron charge, in the vicinity of nucleus, with and without the screening of bound electrons:

$$\delta \equiv [V_{\text{Coul}} - V_{\text{screened}}]_{r \to 0} . \tag{14}$$

Replacing the screened eigenvalue ε by this shifted energy, according to Eq. (13), and expanding the screened Dirac equation at small distances, we find the leading coefficients of the wave functions, as function of this shifted energy, are exactly the same as for the point Coulomb wave functions, as function of point Coulomb eigenvalues. (Here, by "leading coefficients," we mean the first two or three coefficients in the small-distance expansion of wave functions.) This says that the wave function's shape at small distances can be characterized primarily by the shifted energy. Since the screened energy ε can be numerically calculated and δ can be fairly well determined, this shifted energy provides an effective way to describe screening at Compton wavelength distances. Nevertheless, further screening effects still exist in coefficients of higher-order terms in the small-distance wave-function expansion, which cannot be described by this shifted energy. We use APT to provide an estimate of these remaining screening effects.

The method of APT is based on a smoothed description of the potential inside an atom, as a function of one parameter λ, having the form

$$V(r) = -\frac{a}{r}[1 + V_1(\lambda r) + V_2(\lambda r)^2 + V_3(\lambda r)^3 + \cdots] . \tag{15a}$$

Here $\lambda = 1.13\alpha Z^{1/3}$ is a parameter characterizing the screening, in the sense that λ^{-1} determines the range of the short-distance screened potential V and can be used to characterize the dimensions of the neutral atom. The value of λ^{-1}, which evidently depends on Z, is a few tens of electron Compton wavelengths. The V_n coefficients, which characterize the screening due to the atomic electrons, can be found for either analytic potentials (say, the Yukawa potential) or fitted for numerical potentials (e.g., Hartree-Slater potential). Generally, the appropriate choice of V_n does depend on the region of distances of interest. Here the important region corresponds to electron Compton wavelength distances, while for low-energy photoeffect, the V_n should be taken to characterize the entire interior of the atom,[8] particularly the dominant regions for inner shells.

Although APT is quite successful in the analytic description of screened potentials, wave functions, eigenvalues.[8] etc., it is less useful in discussing screening effects in high-energy-limit photoionization and bremsstrahlung. Screening effects on the potential at Compton wavelength distances are not well characterized by a polynomial expansion. Electron wave functions behave as $r^{\gamma-1}$ at such distances, where $\gamma = (\kappa^2 - a^2)^{1/2}$ is not integer. The resulting behavior of the charge density implies similar features in the potential. V_1 is well determined, but not higher V coefficients. To overcome this difficulty, we adopt the following two measures: (i) We use the shifted energy ε', as discussed above, to primarily characterize the screened wave functions, and (ii) we use APT, reduced to a quadratic potential fit, to provide an estimate of the magnitude of residual screening effects.

Given our concern here for Compton wavelength distances, it is more transparent if we interpret the expansion (15a) as an expansion in terms of the quantity (ar). Defining $\Lambda_n \equiv V_n \lambda^n / a^n$, the expansion of the potential can be rewritten, from (15a), as

$$V(r) = -\frac{a}{r}(1 + \Lambda_1 ar + \Lambda_2 a^2 r^2 + \Lambda_3 a^3 r^3 + \cdots) . \tag{15b}$$

(The Λ_n, however, are Z dependent while the V_n were essentially Z independent.) With the V_n coefficients of unity and $\lambda/a = 1.13/Z^{2/3} < 1$, the Λ_n are generally small. When we calculate the transition cross sections, we will expand in a and keep all terms through relative order a^3. It turns out [see Table I and Eqs. (29) and (30)] that the Λ_3 and higher Λ_n coefficients do not occur in the cross sections through this order in a.

Finally, from Eqs. (14) and (15b), it is immediately obvious that in Eq. (14) $\delta = \Lambda_1 a^2$. This identity enables us to use the knowledge of Λ_1, provided by APT, to determine δ and therefore the shifted energy ε'.

TABLE I. Expansion coefficients for the bound wave functions.

	$ns_{1/2}$	$np_{1/2}$	$np_{3/2}$
A_0	1	$a^2(1+a^2/4)/2$	1
A_1	$-(1+a^2 5/12)+a^2 u 5/12$	$2[1-a^2(\frac{1}{6}+u/4)]/3$	$-[1+9a^2(\frac{1}{4}-u)/20]/2$
A_2	$\frac{1}{3}+u/6$	$-[1+a^2(\frac{1}{3}-3\Lambda_2/4-u)]/3$	$(1+u)/10$
A_3	$-(1+3\Lambda_2)/18-u/9$	$(1+u)/15$	$-(1+10\Lambda_2+7u/2)/90$
A_4		$-(1+10\Lambda_2+7u/2)/135$	
B_0	$-\frac{1}{2}-a^2/8$	1	$-(1+a^2/16)/4$
B_1	A_2	$-2[1+a^2(\frac{1}{3}-5u/8)]/3$	A_2
B_2	$3A_3/2$	$5A_3/2$	$3A_3/2$
B_3		$3A_4$	

2. *Bound wave-function shapes at small distance*

Bound-state wave functions can be written in the form

$$\phi_{\varepsilon\kappa m}(\mathbf{r})=\frac{1}{r}\begin{bmatrix} if_{\varepsilon\kappa}(r) & \Omega_{\kappa m}(r) \\ -g_{\varepsilon\kappa}(r) & \Omega_{-\kappa m}(r)\end{bmatrix}, \tag{16}$$

where the angular functions $\Omega_{\kappa m}$ are simultaneous eigenfunctions of J^2, L^2, and J_z, and κ is defined by

$$(1+\sigma L)\Omega_{\kappa m}=\kappa\Omega_{\kappa m}\ , \tag{17}$$

so that

$$\kappa=\pm(j+\tfrac{1}{2})=\begin{cases}-(l+1), & \text{when } j=l+\tfrac{1}{2}\ , \\ l, & \text{when } j=l-\tfrac{1}{2}\ .\end{cases} \tag{18}$$

Expanding both $f(r)$ and $g(r)$ in terms of ar, at Compton wavelength distances we have

$$\begin{bmatrix} f(r) \\ g(r)\end{bmatrix}=Nr^{\gamma}\sum_{n=0}^{\infty}\begin{bmatrix} A_n \\ B_n\end{bmatrix}(ar)^n\ , \tag{19}$$

where $\gamma=(\kappa^2-a^2)^{1/2}$. The nth term of these expansions first contributes to the cross section in order a^n or higher, and hence to any desired order in a, it is sufficient to replace the infinite sums in Eq. (19) by finite polynomials in ar.

