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UNDERSTANDING ATOMIC PROCESSES IN TERMS OF COULOMB SINGULARITIES

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Many aspects of high-energy atomic processes can be described in terms of singularities of a many-body Hamiltonian using the generalized asymptotic Fourier transform (AFT) theory. The study of matrix elements in different kinematic regimes is related to the study of singularities (points of nondifferentiability) of the wave functions and the e–γ interaction. These singularities reflect the singularities of the many-body Hamiltonian. We illustrate the principles of the AFT approach in the simple example of photoabsorption by the electron bound in a potential with a Coulomb singularity. We exhibit two general results that are important for any many-body system: 1) the quality of approximate results in different forms («gauges») depends on the quality of the description of the wave functions in the vicinity of singularities and 2) due to the character of the Coulomb singularity, photoabsorption cross sections converge slowly to their asymptotic form as the energy increases. But the slowly converging behavior of these cross sections is due to one common factor (the Stobbe factor), which can be obtained analytically in terms of the characterization of the vicinity of the singularity. The common Stobbe factor explains why ratios of cross sections converge more rapidly than the cross sections themselves.

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1. INTRODUCTION

High-energy atomic processes can be described in terms of singularities of the many-body Hamiltonian. The asymptotic Fourier transform (AFT) theory [1, 2] can provide such a description. In this paper, we apply the AFT approach to photoabsorption (at high but nonrelativistic energies) in a simple atomic system, the electron in a potential with a Coulomb singularity. This serves to illustrate general points that are important in a variety of more complex systems. In particular, we illustrate: 1) dependence of the required wave function quality on the interaction form («gauge») utilized and 2) extraction of a common factor (the Stobbe factor) that contains all slow convergence of the matrix elements to their high-energy limit.

The study of single-photon ionization processes resulting in single [3, 4] or multiple [5, 6] ionization of an atom is of fundamental and practical importance. New experimental possibilities, modern synchrotron sources and experimental methods [7] result in better understanding of the electron correlation effects in complex systems and in processes involving these systems [8–12]. Recently, we have proposed a unified description [1, 2] of the processes of high-energy[1)] ionization by photoabsorption, based on the mathematically well founded AFT theory. The idea is based on the close relation

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[1)] By high energy, we mean that the photon energy $\omega \gg E_B$ (where E_B is the binding energy of the state that is ionized), but still $\omega \ll m$ (for a nonrelativistic description of electrons).

between high-energy photoabsorption matrix elements and the AFT of functions with singularities (by a singularity, we mean a point where a function is not differentiable).

According to the AFT theory, the asymptotic Fourier transform of a function with singularities is determined by the behavior of the function in the vicinity of these singularities [13, 14]. Because photoabsorption at high photon energies requires at least one large outgoing electron momentum p, we can generally argue that the analysis is equivalent to the analysis of the asymptotic forms of Fourier transforms (FT). A slow asymptotic decrease for large p, such as $1/p^n$ for example, of the FT of a well-localized function, results only from singularities of that function. By studying singularity structures of the wave functions, which follow from the Schrödinger equation, one is then able to address various, quite general, issues of the matrix element (such as the interaction-form dependence of approximate matrix elements and the nature of convergence with energy to high-energy forms) without needing the full knowledge of the many-body wave functions. The AFT approach has been applied to double ionization [1] of He-like systems and single ionization of more complex atoms [2].

In this paper, we describe this approach to photoabsorption (and perhaps other related) processes at high but nonrelativistic energies. We use the example of single ionization within a central field independent particle approximation (IPA) model and assume that the IPA potential near the nucleus is point Coulomb. We use this simple and familiar model in order to illustrate the main points of our general approach in the context of a relatively simple and familiar situation where most features can clearly be seen. We view the idea of the AFT approach very general, and by presenting it in a relatively simple situation we want to motivate its application to other processes. The kinematic situations that occur in high-energy photoabsorption can also occur in other processes, e.g., in charged particle scattering. In such situations, the AFT approach connects matrix element of the process with the singularities of the system involved in the process.

Another important motivation in considering the simple system is to illustrate and emphasize two often neglected points, which are general for any photoabsorption process, and for which purpose an IPA model is sufficient. The first point is concerned with how the quality of approximate results depends on both the quality of approximate wave functions used and the interaction form chosen. For example, a plane-wave description of fast electrons is generally inadequate, as discussed in [15–18]. The second point is that due to the Coulomb singularity, any high-energy photoabsorption cross section (for ionization of a system with an interaction having a Coulomb singularity) has the Stobbe factor, which must be extracted in order to obtain a fast convergence of the results. This is very important for high-energy studies of photoabsorption. For example, because absolute measurements at higher energies are less accurate than at lower energies, the high-energy results are often obtained from lower energy results assuming some asymptotic behavior. It is sometimes assumed [5, 19] that at some finite energy (not taken sufficiently high), the cross sections for photoabsorption follow the leading-order Born result. This causes errors in reported cross sections.

We consider the adequacy of various forms of matrix elements (length (L), velocity (V) or acceleration (A) forms) in using approximate wave functions of various qualities in the vicinity of a singularity. We demonstrate that nonrelativistic IPA high-energy photoabsorption is determined (up to corrections $O(1/p^2) \approx O(1/\omega)$, where p is the outgoing electron momentum) by the initial state normalization and the point Coulomb singularity. This result is form-independent, but whether the information about the singularity comes from the interaction (as in the A-form) or from the initial and final state (as in the L- and V-forms), is form-dependent. In such a way, we are able to identify necessary conditions for all the three forms to give the correct high-energy result in the IPA case. We also explicitly obtain the order of magnitude of the error resulting from the error in the description of the wave functions in the vicinity of the singularity. We consider this at two levels of accuracy (depending on the accuracy of the description of the wave functions in the vicinity of the singularity). We first consider the leading-order results in $1/p$ that can be obtained by taking a simple description of the wave functions in the vicinity of the singularity. To illustrate the source of the general Stobbe factor, we then use a description that completely includes the strong e–N Coulomb interaction.

We begin in Sec. 2 with a general discussion of the AFT of singular functions. We discuss the connection with the photoabsorption matrix element and differences (modifications of the asymptotic AFT) required due to the presence of Coulomb functions. In Sec. 3, we begin the discussion of the behavior of the photoeffect matrix element in an IPA potential. Here, we take the simplest description of the wave functions, which provides an illustration of the main ideas. In Sec. 4, we consider the simplest case, photoabsorption by an s-

state in a purely Coulomb potential, neglecting retardation in order to make comparison with the well-known results obtained in the Born expansion approach. We there illustrate our AFT approach in more detail. In Sec. 5–7, we remove the constraints of the simplest case, identifying the resulting additional features. We show how the approach works for non-s-states (Sec. 5) and for a general IPA potential with a point Coulomb singularity (Sec. 6). We discuss relativistic and retardation contributions in Sec. 7. Finally, in Sec. 8, we show how more accurate results (together with a measure of their error) can be obtained by fully including in the wave functions the interactions that are strong in the vicinity of the singularity (e–N). We also assess the importance of the contributions arising from interactions that are weak in the vicinity of the singularity (screening, or correlations more generally). We discuss the convergence of the results to asymptotic forms with increasing energy. We explicitly obtain a common factor (the Stobbe factor) arising from the e–N interaction that contains all the slowly converging behavior. This explains why ratios of cross sections converge to asymptotic forms much more rapidly than the cross sections themselves. In Sec. 9, we summarize our conclusions.