To determine the A,B coefficients, we may start from the wave equation

$$\begin{cases}\dfrac{df}{dr}+\kappa\dfrac{f}{r}-\left(\varepsilon_c+1+\dfrac{a}{r}\right)g=[(\varepsilon-\varepsilon_c)-(V-V_c)]g\ , \\ \dfrac{dg}{dr}-\kappa\dfrac{g}{r}+\left(\varepsilon_c-1+\dfrac{a}{r}\right)f=-[(\varepsilon-\varepsilon_c)-(V-V_c)]f\ ,\end{cases} \tag{20}$$

where $V_c=-a/r$ is the point Coulomb potential and

$$\varepsilon_c=[1+a^2/(n-|\kappa|+\gamma)^2]^{-1/2} \tag{21}$$

is the point Coulomb eigenvalue. Note that $(\varepsilon,\varepsilon_c)$ represents the eigenvalue (including rest mass energy) and (E,E_c) will be used to denote the binding energy, all in the unit of $m_c c^2$. The subscript c stands for a Coulombic quantity. Define

$$u\equiv 2(E-\Lambda_1 a^2)/a^2\ , \tag{22}$$

and substitute (20) into (21), obtaining recurrence relations. Specifying the value of one coefficient, say let $A_0=1$ or $B_0=1$, we can get all of the coefficients A_i,B_i rather easily from these recurrence relations. These coefficients are presented in Table I, with the choice $A_0=1$ for $ns_{1/2},np_{3/2}$ states and $B_0=1$ for the $np_{1/2}$ state. [According to the criterion of our expansion, in the $j=l-\frac{1}{2}$ cases we do not keep the pairs associated with a^4 (or higher power terms in a) for these coefficients.] The different choice for the $np_{1/2}$ case is made because, for the $j=l-\frac{1}{2}$ cases, $g(r)$ is bigger than $f(r)$ at small distances. In this case we will also need more terms in the polynomial expansion to obtain the same relative accuracy in the cross section, as shown in Table I.

The quantity u, as defined by Eq. (22), is essentially the screened binding energy (with the "outer screening" term $\Lambda_1 a^2$ subtracted). An additive constant term in the potential, as outer screening, does not affect the wave functions, and thereby the resulting cross sections, although it does change the eigenvalues. The quantity u is of the order of unity.

3. *Small-distance behavior of high-energy continuum wave functions*

Now we consider how to calculate the needed portion of the APT continuum wave functions. From Eq. (6) we have

$$\begin{aligned}\chi(\mathbf{r})-\chi(\mathbf{r}')&=\int_z^{\infty}V(\rho,z'')dz''-\int_{z'}^{\infty}V(\rho,z'')dz'' \\ &=\int_z^{z'}V(\rho,z'')dz''\ .\end{aligned} \tag{23}$$

Writing $V(r)$ in terms of cylindrical coordinates we obtain, through order α^3,

$$\chi(\mathbf{r})-\chi(\mathbf{r}')=-a(\chi_0+\chi_1\Lambda_1+\chi_2\Lambda_2+\chi_3\Lambda_3)\,|_{z''=z}^{z''=z'}\ , \tag{24}$$

where

$$\begin{aligned}\chi_0&=\ln[(z''+r)/\rho]\ , \\ \chi_1&=az''\ , \\ \chi_3&=a^2\{z''r+\rho^2\ln[(z''+r)/\rho]\}/2\ , \\ \chi_3&=a^3z''(\rho^2+z''/3)\ .\end{aligned} \tag{25}$$

Inserting (24) and (25) in Eq. (12), we obtain

$$g(r,r')=g_0+g_2\Lambda_2+g_3\Lambda_3\ , \tag{26}$$

where

$$\begin{aligned}g_0&=\varepsilon'(z-z')+a\ln[(z+r)/(z'+r')]\ , \\ g_2&=a^3\{zr-z'r'+\rho^2\ln[(z+r)/(z'+r')]\}/2\ , \\ g_3&=a^4[\rho^2(z-z')+(z^3-z'^3)/3]\ ,\end{aligned} \tag{27}$$

with shifted screened bound-state energy $\varepsilon'=\varepsilon+a^2\Lambda_1$ where $a^2\Lambda_1$ comes from the second term of Eq. (24), and the screened bound-state energy ε comes from the first term of Eq. (12). It is worth mentioning that the results (26) and (27) can be obtained directly from Eq. (7).

4. *Formalism of the calculation*

Using Eq. (26), we can rewrite Eq. (10) as

$$I=I_0+I_2\Lambda_2+I_3\Lambda_3\ , \tag{28}$$

where

$$I_0=\int dz\,dz'\,\rho\,d\rho\,F(\mathbf{r},\mathbf{r}')e^{ig_0}\ , \tag{29}$$

$$I_n=\int dz\,dz'\rho d\rho\,F(\mathbf{r},\mathbf{r}')e^{ig_0}ig_n,\quad n=2,3\ . \tag{30}$$

It is found that I_3 contributes only in relative order a^4 or higher to the cross section, so it will not be needed. The calculations of I_0 and I_2 can be carried out analytically using the technique discussed in Refs. 4 and 11. For the $ns_{1/2}$, $np_{1/2}$, and $np_{3/2}$ bound states the function $F(\mathbf{r},\mathbf{r}')$ defined by Eq. (11) can be written in the form[11]

$$4\pi r r' F(\mathbf{r},\mathbf{r}') = \begin{cases} ff'+gg'\cos(\theta-\theta')+ifg'\cos\theta'-if'g\cos\theta & \text{for } ns_{1/2} \\ ff'\cos(\theta-\theta')+gg'+ifg'\cos\theta-if'g\cos\theta' & \text{for } np_{1/2} \\ 2ff'\cos(\theta-\theta')+gg'[3\cos^2(\theta-\theta')-1]+ifg'[3\cos(\theta-\theta')\cos\theta'-\cos\theta] \\ -if'g[3\cos(\theta-\theta')\cos\theta-\cos\theta'] & \text{for } np_{3/2} , \end{cases} \tag{31}$$

where

$$\begin{aligned} &\cos\theta = z/r , \\ &\cos\theta' = z'/r', \quad \text{with } \rho' = \rho \\ &f' = f(r') , \\ &g' = g(r') . \end{aligned} \tag{32}$$

Substituting Eq. (31) into Eqs. (29) and (30), making the transformations

$$\begin{aligned} z &= \rho\sinh(x+i\pi/2) , \\ z' &= \rho\sinh(y-i\pi/2) , \end{aligned} \tag{33}$$

performing the integration over ρ, and returning the contours to the real axis, we get

$$I_0 = N^2 \frac{\exp(-\pi a)\Gamma(2\gamma+2)}{4\pi(\varepsilon')^{2\gamma+2}} \sum_{n=0}^{i} \frac{1}{(\epsilon')^n} \frac{\Gamma(2\gamma+2+n)}{\Gamma(2\gamma+2)} J_n , \tag{34a}$$

$$I_2 = N^2 \frac{\exp(-\pi a)\Gamma(2\gamma+2)}{4\pi(\varepsilon')^{2\gamma+2}} \sum_{n=2}^{i} \frac{1}{(\epsilon')^n} \frac{\Gamma(2\gamma+2+n)}{\Gamma(2\gamma+2)} \tilde{J}_n , \tag{34b}$$

where $i=4$ for $ns_{1/2}, np_{3/2}$ and $i=6$ for $np_{1/2}$, since the leading term in I_0 is of order a^2 higher in the $np_{1/2}$ case. In Eq. (34), J_n and $\tilde{J}_n$ are integrals, generally of the form

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{G(x,y)}{(\cosh x+\cosh y)_k}, \quad k = 4.5, \ldots, 10 \tag{35}$$

where $G(x,y)$ is some even function of x and y involving various combinations of terms such as $(\sinh x_i)^m$, $(\cosh x_i)^m$, x_i^m, $(\ln \sinh x_i)$, $\ln(\cosh x_1+\cosh x_2)$, and the step function

$$\Theta(x_i) = \begin{cases} 1, & \text{when } x_i > 0 \\ -1, & \text{when } x_i < 0 , \end{cases} \tag{36}$$

etc., where $m=0,1,2$ and $x_1=x$, $x_2=y$. The integrals can be performed with routine methods, and one then has analytic expressions for the cross sections.

III. RESULTS AND DISCUSSION

A. Results

The major effort in calculation is to perform the integrals contained in Eq. (34). The expressions for the integrands are too lengthy to present. Here we give our final analytic expressions for the photoionization cross sections, keeping all terms of an expansion in a through a^3, assuming the potential at small distances can be characterized by a polynomial expansion in (ar). For the $ns_{1/2}$ case, we have

$$\sigma_{ph} ns_{1/2} = \sigma_0 \frac{\exp(-\pi a)}{4a^3} N^2 P_{ns_{1/2}} , \tag{37}$$

where

$$\begin{aligned} P_{ns_{1/2}} = 1 &- \frac{4\pi}{15}a + a^2\left(\tfrac{139}{720}\pi^2 + \tfrac{4}{3}u - \tfrac{4}{3}\Lambda_2 + \tfrac{373\,729}{150\,000}\right) , \\ &+ \pi a^3\left(\tfrac{77}{720}\pi^2 - \tfrac{148}{315}u - \tfrac{46}{105}\Lambda_2 - \tfrac{310\,769}{328\,125}\right) . \end{aligned} \tag{38}$$

Here $\sigma_0 = 4\pi a^5\alpha/k$ is the high-energy limit of Sauter's formula[4] and the normalization N is best obtained through numerical calculation.

For the $np_{1/2}$ case, the "small" component $g(r)$ of the bound-state wave function is bigger than the "large" component $f(r)$ at small distances. The smallness of A_0 ($\propto a^2$) results in the involvement of more coefficients, since we want to keep the expansion to the same relative order (a^3). This means also that more integrals need to be performed to get the cross section. The final result for this case is

$$\sigma_{ph}(np_{1/2}) = \sigma_0 \frac{\exp(-\pi a)}{4a} N^2 P_{np_{1/2}} , \tag{39}$$

where

$$\begin{aligned} P_{np_{1/2}} = 1 &+ \frac{4\pi}{9}a + a^2\left(\tfrac{19}{432}\pi^2 + \tfrac{148}{135}u - \tfrac{76}{27}\Lambda_2 + \tfrac{481\,187}{450\,000}\right) \\ &+ \pi a^3\left(-\tfrac{5}{432}\pi^2 + \tfrac{172}{315}u + \tfrac{3854}{945}\Lambda_2 + \tfrac{288\,557}{590\,625}\right) . \end{aligned} \tag{40}$$

Finally, the photoionization cross section from the $np_{3/2}$ subshell is

$$\sigma_{\rm ph}(np_{3/2}) = 2\sigma_0 \frac{\exp(-\pi a)}{a^3} N^2 P_{np_{3/2}} , \tag{41}$$

where

$$\begin{aligned} P_{np_{3/2}} = 1 &- \frac{33\pi}{140}a + a^2\left(-\tfrac{2981}{13\,440}\pi^2 + \tfrac{13}{6}u - \tfrac{17}{6}\Lambda_2 + \tfrac{178\,743}{100\,000}\right) \\ &+ \pi a^3\left(\tfrac{281}{4480}\pi^2 - \tfrac{233}{420}u - \tfrac{67}{140}\Lambda_2 - \tfrac{135\,836\,399}{294\,000\,000}\right) . \end{aligned} \tag{42}$$

In addition to these analytic formulas for high-energy-limit photoionization cross sections, here we also present analytic formulas for the ratios of subshell cross sections, for fixed l and j, varying the principal quantum numbers. Defining $R_{nlj}(n',n) = P_{n'lj}/P_{nlj'}$, we have, from Eqs. (38), (40), and (42),

TABLE II. Comparison between numerically calculated I_0/G, obtained from Eq. (33), and the same quantity given by the analytic result, Eq. (40), for the $2p_{1/2}$ case. Here $G=a^4N^2\exp(-\pi a)/4\pi$ and the coefficients C_1,C_2,C_3 are defined by Eq. (40).