2. GENERAL CONSIDERATIONS

In general, the final-state wave function in high-energy photoionization of a many-electron atom is of the form $\exp(i\mathbf{p}\cdot\mathbf{r}_1)\Phi_{\mathbf{p},\lambda}$, where $\mathbf{p}$ denotes the large momentum of one ejected electron (there must be at least one), $\mathbf{r}_1$ is its space coordinate, and λ denotes quantum numbers of other electrons in the final state. Because the outgoing electron wave function is described by a plane wave and incoming spherical waves at large distances (with appropriate long-range Coulomb logarithmic factors), these oscillations limit the range in $\mathbf{r}_1$ that contributes to the matrix element integral, which can be viewed as a FT in the electron momentum $\mathbf{p}$ of slowly varying functions. (Because we have assumed nonrelativistic energies, there are no oscillations of any retardation factor in the interaction in this range.) We discuss the remaining p-dependence in the Coulomb wave function in this range below. Because large ω necessarily implies large $\mathbf{p}$, the study of the photoabsorption matrix element at large energies is equivalent to the study of the asymptotic form of the FT.

The study of the asymptotic form of the FT arising in our problems is based on the theory of generalized functions [13]. By definition [14], a good function f is an infinitely differentiable function of n variables such that

$$R^l \frac{\partial f}{\partial x^{\alpha_1}\partial x^{\alpha_2}\ldots\partial x^{\alpha_n}} \to 0, \quad R\to\infty \tag{1}$$

for any l and m and any choice of the indices $\alpha_1, \alpha_2, \ldots, \alpha_n$ (with $\alpha_1+\alpha_2+\ldots+\alpha_n = m$), where $R \equiv (x_1^2+x_2^2+\ldots+x_n^2)^{1/2}$. (In the terminology of [14], these are called χ functions.) The theorem [13, Theorem 2, p. 15] says that the FT of a good function is a good function [13, 14]. This implies that asymptotically, the Fourier transform $g(p_1,\ldots,p_n)$ of a good function decreases faster than any power of $p \equiv (p_1^2+p_2^2+\ldots+p_n^2)^{1/2}$. We call this the AFT theorem. An example of such a function in three dimensions is given by $f_1(\mathbf{r}) = \exp(-r^2)$. For large p, the FT $F_1(\mathbf{p}) \propto \exp(-p^2/2)$ of this function decreases exponentially, i.e., faster than any power of $1/p$, in accordance with the AFT theorem.

The functions that appear in our photoionization matrix elements, even for the photoionization of a particle in a potential, are well localized (because the bound state is localized), but are singular [20], i.e., nondifferentiable, at coalescence points. The wave functions, which are eigenstates of a many-body Hamiltonian with Coulomb interactions, have singularities at the singularities of the Hamiltonian, which are located at points where the particles coalesce. We use the term coalescence points for the locations of these singularities. In general, there are double coalescence points where two particles meet[2] and multiple coalescence points where more than two particles coincide. The properties of wave functions in the near vicinity of these singularities, which are well understood for bound states [20, 21], can be extracted from the Schrödinger equation. They are known as coalescence properties, and for s-states, they are often called Kato cusp conditions. We use the term Kato cusp conditions more generally, to denote exact behavior of the wave functions at a two-particle singularity. (There must also be singularities in the e–γ interaction operator, depending on the form that we take.)

In the vicinity of a singularity, the functions whose FT is calculated can be written in terms of simpler functions f_s (with s standing for «simple») whose FT is known and a remainder O whose FT is asymptotically

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[2] Finite nuclear size does not affect our conclusions in any way because the distances probed at nonrelativistic energies are much larger than the size of the nucleus. A finite nuclear size cannot be relevant for photoabsorption (when the total cross section is considered, for example) even at ultrarelativistic energies, see Sec. 7.

negligible. We call this the partitioning (f_s+O) of functions. According to the theory of generalized functions, the FT of a generalized function with singularities is approximated by the FT of these simpler functions f_s, while the size of the FT of the remainder O gives a measure of the accuracy of the approximation. The point is that by taking f_s more accurately in the vicinity of the singularity, we can in principle achieve arbitrary accuracy [14, Theorem 19, p. 52]. A simple example of such a singular function is given by $f_2(\mathbf{r}) = \exp(-r)$. The FT of this function is $F_2(\mathbf{p}) \propto (1+p^2)^{-2}$, which indeed decreases as a power of p. By partitioning f_2 in terms of polynomials[3] in r and using

$$\lim_{\varepsilon\to 0} \int \exp\left[-(\varepsilon r + i\mathbf{p}\cdot\mathbf{r})\right] r^n d^3r = \\ = \frac{4\pi(n+1)!}{(ip)^{n+3}} \begin{cases} 0, & \text{even } n \ge 0, \\ 1, & \text{odd } n > 0 \end{cases} \qquad (2)$$

(where we assume that $p \neq 0$, and therefore do not include δ-function terms), we reproduce the expansion of $F_2(\mathbf{p})$ in powers of $1/p$. If we used some other partitionings, we would not obtain powers in $1/p$, but rather some other function of p, depending on the nature of f_s used. The point is that the asymptotic FTs of such simpler functions approach the exact FT for large p and the FT of the remainder vanishes faster, in accordance with the theory of the FT of generalized functions.

This is an illustration of the general idea. The functions that appear in our matrix element can be written in terms of simpler functions, which are required by the Kato conditions to have the Coulomb behavior in the vicinity of a two-particle singularity, as explained below. In obtaining leading-order results, or in simple cases that we consider for illustration, we use polynomials in r (the interparticle distance) as our simpler functions. These polynomials can be viewed as expansions in r (which can exist in IPA potentials). But in more general situations (with more electrons involved, e.g., as considered in [1]) we cannot assume that singular functions are expandable in infinite series in r in the vicinity of any singularity. In such cases, we can still partition a singular function in the vicinity of a singularity into a simple function (perhaps a polynomial or the Coulomb function) and a remainder, which may not necessarily be expandable but which vanishes faster than the simple function as r approaches the singularity. In obtaining our full IPA results in Sec. 8, partitioning in terms of Coulomb functions is required (because all orders in the e–N interaction are required). Such a choice is sufficient for our purposes; it gives accurate results neglecting the order $m\alpha^2/p^2$ (we use the system of units $\hbar = c = 1$) and allows us to collect all Coulomb slowly converging terms in (powers of) $\pi a/p$ (when full Coulomb functions are used), $a = mZ\alpha$, where Z is the nuclear charge and m is the electron mass. If better accuracy is required, one must go beyond functions with the Coulomb shape in the vicinity of a singularity.

Expansion of wave functions around the origin (which is the position of the e–N singularity) in terms of polynomials has been used previously in both single and double ionization by photoabsorption [16, 17, 22, 23] and in collisions [23]. Here, we illustrate generalizations of these approaches using the AFT theory [1, 2]. We can partition (e.g., use Coulomb functions, which are much better functions than polynomials near the singular point) around singular points that do not have to be at the origin in general and consider all singularities on the same footing. An important point of this approach is that it clarifies which singularities must be considered for these partitionings (there are more than one singularity in many-body wave functions and interactions in general [1]). As shown in [1], the singularities that must be considered are determined by the kinematics of outgoing electron momenta, identifying situations in which the number of the asymptotic FTs is minimized. Another important point of our approach is that we start from exact matrix elements (with exact wave functions) and extract and collect all contributions in the leading power of $1/p$, which determine the high-energy behavior (and the leading corrections in some cases). With our approach, we identify the dominant terms and avoid losing any of them; we also avoid uncontrolled introduction of spurious contributions. It is illustrated in [1] how both these problems have arisen in the use of approximate wave functions.

There is however a point of difference between our asymptotic matrix element and the asymptotic FT. Namely, after isolating the fast oscillating terms of the plane wave, the function left in the integrand still depends on the large momentum variable $\mathbf{p}$ (coming from the final-state wave function) through the pr-dependence (as for example in confluent hypergeometric functions in the Coulomb case). It might therefore be more appropriate to talk about a generalization of the FT. We see in what follows that this additional p-dependence is not a problem. The Coulomb modification of the FT results, as we demonstrate in Sec. 8,

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[3] Polynomial partitioning requires a convergence procedure; we multiply each term in f_s with $\exp(-\varepsilon r)$ and let $\varepsilon \to 0$ after the integration is performed. This is consistent with the definition of the FT of generalized functions [14, p. 33].

in a slowly converging factor, the Stobbe factor.

Accurate evaluation of the matrix element at high energies requires knowledge of both initial and final state electron wave functions at the singular point or at all singular points in general, if one goes beyond the IPA. However, how much of this knowledge is actually needed in a given calculation depends on the form of the matrix element used for that calculation. As we demonstrate in considering the leading-order result, only the normalization of the initial wave function at the e–N coalescence is required if the A-form is used. With other forms (V and L), we generally need further information about both the initial and final states. The exception is for the s-state ionization in the V-form, for which we need only the normalization and slope of the initial state at the coalescence. In any case, this knowledge gives us the leading contribution of the high-energy matrix element, which is generally accurate to the relative order $O(\pi m Z\alpha/p)$.

3. SINGULARITIES OF THE IPA MATRIX ELEMENT INTEGRAND

For a single electron in a potential, in the lowest order of the electron–photon interaction, the matrix element for photoionization by photoabsorption is given by (in units $\hbar = c = 1$)

$$M = \int \Psi_{\mathbf{p}}^{(-)*}(\mathbf{r}) I(\mathbf{r}) \Psi_i(\mathbf{r}) d^3r, \tag{3}$$

where $\Psi_i(\mathbf{r}) = R_{nl}(r) Y_l^m(\hat{\mathbf{r}})$ is the initial bound state normalized to unit integrated probability density (the hat denotes the unit vector), $\Psi_{\mathbf{p}}(\mathbf{r}) = \exp(i\mathbf{p}\cdot\mathbf{r})\Phi_{\mathbf{p}}^{(-)}(\mathbf{r})$ is the final electron continuum state normalized on the momentum scale (to asymptotically approach a distorted plane wave of the momentum $\mathbf{p}$ with the amplitude $(2\pi)^{-3/2}$), and $I(\mathbf{r})$ is the interaction operator, given in the three commonly used forms (keeping retardation to all orders) as

$$I_V = -ie^{i\mathbf{k}\cdot\mathbf{r}} \boldsymbol{\epsilon}\cdot\nabla, \tag{4}$$

$$I_L = im\left(\omega - \frac{k^2}{2m}\right) \boldsymbol{\epsilon}\cdot\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} - e^{i\mathbf{k}\cdot\mathbf{r}}(\boldsymbol{\epsilon}\cdot\mathbf{r})(\mathbf{k}\cdot\nabla), \tag{5}$$

$$I_A = \left(\omega - \frac{k^2}{2m}\right)^{-1} \times \\ \times \left[ie^{i\mathbf{k}\cdot\mathbf{r}}(\boldsymbol{\epsilon}\cdot\nabla)V(r) - \frac{1}{m}e^{i\mathbf{k}\cdot\mathbf{r}}(\mathbf{k}\cdot\nabla)(\boldsymbol{\epsilon}\cdot\nabla)\right]. \tag{6}$$

Here, $\boldsymbol{\epsilon}$ is the photon polarization and $V(r)$ is an IPA potential energy of the type $V(r) = -(Z\alpha/r)S(r)$, where $S(r)$ is a screening function, which we assume[4] can be described as a polynomial in r for small r, $S(r) = (1+s_1 r + s_2 r^2 + \ldots)$; the potential therefore has only a Coulomb divergence and is differentiable except at $\mathbf{r} = 0$. The singularity of the potential energy results in singularities in the wave functions $\Psi_{\mathbf{p}}$ and Ψ_i. These functions are not differentiable at the origin. The e–γ interaction operator in the L- and V-forms is regular in this sense, while in the A-form it is singular because it involves the singular potential $V(r)$, Eqs. (4)–(6). The large-p behavior of the Fourier transform of a slowly varying function of r is determined by its behavior near the coalescence point (because $pr \sim 1$, large p corresponds to small r) and only depends on the singular parts of the function. We thus partition the functions $\Psi_i(\mathbf{r})$ and $\Phi_{\mathbf{p}}^{(-)}(\mathbf{r})$ around the coalescence point $\mathbf{r} = 0$ (the only singular point here). The small-r behavior of these slowly varying portions of the integrand determine the AFT.

The partitioning $f_s + O$ in terms of polynomials of the initial (bound) state with quantum numbers (n, l, m) in an IPA potential with the Coulomb singularity is

$$\Psi_i(\mathbf{r}) = N_i^{IPA} r^l \times \\ \times \left[1 - \frac{a}{l+1} r + \lambda_2 r^2 + \lambda_3 r^3 + O(r^4)\right] Y_l^m(\hat{\mathbf{r}}). \tag{7}$$

In the simple function f_s (in which the terms are alternately regular and singular, with the regular first term, $r^l Y_l^m(\hat{\mathbf{r}})$), the first two terms are determined solely by the Coulomb singularity of the potential and are therefore known independently of the screening, except for the overall normalization factor N_i^{IPA} (which depends on the choice of the IPA potential). Higher-order terms in f_s in Eq. (7) depend on the screening of the IPA potential, which determines the λ_i coefficients. The fact that the first two terms in the parenthesis in Eq. (7) are determined by the Coulomb singularity is well known; it is a special case of the general behavior of wave functions at coalescence points of many-electron atoms [20, 21]. Namely, in the description of a bound-state many-electron atom wave function around any coalescence (which includes any electron–electron coalescence) in terms of the relative coordinate of the

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[4] Here, we assume a potential that can be expanded in integral powers of r in the vicinity of a singularity. Using a potential that is expandable in nonintegral powers of r (e.g., the Thomas–Fermi potential $V_{TF} = -Z\alpha/r + C_{TF} + O(\sqrt{r})$, where C_{TF} is a constant) would lead to nonintegral powers of $1/p$.

two coalescing particles, the first two terms are determined by the singularity of the corresponding part of the Coulomb potential, up to an overall factor, and there is a remainder that vanishes more rapidly than linearly in the coordinate. These two terms and the normalization constant are all that we need from the initial-state wave function (we also need information from the final state) in order to determine the leading contribution in $1/p$ to high-energy photoabsorption in any form.