	Analytic result			
a	$1+C_1a$	$1+C_1a+C_2a^2$	$1+C_1a+C_2a^2+C_3a^3$	Numerical result
0.01	1.014	1.014	1.014	1.014
0.05	1.070	1.074	1.074	1.074
0.10	1.140	1.157	1.159	1.160
0.20	1.279	1.350	1.363	1.371
0.30	1.419	1.579	1.622	1.662
0.40	1.559	1.843	1.946	1.991

$$R_{s_{1/2}}(n',n)=1+a^2 4(u-u)/3-\pi a^3 4(u'-u)/35\ , \tag{43}$$

$$R_{p_{1/2}}(n',n)=1+a^2 148(u'-u)/135 +\pi a^3 100(u'-u)/1701\ , \tag{44}$$

$$R_{p_{3/2}}(n',n)=1+a^2 13(u'-u)/6-\pi a^3 37(u'-u)/840\ . \tag{45}$$

Here u (and u') depend on the quantum number n (and n') [see Eq. (22)]. It is interesting to see that the extra screening enters the ratios of subshell cross sections only through the energy difference $u'-u=2(E'-E)/a^2$, at the level of our expansion.

B. Checks and tests

Compared to the existing results.[4,5,10,11,13] the cross sections given in this work include higher-order expansion terms in a, general n dependence and screening-dependent terms. All the calculations which lead to these new features have been independently checked. As an example, we show in Table II for the $2P_{1/2}$ case the numerically calculated I_0/G and the same quantity given by the analytic formula Eq. (40), with the expansion through increasing orders of a. Here $G=a^4N^2\exp(-\pi a)/4\pi$.

As a further check of our analytic cross-section formulas, we have compared these predictions for the subshell ratios with the existing finite-energy numerical data.[14] It is of course not reasonable to expect the high-energy-limit predictions to give the right energy dependence for cross sections in the relatively low-energy region, where in fact numerical data exist (the MeV region). However, in examining the existing numerical data we have noticed that the subshell ratios of the photoionization cross sections reach high-energy-limit behavior at much lower energy than the cross sections themselves, a phenomenon observed before in other situations.[15,16] The leading term of the photoionization cross section in a $1/k$ expansion is the same for the transitions from all subshells: $1/k$, where k is the photon energy. This energy dependence is canceled in a subshell ratio, so that all such ratios become constant at high energy. However, it appears that the next term(s), whose coefficient(s) is (are) presently unknown, probably cancel(s) as well. Using Scofield's table.[14] we see this phenomenon for many outer subshells. As an example, we show a few subshell ratios for finite-energy photoionization cross sections (Sn, $Z=50$) in Table III. We see that the σ_{4s}/σ_{3s} ratio is quite constant when the photon energy varies from 200 to 1500 keV (relative error less than 0.1%). The ratios $\sigma_{4p_{1/2}}/\sigma_{3p_{1/2}}$ and $\sigma_{4p_{3/2}}/\sigma_{3p_{3/2}}$ are also almost constant. However, when different j are involved, the subshell ratios do not show high-energy-limit behavior in this energy range. Using Scofield's data as an example again, we also show the $\sigma_{4p_{1/2}}/\sigma_{4p_{3/2}}$ ratios for Sn in Table III. Apparently, this ratio has not yet stabilized. This comparison suggests that the coefficient(s) of the next term(s) in the expansion in $1/k$ depends on j considerably.

If we assume these stabilized subshell ratios are the high-energy-limit values, we can compare them with our predictions. The agreement is excellent (see Sec. IV), and this suggests the accuracy of our calculations.

C. Discussion of the results

1. *Extra screening effects and their n dependence*

Here we discuss extra screening effects and their n dependence. By extra screening we mean the ratio between a screened and a Coulomb cross section, after normalizations are removed. First, we present the analytic expressions for extra screening, followed by some numeri-

TABLE III. Photoionization subshell ratios for tin ($Z=50$) (Ref. 14).

$E_{\rm ph}$ (keV)	σ_{4s}/σ_{3s}	$\sigma_{4p_{1/2}}/\sigma_{3p_{1/2}}$	$\sigma_{4p_{3/2}}/\sigma_{3p_{3/2}}$	$\sigma_{4p_{1/2}}/\sigma_{4p_{3/2}}$
200	0.2035	0.1877	0.1858	0.8389
500	0.2037	0.1879	0.1865	0.9108
1000	0.2037	0.1878	0.1868	0.8850
1500	0.2037	0.1880	0.1865	0.8549

TABLE IV. Extra screening: $ns_{1/2}$, $np_{1/2}$, $np_{3/2}$ cases.

Z	$1,2j$	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$
13	0,1	1.0010	1.0027	1.0038			
	1,1		1.0031	1.0042			
	1,3		1.0040	1.0062			
50	0,1	1.0029	1.0099	1.0157	1.0197	1.0224	
	1,1		1.0093	1.0155	1.0198	1.0225	
	1,3		1.0189	1.0328	1.0423	1.0484	
82	0,1	1.0001	1.0072	1.0137	1.0186	1.0222	1.0247
	1,1		1.0079	1.0180	1.0254	1.0308	
	1,3		1.0257	1.0518	1.0716	1.0860	

cal results for a number of elements and a comparison of extra screening with the normalization screening. Afterwards, we will discuss the n dependence of the extra screening and the connection with bremsstrahlung.

Defining $S_{nlj} \equiv P_{nlj}/P_{nlj}^{\text{Coulomb}}$, where the P_{nlj} are given by (38), (46), (42), and P_{nlj}^{Coulomb} are defined as the Coulomb P's, we have

$$S_{ns_{1/2}} = 1 + a^2[4(u-u^c)/3 - 4\Lambda_2/3] - \pi a^3[4(u-u^c)/35 + 50\Lambda_2/63] , \quad (46)$$

$$S_{np_{1/2}} = 1 + a^2[148(u-u^c)/135 - 76\Lambda_2/27] + \pi a^3[100(u-u^c)/1701 + 45\,326\Lambda_2/8505] , \quad (47)$$

$$S_{np_{1/2}} = 1 + a^2[13(u-u^c)/6 - 17\Lambda_2/6] - \pi a^3[37(u-u^c)/840 + 321\Lambda_2/280] , \quad (48)$$

where u^c is the Coulomb u. It is clear that the extra screening effects start to appear with the a^2 term in all three cases; only two quantities, namely, $\Delta u \equiv u - u^c$ and Λ_2, characterize the screening dependence for all cases. Before we discuss the characteristic importance of these two quantities, we give a few numerical examples of extra screening and its comparison with the normalization screening.