In the final-state electron wave function, the situation is very similar, except that the normalization is not affected by screening in the limit of high momenta. According to [24–27], the wave function of a high-energy continuum electron state of momentum $\mathbf{p}$ in the vicinity of the Coulomb singularity of the IPA potential is essentially of a Coulomb form. As shown in [27] using the analytic perturbation theory, the corrections to the Coulomb wave function due to screening in the vicinity of the nucleus ($r \ll 1/a$, where $a = mZ\alpha$ characterizes the unscreened nuclear charge) decrease with the electron momentum as $O(1/p^2)$ relative to the Coulomb functions. This means that in the vicinity of the Coulomb singularity ($r \ll 1/a$), the wave function representing the outgoing electron of momentum $p \gg a$ can be written, following [25, 27], as

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C e^{i\mathbf{p}\cdot\mathbf{r}} \left[{}_1F_1\left(-i\frac{a}{p}, 1, -ipr(1+\cos\vartheta)\right) + + O\left(\frac{1}{p^2}; pr, \cos\vartheta, s_i\right)\right], \quad (8)$$

where $\cos\vartheta = \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}$, the first term in the right-hand side is the Coulomb term while the second term is the remainder, which vanishes faster than $1/p$ (denoted by $1/p^2$ in O). The functional dependence of O is also shown; the remainder contains all information on screening, symbolized by the coefficients s_i characterizing the small-distance behavior of the screened potential. According to the analytic perturbation theory [25, 27], an even more accurate continuum wave function of the Coulomb shape is obtained in the region $r \ll 1/a$ by shifting the electron momentum in Eq. (8) from p to p_C, by an amount determined by the parameters of the screened potential, and by replacing the normalization N_p^C (if the momentum scale normalization is used) by $\sqrt{p_c/p}\,N_{p_C}^C$. However, although such a Coulomb function is more accurate, its error still decreases as $1/p^2$ with large momentum p. We therefore do not need it here, but we use it in Sec. 8.

The result in Eq. (8) is important for our approach because as we show below, it implies that the terms in the partitioning of the final state around the coalescence that contribute to the high-energy matrix element are not affected by screening. We show this to the leading order in $1/p$, further simplifying f_s in the partitioning of Eq. (8). Because distances involved in the process are $r \sim 1/p$ and because we consider high energies for which $p \gg mZ\alpha$, while the wave functions are considered at fixed pr, the terms that are important for our discussion here involve terms up to linear in the parameter $mZ\alpha/p$, with further terms contributing to higher orders in 1/p. We write

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C e^{i\mathbf{p}\cdot\mathbf{r}} \left[1 - i\frac{a}{p} g^{(-)}\left(i(pr + \mathbf{p}\cdot\mathbf{r})\right) + + O\left(\frac{1}{p^2}; pr, \cos\vartheta, s_i\right)\right], \quad (9)$$

where O includes all contributions of the order a^2/p^2 and higher-order contributions from the full Coulomb function in Eq. (8), and

$$g^{(-)}(i\xi) = -\frac{1}{2\pi i}\oint_\Gamma e^{-i\xi t} \ln\left(\frac{t-1}{t}\right)\frac{dt}{t} = = \int_0^1 \left(e^{-i\xi t} - 1\right)\frac{dt}{t} \quad (10)$$

determines all contributions of the order a/p to the full Coulomb wave function for $pr \sim 1$. Here, Γ is a counterclockwise oriented closed contour encircling the cut $[0, 1]$. By inserting Eqs. (9) and (7) in Eq. (3), we obtain a series of integrals of functions that contain powers of r, the $g^{(-)}$ function, and angular functions. The function $g^{(-)}(i\xi)$ is needed in calculating the leading contribution to the high-energy matrix element in general. It contains p-dependence through pr, which may appear undesirable, at first sight, if we want to view this high-energy matrix element as a FT. It follows from explicit calculations, however, that there is no additional p-dependence in a FT integral also involving $g^{(-)}$ function despite the p-dependence of the $g^{(-)}$ function.

The factor $\exp(-\varepsilon r)$ is introduced in order to achieve a convergent integration of each term in the series; after the integration is performed, the limit $\varepsilon \to 0$ is taken. As noted in Sec. 2, this procedure is consistent with the definition of the FT of generalized functions [13]. For the AFT theorem (and we also assume for the AFT involving the $g^{(-)}$ function), we must understand the singularities of the integrand. The singularity properties of the wave functions are immediately identifiable in these series, which involve powers of r

and angular functions such as powers of $\hat{\mathbf{p}}\cdot\hat{\mathbf{r}} = \cos\vartheta$ and spherical harmonics. For example, r and $\cos\vartheta$ are singular at the origin (as functions of x, y, and z), but their product is not ($r\cos\vartheta = z$), nor are their squares (we also note that $r^l Y_l^m$ is regular).

We see in what follows that the leading contribution to the high-energy matrix element can be obtained in any form using only the first two terms in f_s of the respective partitioning of the initial and final state in Eqs. (7) and (9), while neglecting some of these first two terms may lead to erroneous results in some forms. Higher-order terms in the expansion give higher-order contributions in $1/p$, as is explained below and is demonstrated using simple examples in Secs. 4 and 5. To the leading order in $1/p$, the form-independent high-energy matrix element for photoabsorption in an IPA model is obtained from

$$M = N_i^{IPA} N_p^{C*} \lim_{\varepsilon\to 0} \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r) \times \\ \times \left[1 + i\frac{a}{p} g^{(-)*}\left(i(pr + \mathbf{p}\cdot\mathbf{r})\right)\right] I(\mathbf{r}) r^l \times \\ \times \left[1 - \frac{a}{l+1} r\right] Y_l^m d^3 r, \quad (11)$$

where $I(\mathbf{r})$ can take forms like Eqs. (4)–(6), which also contain different powers of r and angular functions.

Expression (11) is a form-independent term that gives the leading order in $1/p$ for large p. We see from Eq. (11) that the only difference from the purely Coulomb case is in the initial-state normalization, which depends on the IPA potential. All other terms are determined by the Coulomb singularity. Therefore, in an IPA model with a Coulomb singularity, information about screening persists at high energies only in the initial-state normalization. This behavior for high-energy photoabsorption in an IPA potential is known [26], but it is just one aspect of the persistence of the electron–electron interaction in high-energy photoabsorption, discussed within the AFT approach for two-electron atoms in [2].

In a matrix-element form, in which the interaction operator is regular (such as the V-form and L-form, to be denoted by I_V^R and I_L^R) rather than singular (as in the A-form, I_A^S), the contribution from the term in the integrand involving the first terms of the simple functions f_s of both the partitionings of Ψ_i and of $\Phi^{(-)}$ vanishes for any l (while in the A-form, this term gives the leading nonvanishing contribution). The leading nonvanishing contributions in such forms (L or V) involve the product of the first term from $\Phi^{(-)}$ (which is regular, to be denoted as R_f) with the second term in Ψ_i (singular, S_i) and the product of the second term from $\Phi^{(-)}$ (singular, S_f) with the first term in Ψ_i (regular, R_i). These two contributions are of the same order in $1/p$. In summary, in the leading order in $1/p$, we obtain the nonvanishing contribution from

$$M = \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r)\,[R_f + S_f] \times \\ \times \begin{bmatrix} I_L^R \\ I_V^R \\ I_A^S \end{bmatrix} [R_i + S_i] \to \\ \to \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r) \begin{bmatrix} R_f I_L^R S_i + S_f I_L^R R_i \\ R_f I_V^R S_i + S_f I_V^R R_i \\ R_f I_A^S R_i \end{bmatrix}. \quad (12)$$

We explicitly evaluate Eq. (11) for an H-like potential in the next two sections, and we discuss the obtained leading-order results further, comparing them with the Born-approximation results in different forms. The two approaches must of course agree. We note that the results in Eqs. (11) and (12) reflect the importance of the singularity region. This means that if one wants to improve results, one needs to partition functions in terms of functions that better describe the behavior in the vicinity of the singularity. (This is only one of the points of distinction from a perturbative approach, e.g., the Born expansion. The Born expansion gives the same weight to all regions, while the AFT approach tells us that the singularity region is important for high-energy photoabsorption.) Partitioning of the wave functions in terms of functions that are more accurate in the vicinity of the singularity provides more accurate results. The results in Sec. 8, for example, are obtained using partitioning in terms of Coulomb functions (which include the e–N interaction to all orders).