Using the analytic formula (46), (47), and (48), together with numerical binding energies (obtained from Liberman's[17] code with Kohn-Sham exchange) and Λ_1 and Λ_2 coefficients (obtained by a least-squares fit to the same Kohn-Sham potential), we obtain the "extra screening" for photoionization cross sections from $ns_{1/2}$, $np_{1/2}$, and $np_{3/2}$ subshells for various atoms (Table IV).

From Table IV we see the extra screening beyond normalization does exist, usually at, or for low Z less than, the few percent level. This reflects the fact that even at Compton wavelength length distances there is still deviation of the potential from the point Coulomb potential. A comparison between the normalization screening and extra screening is presented (for low-, medium-, and high-Z elements) in Table V. In all cases the normalization screening is much larger, although the extra screening is significant in many cases (for large n and for $p_{3/2}$).

The extra screening shows significant n dependence. This is of course related to the way it enters the wave functions and the cross sections. From Table I we see that only two quantities, i.e., u and Λ_2, contain screening. However, u dominates for all cases, as indicated by Table V, showing the comparison between

$$\Delta u = u - u^c = 2(E - E^c - \Lambda_1 a^2)/a^2 \quad (49)$$

and

$$\Delta\Lambda_2 = \Lambda_2 - \Lambda_2^c = \Lambda_2 , \quad (50)$$

for a few atoms ($Z=13$, 50, and 82), for $ns_{1/2}$ states. (The numbers inside the parentheses, right-hand column, show the variation of Λ_2 due to the uncertainty of Λ_2 in least-squares fits at Compton wavelength distances.) The major extra screening is carried by Δu, and it is this quantity we should focus on in order to understand the n dependence of extra screening. Meanwhile we may ignore the variation of Λ_2 (due to its uncertainty) since this variation is almost always less important than Δu.

TABLE V. Comparison between normalization screening and extra screening for low-, medium,-, and high-Z elements (occupied states only).

Initial state	$Z=13$		$Z=50$		$Z=82$	
	Nor. Scr.	Ext. Scr.	Nor. Scr.	Ext. Scr.	Nor. Scr.	Ext. Scr.
$1s_{1/2}$	0.9505	1.0010	0.9810	1.0029	0.9861	1.0001
$3s_{1/2}$	0.1582	1.0038	0.5399	1.0157	0.6799	1.0137
$3p_{1/2}$	0.0580	1.0042	0.4436	1.0155	0.6074	1.0180
$3p_{3/2}$	0.0579	1.0062	0.4287	1.0328	0.5677	1.0518
$5s_{1/2}$			0.0580	1.0224	0.1826	1.0222
$5p_{1/2}$			0.0248	1.0225	0.1359	1.0308
$5p_{3/2}$			0.0218	1.0484	0.1143	1.0860

Δu can be regarded as composed of two parts, the screening energy shift (n-dependent term) $\Delta E = E^s - E^c$ (negative always) and the n-independent term $-\Lambda_1 a^2$ (which is positive since Λ_1, representing the outer electron screening of the nuclear potential, is negative). The absolute value of ΔE decreases with the increase of n and approaches zero, primarily due to the fact that both screened and Coulomb binding energies approach the threshold monotonically. Meanwhile, $-\Lambda_1 a^2$ is always greater than $|\Delta E|$, a result connected with the fact that $\Lambda_1 a^2$ is the potential-energy shift seen by a test charge at Compton wavelength distances and $E^s - E^c$ is the level shift due to screening determined, generally speaking, at much more outer distances (depending on the quantum number n). Consequently, Δu is a positive quantity and approaches the limit $-2\Lambda_1$ when $n \to \infty$ as shown in Table VI. The maximum extra screening carried by Δu occurs in this limit. (Incidentally, this limit is also the limit for the bremsstrahlung tip; see Sec. IV for details.) This agrees with what we see in Table IV: The extra screening effects increase with n, but within the few percent range.

2. *Comparison with finite-energy numerical results*

As we have already mentioned, the finite-energy numerical photoionization cross sections, and particularly their ratios, begin to show certain high-energy-limit behavior in the MeV region. It is therefore interesting to compare the predictions from our high-energy-limit formulas with the existing high- (but finite) energy data. In Table VII we present ratios obtained (i) from Scofield's numerical data, (ii) from normalization theory,[6] and (iii) from this work, for various elements. Normalization theory predicts that the high-energy limit of such ratios, varying principal quantum number for fixed (lj), is just the square of the ratio of corresponding normalizations:

$$\frac{\sigma_{nlj}}{\sigma_{n'lj}} = \frac{N^2_{nlj}}{N^2_{n'lj}} , \tag{51}$$

so that the knowledge of the screened normalizations immediately provides the ratio. We can see from Table VII that the normalization theory results agree quite well with the numerical ones. The difference of this work compared to normalization theory lies in the inclusion of "extra n dependence" and "extra screening," namely,

$$\sigma_{\text{this work}} = \sigma_{\text{nor theo}} \Delta_{\text{extra } n \text{ dependence}} \Delta_{\text{extra screening}}$$

where $\Delta_{\text{extra } n \text{ dependence}}$ is defined as P^{Coulomb}_{nlj}, and $\Delta_{\text{extra screening}}$ is given by Eqs. (46), (47), and (48). As a matter of fact, extra n dependence has been studied in Refs. 4 and 5 for the $ns_{1/2}$ case with $n = 1,2$. From Table VII we can see clearly that, with these two effects included, the results of this work agree with the numerical data better than the normalization theory results do, although normalization theory correctly gives the dominant effects.

Finally, we should mention that a similar comparison with the finite-energy numerical results, but for the ratio between the subshells with same n,l but different j, would be very interesting since the normalization screening of this ratio is relatively small and the extra screening has a better chance to be visible. However, this ratio does not reach its high-energy-limit behavior as early as the others discussed before (for which l and j are kept constant). We note this suggests that the coefficient of the next term in the expansion in terms of $1/k$, of order $1/k^2$, depends on j considerably.

IV. HIGH-FREQUENCY REGION OF THE SPECTRUM OF ELECTRON BREMSSTRAHLUNG

A. The analytic continuation between photoeffect and bremsstrahlung

The relationship between the high-frequency end-point region of the bremsstrahlung spectrum (almost all incident

TABLE VI. Decomposition of Δu and comparison between Δu and Λ_2.

		Decomposition of Δu (keV)			Comparison between Δu and Λ_2		
Z	n	$\Delta E_{ns_{1/2}}$	$\Delta E_{np_{1/2}}$	$-\Lambda_1 a^2$	$\Delta u_{ns_{1/2}}$	$\Delta u_{np_{1/2}}$	Λ_2
13	1	−0.7996		0.9052	0.0459		−0.036(0.022)
13	3	−0.2465	−0.2514	0.9052	0.2865	0.2842	−0.036(0.022)
13	∞	0.0000	0.0000	0.9052	0.3936	0.3936	−0.036(0.002)
50	1	−6.2691		6.8535	0.0172		−0.0032(0.01)
50	3	−3.0699	−3.1863	6.8535	0.1112	0.1078	−0.0032(0.01)
50	5	−1.3804	−1.3874	6.8535	0.1609	0.1606	−0.0032(0.01)
50	∞	0.0000	0.0000	6.8535	0.2014	0.2014	−0.0032(0.01)
82	1	−13.6727		15.0842	0.0154		0.0031(0.004)
82	3	−7.5036	−7.7836	15.0842	0.0829	0.0798	0.0031(0.004)
82	5	−3.7781	−3.8196	15.0842	0.1236	0.1231	0.0031(0.004)
82	∞	0.0000	0.0000	15.0842	0.1648	0.1648	0.0031(0.004)

TABLE VII. Comparison of cross-section ratios obtained by numerical calculation (Ref. 14), normalization theory, and this work.

Z	$\sigma(n,l,2j)/\sigma(n',l,2j)$	Numerical result (Ref. 14)	Normalization theory	Extra n dependence	Extra screening	This work
8	(201)/(101)	0.057 06	0.057 16	0.9967	1.0007	0.057 01
20	(301)/(201)	0.1323	0.1325	0.9963	1.0019	0.1323
50	(401)/(301)	0.2037	0.2044	0.9933	1.0039	0.2038
75	(501)/(401)	0.1815	0.1818	0.9951	1.0036	0.1816
92	(601)/(501)	0.2064	0.2064	0.9974	1.0023	0.2064
92	(501)/(401)	0.2575	0.2584	0.9951	1.0031	0.2579
92	(501)/(301)	0.069 63	0.070 75	0.9844	1.0073	0.070 16
50	(411)/(311)	0.1880	0.1888	0.9935	1.0041	0.1883
74	(511)/(411)	0.1546	0.1551	0.9940	1.0046	0.1549
50	(413)/(311)	0.1864	0.1875	0.9961	1.0090	0.1866
74	(513)/(413)	0.1482	0.1486	0.9858	1.0114	0.1482

kinetic energy radiated) and the atomic photoelectric effect was discussed some time ago by Fano, Koch, Motz,[9] McVoy and Fano,[18] and Pratt.[10] Through detailed balance, photoeffect, involving emission of an electron from a (n,j,l,m) state, is related to direct radiative recombination (DRR), filling a vacancy in a (n,j,l,m) state. The matrix element for DRR, involving a final negative binding energy state ($\varepsilon_n < 1$), may be analytically continued to the corresponding bremsstrahlung matrix element involving a positive kinetic energy final state ($\varepsilon > 1$). Evidently, knowledge of the photoionization cross section in the high-energy limit also provides predictions for the corresponding bremsstrahlung cross sections.

The differential cross section for an incident electron (with momentum $\mathbf{p}$ and total energy ε_p) to radiate a photon (with momentum $\mathbf{k}$ and energy $\hbar\omega = \hbar ck = k$), in the situation that the final electron is not observed, can be expressed as a sum of cross sections into final electron states of definite angular momentum (j,l,m) as

$$d\sigma_{\text{brem}} = \sum_{j,l,m} d\sigma_{\text{brem}}^{jlm} ,$$

where

$$d\sigma_{\text{brem}}^{jlm} = (2\pi)^{-2} p^{-1} \varepsilon_p \mid H_{\text{brem}}^{jlm} \mid^2 d^3k \, \delta(\varepsilon_p - k - \varepsilon) , \quad (52)$$

$$H_{\text{brem}}^{jlm} = -e(2\pi/k)^{1/2} \int d^3r \, \psi_{\text{final}}^{*}(\varepsilon,j,l,m) \boldsymbol{\alpha}\cdot\mathbf{e}^{*} \times \exp(-i\mathbf{k}\cdot\mathbf{r}) \psi_{\text{int}} , \quad (53)$$

and $\varepsilon_p > 1$ is the total energy of the outgoing electron. (Near the hard photon end point of the spectrum, if the incident electron kinetic energy is not low, the expansion in j,l,m converges rapidly; for high incident energies it is dominated by s waves and p waves in the final electron.) The differential cross section for an incident photon (with momentum $\mathbf{k}$ and energy $\mathbf{k}$) to eject an electron (with momentum $\mathbf{p}$ and energy ε_p) from a bound state (n,j,l,m) of an atom (or ion) is

$$d\sigma_{\text{phot}}^{jlm} = (2\pi)^{-2} \mid H_{\text{phot}} \mid^2 d^3p \, \delta(\varepsilon_p - k - \varepsilon) , \quad (54)$$

where

$$H_{\text{phot}}^{*jlm} = -e(2\pi/k)^{1/2} \int d^3r \, \psi_{\text{int}}^{*}(n,j,l,m) \boldsymbol{\alpha}\cdot\mathbf{e}^{*} \times \exp(-i\mathbf{k}\cdot\mathbf{r}) \psi_{\text{final}} , \quad (55)$$

and $\varepsilon < 1$ is the total energy of the bound electron. The high-energy continuum wave function is normalized to unit volume (both in bremsstrahlung and in photoionization) and to an energy δ function for the outgoing (low-energy) electron of the bremsstrahlung. As to the bound state, it is normalized so that $\int \mid \psi \mid^2 d^3r = 1$.