The integrals involved in evaluating Eq. (11) are elementary and are of two types. The integrals that involve the first term in the square brackets from the final state and powers of r and products of spherical harmonics from the e–γ interaction and the initial state[5] are given by

$$J_1 = \lim_{\varepsilon\to 0} \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r) r^n Y_L^M(\hat{\mathbf{r}}) d^3 r = \\ = \frac{2\pi(n+2)!}{(ip)^{n+3}} Y_L^M(\hat{\mathbf{p}}) f_{n+3}^L, \quad (13)$$

where

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[5] These products of spherical harmonics can be combined into one Y_L^M.

$$f_k^L = \int\limits_{-1}^{1} \frac{P_L(x)dx}{(x - i\varepsilon)^k} \tag{14}$$

and $P_L(x)$ is the Legendre polynomial. The integrals of the second type, involving $g^{(-)}(i(pr + \mathbf{p}\cdot\mathbf{r}))$ from the final state and powers of r and products of spherical harmonics from the e–γ interaction and the initial state, are given by

$$\begin{aligned} J_2 &= \\ &= \lim_{\varepsilon\to 0} \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r) g^{(-)*}(i(pr + \mathbf{p}\cdot\mathbf{r})) r^n Y_L^M d^3r = \\ &= \frac{2\pi(n+2)!}{(ip)^{n+3}} Y_L^M(\hat{\mathbf{p}}) h_n^L, \end{aligned} \tag{15}$$

where

$$\begin{aligned} h_n^L = \int\limits_{-1}^{1} dx\, P_L(x) \times \\ \times \left\{ \sum_{j=0}^{n+1} \frac{(-1)^{n-j}(x - i\varepsilon)^{n+2-j} - 1}{(n+2-j)(x - i\varepsilon)^{n+3}} + \right. \\ \left. + \frac{i\pi + \ln(x - i\varepsilon)}{(x - i\varepsilon)^{n+3}} \right\}. \end{aligned} \tag{16}$$

In performing the radial integration in Eq. (15), we used the integral form (the second form in Eq. (10)) of the function $g^{(-)}(i(pr + \mathbf{p}\cdot\mathbf{r})$. The integrations over x in Eqs. (14) and (16) are elementary, and we evaluate them for specific L in Secs. 4 and 5.

Expressions (13) and (15) show how higher powers in r lead to higher powers in $1/p$. We note that while J_2 gives a nonzero result for any n and L (because g contains both regular and irregular terms), J_1 is zero for n and L for which $r^n Y_L^M$ is regular, in accordance with the AFT theorem. Therefore, depending on the form used, at least one of the two first terms in the f_s functions of electron states gives a contribution to the leading order of the matrix element, while all further terms beyond the first two give higher-order contributions.

4. THE SIMPLEST CASE: GROUND STATE IONIZATION OF AN H-LIKE ATOM

We now discuss how the leading contribution to the matrix element is obtained in the three forms in Eqs. (4)–(6), in the simple and familiar case of photoionization of the ground state of an H-like atom with retardation neglected.

When we neglect retardation and use the nuclear Coulomb potential, the A-, V-, and L-forms of the matrix element are obtained using

$$I_A = \frac{iZ\alpha}{\omega} \frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{r}}}{r^2}, \quad I_V = -i\boldsymbol{\epsilon}\cdot\nabla, \quad I_L = im\omega\boldsymbol{\epsilon}\cdot\mathbf{r} \tag{17}$$

for the interaction operators, where ω is the photon energy and $\boldsymbol{\epsilon}$ is the photon polarization. The V- and L-forms of the interaction operator are regular, but the A-form is not, because it was obtained by taking the gradient of the potential. We note that the A-form is irregular at the origin both because it is divergent and because its value near the origin depends on the direction of approach.

As we have seen, the large-p asymptotic behavior of the FT of a slowly varying function of r is determined by its behavior near the coalescence point; it only depends on the singular parts of the function in the small-r limit. We therefore begin by partitioning the functions $\Psi_i(\mathbf{r})$ and $\Phi_{\mathbf{p}}^{(-)}(\mathbf{r})$ around the coalescence point $\mathbf{r} = 0$ (the only singular point here). We write

$$\begin{aligned} &\Psi_i(\mathbf{r}) = N_i(1 - ar + \ldots), \\ &\Phi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C \left(1 - i\frac{a}{p} g^{(-)}\left(i(pr + \mathbf{p}\cdot\mathbf{r})\right) + \ldots\right). \end{aligned} \tag{18}$$

If we proceed as described in the previous section, we obtain the familiar high-energy expression, which is usually obtained in the V-form by assuming that the energetic outgoing electron can be regarded free and can be represented by a plane wave [28–30]. But in our procedure, we must be more careful and must not make such an assumption, which is incorrect in general (e.g., for non-s-states or even for s-states in the L-form).

Substituting Eqs. (18) and (17) in the matrix element in Eq. (3), we obtain a series of integrals involving powers of r and powers of $\cos\vartheta$. (We choose the $\mathbf{p}$ direction as the z axis in this integration, and only functions of $\cos\vartheta$ therefore appear). Applying $\boldsymbol{\epsilon}\cdot\nabla\Psi_i = \epsilon\cdot\hat{\mathbf{r}}\ (-a + a^2 r + \ldots)$, we obtain integrals of the two types in Eqs. (14) and (16). The integral involving the first term from f_s of the partitioning of $\Phi_p^{(-)}$ and terms from the partitioning of Ψ_i is [1]

$$\begin{aligned} &\int \exp\left[-(\varepsilon + i\mathbf{p}\cdot\mathbf{r})\right] r^n \boldsymbol{\epsilon}\cdot\hat{\mathbf{r}}\, d^3r = \\ &\qquad = \frac{2\pi(n+2)!\ \boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{(ip)^{n+3}} C_n, \\ &C_n = \begin{cases} -2/(n+1), & \text{even } n \geq -2, \\ 0, & \text{odd } n > -1, \\ i\pi, & n = -1. \end{cases} \end{aligned} \tag{19}$$

We note that the zero result for odd $n > -1$ follows from the AFT theorem because the integrand function is not singular; for even n and for $n = -1$, the integrand function is singular. Integrals involving the term $g^{(-)}(pr, \cos\vartheta)$ in the partitioning of $\Phi_p^{(-)}$ are easily performed using the integral representation in Eq. (10). We obtain [1]

$$\int \exp\left[-(\varepsilon + i\mathbf{p}\cdot\mathbf{r})\right] g^{(-)*}\left(i(pr + \mathbf{p}\cdot\mathbf{r})\right) r^n \boldsymbol{\epsilon}\cdot\hat{\mathbf{r}}\, d^3r = \\ = \frac{2\pi\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{(ip)^{n+3}} D_n, \quad (20)$$

where

$$D_n = 2(n+2)!\ (1 - i\pi)/(n+1)$$

for even $n \geq 0$ and

$$D_n = \sum_{k=0}^{(n-1)/2} \frac{2k+2}{n-2k}$$

for odd $n > 0$, $D_{-2} = i\pi - 2$, and $D_{-1} = -\pi^2/2 - i\pi - 2$.