The matrix elements H_{brem}^{jlm} and H_{phot}^{jlm} are related through analytic continuation. More precisely, if we define "reduced" wave functions as normalized simply to $r^{\gamma-1}$ at the origin (i.e., dividing through by the usual normalization factors at the origin) and "reduced" matrix elements defined in terms of reduced wave functions, then H_{brem}^{jlm} and H_{phot}^{*jlm} represent one analytic function of the energy ε, continued analytically between low continuum energy $\varepsilon > 1$ and bound-state energy $\varepsilon < 1$. Since the boundary conditions on reduced wave functions do not depend on the parameter ε, Poincare's theorem[19] tells us that they are analytic functions of ε. From this it also follows, using the methods of Dillon and Inokuti[20] and Lassettre[21] for the bound-bound–bound-free continuation, that these reduced matrix elements represent one analytic function of ε. (The normalization factors do not continue analytically, and in our applications we are calculating them with numerical methods.)

With a second application of Poincare's theorem, we can obtain results for positron bremsstrahlung from the corresponding results for electron bremsstrahlung. Now the analytic parameter is $a \equiv Z\alpha$, and we continue through zero between positive and negative values to get the two cases. We will be able to go between electron and positron results with the substitution $a \leftrightarrow -a$.

B. General expressions and Coulomb results for high-frequency region of the electron bremsstrahlung spectrum

1. General expressions

From our discussion above and the analytic expressions for the high-energy-limit total photoionization cross sec-

tions, we may readily obtain the high-frequency-region electron bremsstrahlung partial-wave cross section (we will discuss the full spectrum, which is the normal experimental observable, later) in the high-energy limit ($E\rightarrow\infty$):

$$\sigma_{\text{brem}}(s_{1/2})=\sigma_0[\exp(-\pi a)/(4a^3)] \times N^2(s_{1/2})P_{\text{brem}}(s_{1/2}) , \tag{56}$$

$$\sigma_{\text{brem}}(p_{1/2})=\sigma_0[\exp(-\pi a)/(4a)] \times N^2(p_{1/2})P_{\text{brem}}(p_{1/2}) , \tag{57}$$

$$\sigma_{\text{brem}}(p_{3/2})=\sigma_0[\exp(-\pi a)/a^3] \times 2N^2(p_{3/2})P_{\text{brem}}(p_{3/2}) , \tag{58}$$

where $P_{\text{brem}}(s_{1/2})$, $P_{\text{brem}}(p_{1/2})$, and $P_{\text{brem}}(p_{3/2})$ are still given by (38), (40), and (42), except that the binding energy $-E$ contained in u, Eq. (23), should be replaced by the electron kinetic energy T. The N's now are the normalization factors for the low-kinetic-energy outgoing electron. They can be given analytically for the point Coulomb wave function (see below) and we will calculate them numerically for the screened cases. Note that, within Eqs. (56) to (58), only the P's and N's are different from the corresponding quantities for photoionization.

2. *Point Coulomb potential results*

Our formulas can be immediately applied to the point Coulomb case by setting the Λ_1 and Λ_2 coefficients to zero in our expressions for the P's. We obtain in this way an extension of the previous Coulomb results.[10,11,13] Explicitly,

$$\sigma^{\text{Coul}}_{\text{brem}}(s_{1/2})=\sigma_0[\exp(-\pi a)/(4a^3)]N^2_{\text{Coul}}[1-4\pi a/15+a^2(8T)/(3a^2)-139\pi^2/720+\tfrac{373\,729}{150\,000} +\pi a^3(-296T)/(315a^2)+77\pi^2/720-\tfrac{310\,769}{328\,125}] , \tag{59}$$

$$\sigma^{\text{Coul}}_{\text{brem}}(p_{1/2})=\sigma_0[\exp(-\pi a)/(4a)]N^2_{\text{Coul}}(p_{1/2})[1+4\pi a/9+a^2(296T)/(135a^2)+19\pi^2/432+\tfrac{481\,187}{450\,000} +\pi a^3(344T)/(315a^2)-5\pi^2/432+\tfrac{288\,557}{590\,625}] , \tag{60}$$

$$\sigma^{\text{Coul}}_{\text{brem}}(p_{3/2})=\sigma_0[\exp(-\pi a)/a^3]2N^2_{\text{Coul}}[1-33\pi a/140+a^2(13T)/(3a^2)-2981\pi^2/13\,440+\tfrac{178\,743}{100\,000} +\pi a^3(-233T/(210a^2)+281\pi^2/4480-\tfrac{135\,836\,399}{294\,900\,000}] , \tag{61}$$

where the point Coulomb normalizations for the continuum wave functions are,[22] according to our definitions,

$$N_{\text{Coul}}(\kappa)=\begin{cases}\dfrac{G2^\gamma}{\Gamma(2\gamma+1)}[2(\varepsilon+1)]^{1/2}\text{Re}[(\gamma+i\nu)(-\kappa+ia/p)]^{1/2}, & \text{for } s_{1/2},p_{3/2} \text{ states}\\ \dfrac{G2^\gamma}{\Gamma(2\gamma+1)}[2(\varepsilon-1)]^{1/2}\text{Im}[(\gamma+i\nu)(-\kappa+ia/p)]^{1/2}, & \text{for } \textit{the } p_{1/2} \text{ state}\end{cases} \tag{62}$$

with

$$G=e^{\pi\nu/2}\,|\,\Gamma(\gamma+i\nu)\,|\,p^{\gamma-1/2}/(2\pi)^{1/2} . \tag{63}$$

For the bremsstrahlung tip case ($T\rightarrow 0$), as noted in Ref. 11,

$$\lim_{T\rightarrow 0} G=a^{\gamma-1/2} . \tag{64}$$

Since

$$\lim_{T\rightarrow 0}\text{Re}[(\gamma+i\nu)(-\kappa+ia/p)]^{1/2}=(\gamma-\kappa)/2 , \qquad \lim_{T\rightarrow 0}\text{Im}[(\gamma+i\nu)(-\kappa+ia/p)]^{1/2}=a/p , \tag{65}$$

we obtain

$$\lim_{T\rightarrow 0}|N_{\text{Coul}}|^2=\begin{cases}\dfrac{a^{2\gamma-1}2^{2\gamma}}{\Gamma^2(2\gamma+1)}(\gamma-\kappa)^2 , & \\ \text{for } s_{1/2},p_{3/2} \text{ states} & \\ \dfrac{a^{2\gamma-1}2^{2\gamma}}{\Gamma^2(2\gamma+1)}, & \text{for the } p_{1/2} \text{ state} .\end{cases} \tag{66}$$