In both Eqs. (19) and (20), the p-dependence of the results is seen by inspection, resulting from the nature of the scaling in pr. Equation (19) shows that higher powers in r lead to higher powers in $1/p$, but nonvanishing contributions come only from singular terms. We use this behavior in identifying the leading contributions in $1/p$ in our calculations. In the partitioning of the final-state wave function in Eq. (18), the first term is of course regular, while the second term ($g^{(-)}$) is singular. The same is true for the initial state, not only for this s-state, but for any state with angular momentum l for which the first terms of f_s in the partitioning around $\mathbf{r} = 0$ are

$$\Psi_i \sim r^l Y_l^m (1 - ar/(l+1) + \ldots).$$

We further note that in the case of an s-state, the contributions from the first term of Ψ (which is then a constant) vanish in the V-form because of the derivative in the interaction operator $\boldsymbol{\epsilon}\cdot\nabla$. For non-$s$-states, there are nonvanishing contributions from this first term (when multiplied with g from $\Phi^{(-)}$), which must be taken into account in order to obtain the correct high-energy matrix element, which would be missing if a continuum plane wave had been assumed (neglecting the terms in g).

Therefore, in the V-form for the s-state case, the leading contribution involves only the first term in Φ and the second term in the partitioning of the initial state Ψ, justifying the usual calculation involving the plane-wave approximation for the final state. Using Eq. (19), we obtain the familiar result for s-state ionization neglecting retardation (dipole approximation),

$$M = -A\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3} C_0 = 2A\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3}, \quad (21)$$

where $A = 4\pi a N_i N_p^C$.

We now show that we obtain the same result using the same procedure in the L-form. Here, the singularity of the final state also contributes, however, and an incorrect result is obtained if a plane wave is assumed to provide an adequate description of the energetic electron. In terms of our approach, such an assumption would imply taking the term in the integrand involving the first term from the partitioning of Φ and the second term from the partitioning of Ψ. This contribution is

$$6A\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3} C_2 = 4A\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3}$$

(we have put $\omega = p^2/2m$), which is twice the correct result in Eq. (21). But as we have already explained, we must include all terms contributing to the same power in $1/p$. We must therefore include the term in the integrand that involves the second term $g^{(-)}$ from Φ^- and the first term from Ψ_i. This gives the contribution

$$-\frac{A}{4}\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3} D_1 = -2A\frac{\boldsymbol{\epsilon}\cdot\hat{\mathbf{p}}}{p^3}.$$

The sum of the two terms gives the correct high-energy limit, Eq. (21), showing that the L-form and the V-form indeed agree.

Finally, we can calculate the photoeffect matrix element in the A-form using the same procedures. As we have already remarked, the electron–photon interaction operator I_A, Eq. (17), is singular at the origin in this form, with a singularity arising from the singularity of the potential. The leading contribution to the matrix element in Eq. (3) in the A-form comes from the first terms in the partitioning of $\Phi^{(-)}$ and Ψ_i only (a term in the integrand that did not contribute in the L- and V-form due to its regularity, not only for the s-state case, but for any l). All other terms contribute with higher powers in $1/p$. For the s-state, the result in the A-form is easily evaluated with the help of Eq. (19) for $n = -2$, again giving the same result, i.e., Eq. (21). (We note that in the A-form, the next-to-leading term in $1/p$ can also be obtained without referring to screening; it involves $g^{(-)}$ or ar. We use this fact in Sec. 8 in discussing convergence toward the high-energy limit.)

5. BEYOND s-STATES

We now discuss non-s-states, staying within our simple H-like model without retardation, and building on the general features already encountered in the s-state case. We again utilize the AFT theorem, identifying the singular part of the integrand function, and evaluating the dominant contributions through the partitioning of the bound state in Eq. (7) and the partitioning of the final state in Eq. (9) around the electron–nucleus coalescence. The required integrals are given in Eqs. (13) and (14). Now, however, a plane wave does not adequately describe the fast outgoing electron, except in the A-form, in which the electron–photon interaction provides the needed singular behavior for the integrand function.

The leading contribution in $1/p$ to the high-energy photoabsorption matrix element M in Eq. (3), which in the A-form is obtained by taking the leading, regular terms in the partitioning of the initial and final electron states, is

$$\begin{aligned} M_0^{l,m} = {} & \frac{-2imZ\alpha N_i^C l!}{(2\pi)^{3/2}(ip)^{l+3}}\,\frac{4\pi}{3} \times \\ & \times \sum_{\mu} Y_1^{\mu *}(\boldsymbol{\epsilon}) \int d\Omega \frac{Y_1^{\mu}(\hat{\mathbf{r}})Y_l^m(\hat{\mathbf{r}})}{(\cos\vartheta - i\varepsilon)^{l+1}}. \end{aligned} \quad (22)$$

The remaining angular integration involves only elementary integrals (13). For $l = 1$, the case that we discuss below in other forms for illustration, Eq. (22) gives

$$M_0^{1,m} = (-1)^{1-m}\frac{8\pi i a}{p^4} N_i N_p^C Y_1^m(\boldsymbol{\epsilon}). \quad (23)$$

(For simplicity, expression (22) is obtained with the z axes taken in the direction of $\hat{\mathbf{p}}$. Rotation to fixed coordinates must be made in integrating over electron angles.) We note that the part M_0 of the matrix element M is obtained in the A-form using plane waves. In other forms, the calculation of M_0 requires higher-order (singular) terms, from both initial and final states in general. We therefore do not call M_0 the first (plane-wave) Born approximation result, because it is the first Born approximation only in the A-form and is a higher-order Born result in other forms in general.

While a plane wave is sufficient for an initial s-state in the V-form, this is not true for $l > 0$, as we demonstrate. With the V-form, it is convenient to express $\boldsymbol{\epsilon}\cdot\nabla\Psi_i$ as

$$\begin{aligned} \boldsymbol{\epsilon}\cdot\nabla\left[R_l(r)Y_l^m(\hat{\mathbf{r}})\right] = {} & \sqrt{\frac{4\pi}{3}}\sum_{\nu=-1}^{1} Y_1^{\nu *}(\boldsymbol{\epsilon}) \times \\ & \times \left[\sqrt{\frac{l+1}{2l+3}}\langle 1,\nu;l,m|l+1,m+\nu\rangle Y_{l+1}^{m+\nu}(\hat{\mathbf{r}}) \times \right. \\ & \times \left(\frac{d}{dr} - \frac{l}{r}\right)R_l - \\ & - \sqrt{\frac{l}{2l-1}}\langle 1,\nu;l,m|l-1,m+\nu\rangle Y_{l-1}^{m+\nu}(\hat{\mathbf{r}}) \times \\ & \left. \times \left(\frac{d}{dr} + \frac{l+1}{r}\right)R_l\right], \end{aligned} \quad (24)$$

where $\langle 1,\nu;l,m|L,M\rangle$ are the Clebsch–Gordan coefficients. For $l > 0$, the term with the lowest power in r in the partitioning of the function in Eq. (24) around the coalescence ($\mathbf{r} = 0$) is regular, and it comes from the second term of Eq. (24). Therefore, for the L-form, the term $g^{(-)}$ from the final-state function Φ^- also contributes to the lowest order. The exception, for the V-form, is the s-state, as we saw in the previous subsection, because the second term in Eq. (24) is zero and the lowest power in r is singular for $l = 0$.