For this point Coulomb case, our $s_{1/2}$, $p_{1/2}$, and $p_{3/2}$ partial cross sections agree with those of Jabbur and Pratt.[11,13] More precisely, our $s_{1/2}$ result is identical, since the expansion (in terms of a) has been performed to the same order; our $p_{1/2}$ and $p_{3/2}$ results are expanded to two orders higher. This higher-order expansion allows us to see the energy dependence (linear dependence in T to this order in a) of the $p_{1/2}$ and $p_{3/2}$ partial cross sections, just as had been found in the $s_{1/2}$ case. However, in the usual cross section (summed over the partial-wave states of the final electron), these high-order terms in $p_{1/2}$ and $p_{3/2}$ will not be included as we make a consistent expansion through relative order a^3, as those two partial cross

sections are of order a^2 smaller than the $s_{1/2}$ term. Our point Coulomb result for the bremsstrahlung spectrum, given as a function of the kinetic energy of the outgoing electron and as function of nuclear charge Z, hence agrees exactly with the previous work.[11,13]

All of these results, including the normalization factors, can be applied to positron bremsstrahlung with the substitution $a \leftrightarrow -a$. Note in this case the factor G, Eq. (63), goes to zero as ε approaches 1 and so p goes to zero:

$$\lim_{p\to 0} G(-a)=\exp(-\pi a\varepsilon/p)\,|\,a\,|^{\gamma-1/2}\,, \tag{67}$$

corresponding to the fact that the low-energy positron cannot get near the nucleus.

3. *Screening effects*

As with photoionization, the effect of screening on the bremsstrahlung spectrum can be separated into two parts: normalization screening and extra screening. These are defined in exactly the same way as for photoionization, except that the negative binding energy $-E$ should be replaced by the kinetic energy T. We will discuss the two screening effects separately.

a. Normalization screening. A major difference between screened and point Coulomb cross sections at the tip of the bremsstrahlung spectrum arises from the difference between the screened and point Coulomb normalizations for the continuum wave functions. From Eq. (66), we see that the point Coulomb normalization remains finite and of order a^j in the zero kinetic energy limit; by contrast the screened normalization goes to zero for small momentum p and faster with increasing l. These different behaviors, as illustrated in Table VIII, occur mainly in the threshold region (especially within a few eV of the threshold). With increase in the kinetic energy of the outgoing electron, the difference rapidly disappears. When the kinetic energy exceeds a few keV, the difference is less than 1 or 2% (see Table VIII). At such energies, as we will see below, the extra screening becomes more important. For positrons screening will *enhance* the normalization in comparison to the Coulomb result Eq. (67).

b. Extra screening. The extra screening of the partial cross sections, beyond normalization, can be easily calculated from Eqs. (46)–(48) and the Λ coefficients. For a few representative elements and final electron kinetic energies (from 80 keV) to the tip), we tabulate this effect in Table IX. At the tip ($T=0$) extra screening is identical with what we have seen in the high-n limit of the photoionization cross sections (see Table V). Extra screening is usually a few percent in the $j=\frac{1}{2}$ channel, larger for $j=\frac{3}{2}$ in very-high-Z elements. Further back from the tip, the extra screening increases somewhat while the normalization screening is greatly reduced. Except in light elements, the extra screening is larger than normalization screening at keV energies.

Although the partial bremsstrahlung cross sections which we have been discussing are in principle observable, the observed bremsstrahlung spectrum corresponds to a summation over all these partial cross sections. As noted by Pratt and Tseng,[6] the relative contributions of the partial cross sections to the sum decrease with increasing of the angular momentum l, particularly for increasing incident electron kinetic energies, for which the relative contributions are fixed and rapidly decreasing with l as the energy goes to the high-energy limit. For example, when the incident electron kinetic energy is 1.84 MeV, the $s_{1/2}$ partial cross section contributes 65% to the total cross section, the $p_{1/2}$ and $p_{3/2}$ partial cross sections are about 16% each, while the d-wave partial cross sections are less than 1% each. (In light-Z elements the p-wave contribution is also small.) Therefore, in the high-energy limit, we may fairly well represent the total bremsstrahlung cross section by the summation over our three partial cross sections:

$$\sigma_{\text{brem}}=\sigma_{s_{1/2}}+\sigma_{p_{1/2}}+\sigma_{p_{3/2}}\,. \tag{68}$$

By using Eqs. (61), (62), (63), (72), and numerically calculating the needed normalization factors, we can rather easily obtain the screened bremsstrahlung-tip-region spectrum. Screening effects are dominated by the extra screening except in the very tip region (a few eV above threshold), where normalization screening is much more important.

There are few experiments which study the tip region of

TABLE VIII. Ratio of screened to Coulomb normalization as function of outgoing electron kinetic energy T, for Sn ($Z=50$).

	N(screened)/N(Coulomb)		
T (eV)	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$
0.1	0.3955	0.0182	0.0182
1.0	0.5327	0.0786	0.0787
5.0	0.6592	0.2206	0.2209
10.0	0.7115	0.3246	0.3250
20.0	0.7661	0.4479	0.4484
100.0	0.8842	0.7313	0.7320
1000.0	0.9766	0.9422	0.9431
3000.0	0.9907	0.9762	0.9771
10 000.0	0.9968	0.9916	0.9926

TABLE IX. Extra screening contribution to high-frequency region bremsstrahlung cross sections in the limit of high incident electron kinetic energies.

		Extra screening		
Z	T (keV)	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$
	0	1.005	1.005	1.009
13	40	1.006	1.006	1.013
	80	1.008	1.008	1.027
	0	1.028	1.028	1.061
50	40	1.033	1.033	1.092
	80	1.041	1.040	1.192
	0	1.032	1.042	1.115
79	40	1.036	1.049	1.174
	80	1.040	1.057	1.360

the spectrum produced from high-energy incident electrons. For W ($Z=74$) and Th ($Z=90$), with 15.1-MeV incident electrons, the measured values of $k(d\sigma/dk)/Z^2$ at the tip are[23–25] 1.38 ± 0.41 and 1.6 ± 0.16 mb, while the Jabbur-Pratt point Coulomb results are 1.41 and 1.66 mb; our results, including screening, are 1.46 and 1.71 mb. (The kinetic energy of final state electrons is assumed not to be within a few eV of the tip.)

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*Present address: Department of Chemistry, The University of Kansas, Lawrence, KS 66045-0046.

†Present address: 202 Ramblewood Parkway, Mt. Laurel, NJ 08054.

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