For illustration, we consider the initial $l = 1$ case. Inserting expression Eq. (24) for $l = 1$, using a linear polynomial in the partitioning around the coalescence $R_1 = N_i r[1 - (a/2)r + O(r^2)]$, including contributions from the $g^{(-)}$ term, and performing the integration by choosing the direction of $\mathbf{p}$ as the z axis, we obtain the matrix element in the V-form as

$$\begin{aligned} M_V = {} & iaN_iN_p^C Y_1^m(\boldsymbol{\epsilon}) \int \exp(-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r) \times \\ & \times \left[\frac{(-1)^m}{2^{|m|}\cdot 3}P_2(\cos\vartheta)r + \frac{2}{3}r - \frac{i}{p}g^{(-)*} \times \right. \\ & \left. \times\ (ipr(1+\cos\vartheta))\right] d^3r = \\ & = (-1)^{1-m}\frac{8\pi i a}{p^4}N_iN_p^C Y_1^m(\boldsymbol{\epsilon}), \end{aligned} \quad (25)$$

which coincides with the result obtained in the A-form, Eq. (22). Assuming that a plane wave is an adequate representation of the fast electron wave function and therefore neglecting the contribution from the final-state singularity, one would obtain a nonzero result (in the chosen frame, where $\mathbf{p}$ is directed along the z axes) only for the angular momentum projection $m = 0$, and even that result would be erroneous by the factor 2. The contribution to the matrix element in Eq. (25) coming from the g function part is $-8\pi i a N_i N_p^C Y_1^m(\boldsymbol{\epsilon})/p^4$.

In both V- and L-forms, the interaction of the outgoing electron with the potential («final-state interaction») contributes for any $l > 0$. In contrast, in the A-form, the transition operator is singular and only the leading terms (the lowest powers in r) in both initial and final states are needed for any l to obtain the correct leading contribution.

6. SCREENED POTENTIALS

We now demonstrate that the previous results are sufficient to determine the asymptotic behavior of nonretarded photoabsorption in a general central potential to the leading order in $1/p$. The entire previous discussion, although given for a nuclear point Coulomb potential model, is in fact valid for a general IPA potential that has a singularity of the Coulomb potential at the nucleus. Our discussion relied on the behavior of wave functions and interactions at this singularity. For the leading terms in the partitionings that we utilized, these behaviors are the same for an IPA potential as long as it is Coulomb at the singularity. To see the effects of the difference between an IPA potential (with the Coulomb singularity) and a pure Coulomb potential, we consider a potential energy of the type $V(r) = -(Z\alpha/r)S(r)$, where $S(r)$ is a screening function that behaves as $S(r) = (1 + s_1 r + s_2 r^2 + \ldots)$ for small r, as assumed in Sec. 3.

The interaction operators in the L- and V-forms are independent of the potential. In the A-form, we obtain

$$I_A^{IPA} = -\frac{i}{\omega}[V(r), \boldsymbol{\epsilon}\cdot\nabla] = \frac{i}{\omega}\boldsymbol{\epsilon}\cdot\nabla V(r). \qquad (26)$$

The partitioning of I_A^{IPA} around the coalescence gives

$$I_A^{IPA} = \frac{iZ\alpha\boldsymbol{\epsilon}\cdot\hat{\mathbf{r}}}{\omega}\left(\frac{1}{r^2} - s_2 - 2s_3 r + \ldots\right). \qquad (27)$$

We note that the term involving s_2 in Eq. (27), which is regular, contributes three more powers relative to the first term. In contrast, the first term from wave functions involving screening contribute with two more powers in $1/p$.

We thus conclude that in the leading order, the same expression for photoionization at high energies is obtained in the IPA potential and in the Coulomb case (in Sec. 8, we show that this is in fact true in the first two orders). The normalization factors N_i^{IPA} are different, however, and IPA predictions therefore differ from the purely Coulomb case prediction by these factors.

7. RETARDATION AND RELATIVITY

We now discuss the inclusion of retardation. This changes the forms of the interaction operators. In the V-form, the change is simple: the retarded interaction is $I_V = -i\exp(i\mathbf{k}\cdot\mathbf{r})\boldsymbol{\epsilon}\cdot\nabla$, where $\mathbf{k}$ is the photon momentum. In the L- and A-forms, obtained by applying commutator relations to the V-form, the momentum $\mathbf{k}$ also appears in factors multiplying $\exp(i\mathbf{k}\cdot\mathbf{r})$, as can be seen from Eqs. (4)–(6). In evaluating the integrals, we need to specify how to deal with the photon retardation oscillating term $\exp(i\mathbf{k}\cdot\mathbf{r})$ in the e–γ interaction $I(\mathbf{r})$. One way, particularly if retardation to a certain order in $\mathbf{k}$ is considered, is to expand $\exp(i\mathbf{k}\cdot\mathbf{r})$ in powers of $\mathbf{k}\cdot\mathbf{r}$. Another way of dealing with $\exp(i\mathbf{k}\cdot\mathbf{r})$ is to attach it to the fast oscillating term $\exp(-i\mathbf{p}\cdot\mathbf{r})$ and consider the FT in the variable $\Delta = \mathbf{p}-\mathbf{k}$, because $\mathbf{p}-\mathbf{k}$ is large in the nonrelativistic region whenever $\mathbf{p}$ is large, and our arguments using the AFT theorem in the asymptotic region apply. We note here that in the IPA single ionization from the ground state, retardation effects give a contribution of the relative order $(v/c)^2$ [31, 32], where v is the velocity of the outgoing electron, which is of the same order as the relativistic contribution. This fact is used in the case of a two-electron atom [1] to argue that retardation effects have the same relative contribution in single ionization and in double ionization in the region, where the shake-off mechanism is dominant, due to factorization of the matrix element into a (retardation-independent) correlation term and (generally, retardation-dependent) absorption term.

We however note that at relativistic energies, when $\mathbf{p} \sim \mathbf{k}$, neither expanding in k nor assuming Δ large (in comparison to m) is generally valid. It is still true in certain kinematic situations, but these are not dominant for the photoabsorption processes at those energies. Namely, at relativistic energies (and as $\omega \to \infty$), a region around the nucleus of the Compton wavelength distances continues to contribute to photoabsorption, for arbitrarily high energies. This implies that although it is a relatively small region, the final-state wave function in the whole region, not just at the point of coalescence, is needed, and certain knowledge to all orders in a is required [22]. Under the analyticity assumption, the region is characterized by an expansion around the origin, and expansion of the matrix element as a series in a/Δ is still possible. The plane-wave approximation is no longer valid in any form, but partitioning in terms of Coulomb functions is fully justified.

8. CONVERGENCE OF THE CROSS SECTIONS TO THE HIGH-ENERGY LIMIT. THE STOBBE FACTOR

Here, we discuss the rate of convergence toward the exact IPA high-energy limit for the cross sections that we have obtained using the asymptotic behavior of matrix element (11). The ratio of the first correction to the leading contribution is of the order $1/p$, and it gives a very slow convergence of the matrix elements and cross sections. In fact, it converges as $\pi a/p \sim \pi\sqrt{E_K/\omega}$, where E_K is the K-shell binding energy. We note that a slowly converging factor (i.e., converging as $\pi a/p$ relative to the asymptotic constant value) exists in the final-state normalization, which is

$$N_p^C = \frac{1}{(2\pi)^{3/2}}\Gamma\left(1+i\frac{a}{p}\right)e^{\pi a/2p}. \tag{28}$$

But there are also other Coulomb terms with this slow convergence (e.g., the first correction, which is unaffected by screening). In fact, if partitioning of the initial state was performed in terms of polynomials, a similar slowly converging term would come from each term of the polynomial. Because of this and also because of the possibility of large Z, we include the e–N interaction completely in both the initial and final states by partitioning the wave functions in the vicinity of the singularity in terms of Coulomb functions. Formally, this means that we write the initial-state wave function as

$$\Psi_i^{IPA}(\mathbf{r}) = \frac{N_i^{IPA}}{N_i^C}\Psi_i^C(\mathbf{r}) + O\left[(\lambda_2^C-\lambda_2)r^{l+2}\right], \tag{29}$$

where λ_2 (λ_2^C) is the coefficient multiplying the third term in a polynomial partitioning of the IPA (Coulomb) wave function (7), $\Psi_i^C(\mathbf{r})$ is a normalized Coulomb wave function with the same quantum numbers as $\Psi_i^{IPA}(\mathbf{r})$, and $O[(\lambda_2^C-\lambda_2)r^{l+2}]$ represents the difference between the Coulomb and screened third term in a polynomial partitioning of the wave functions and all higher-order differences. The terms represented by O are small, as we discuss below.

For the final state, we take the Coulomb part of Eq. (8), but with a shifted energy and with the corrected normalization [25, 27]. According to [25, 27], as already mentioned, the exact IPA wave function is Coulomb in the vicinity of the e–N singularity. A sufficiently accurate function (containing the dominant terms of the relative order $1/p^2$) is obtained if the shifted momentum p_C is used instead of the true momentum p. The momentum p characterizes the electron at large distances from the nucleus. If we want to describe the screened wave function in the vicinity of the nucleus by a Coulomb function, we must use, according to [25, 27], the shifted momentum p_C. In addition, if the function is normalized on the momentum scale, the normalization is affected and is given by $N_p^{IPA} = \sqrt{p_C/p}\,N_{p_C}^C$. The final state is therefore given by

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = \sqrt{\frac{p_C}{p}}\Psi_{\mathbf{p}_C}^{(-)}(\mathbf{r}) + O\left(\frac{1}{p^2}\right), \tag{30}$$

where the shifted momentum p_C is [25]

$$\frac{p^2}{2m} - \frac{p_C^2}{2m} = |E_B^C| - |E_B^{IPA}|, \tag{31}$$

with E_B^C (E_B^{IPA}) denoting the hydrogen-like (IPA) binding energy of the state that is ionized.

We arrive at the following approximation for the IPA matrix element:

$$M = \frac{N_i^{IPA}}{N_i^C}\sqrt{\frac{p_C}{p}}\int \Psi_{\mathbf{p}}^{C(-)*}(\mathbf{r})I_A(\mathbf{r})\Psi_i^C(\mathbf{r})d^3r + {}$$
$$+ O\left(\frac{1}{p^2}\right) = \frac{N_i^{IPA}}{N_i^C}\sqrt{\frac{p_C}{p}}M_l^C + O\left(\frac{1}{p^2}\right). \tag{32}$$

From Eq. (32), it immediately follows that at high energies,

$$d\sigma^{IPA} = \left(\frac{N_i^{IPA}}{N_i^C}\right)^2 d\sigma^C + O\left(\frac{1}{p^2}\right), \tag{33}$$

where $d\sigma^C$ is the differential cross section obtained from Coulomb H-like wave functions calculated at the shifted momentum p_C and O indicates how rapidly the error decreases. (The momentum p from the phase space cancels p from the factor p_C/p leaving only the shifted momentum p_C in the right-hand side of Eq. (33).) The error in Eq. (33) is determined by the errors in the wave functions. According to the results in [25], the difference between screened and Coulomb functions is very small when unnormalized functions (with the same first coefficient in the expansion taken) are compared; for potentials with a polynomial expansion, this difference decreases as $1/p^2$ for small r[6].

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[6] We note that the use of a potential that cannot be expanded in integral powers of r might not give a small correction vanishing as $1/p^2$, as given in Eq. (33). For example, the Thomas–Fermi potential (see footnote 4) leads to a correction vanishing slower, i.e., as $1/p^{3/2}$. However, the Thomas–Fermi model fails in the vicinity of the nucleus (which is the region determining high-energy photoabsorption), where it predicts a too large electron density, see, e.g., B. G. Englert and J. Schwinger, Phys. Rev. A **29**, 2331 (1984).

This implies that dominant terms of the relative order $1/p^2$ are collected. We illustrate the fast convergence of this procedure for the cases involving low-Z atoms (He) and outer shells of higher-Z atoms (the L-state of Ne).

For Coulomb states, the integrals in Eq. (32) can be evaluated analytically. As illustrative examples, we have the cross section per electron for the electron ionization from the $1s$, $2s$ and $2p$ shells [15]

$$\sigma^C_{1s} = \frac{32\pi a^5 \alpha p}{3m^3\omega^3(p^2+a^2)} 2\pi \frac{a}{p} \left[\exp \frac{a}{p}\left(\pi - 4\,\mathrm{arctg}\,\frac{p}{a}\right)\right] \times \left[\exp\left(\frac{\pi a}{p}\right) - \exp\left(-\frac{\pi a}{p}\right)\right]^{-1}, \qquad (34)$$

$$\sigma^C_{2s} = \frac{4\pi a^5 \alpha p (p^2+a^2)}{3m^3\omega^3[p^2+(a/2)^2]^2} 2\pi \frac{a}{p} \times \exp\left[\frac{a}{p}\left(\pi - 4\,\mathrm{arctg}\,\frac{2p}{a}\right)\right] \times \left[\exp\left(\frac{\pi a}{p}\right) - \exp\left(-\frac{\pi a}{p}\right)\right]^{-1}, \qquad (35)$$

$$\sigma^C_{2p} = \frac{\pi a^7 \alpha p [p^2+(11/12)a^2]}{3m^3\omega^3[p^2+(a/2)^2]^3} 2\pi \frac{a}{p} \times \exp\left[\frac{a}{p}\left(\pi - 4\,\mathrm{arctg}\,\frac{2p}{a}\right)\right] \times \left[\exp\left(\frac{\pi a}{p}\right) - \exp\left(-\frac{\pi a}{p}\right)\right]^{-1}. \qquad (36)$$

To illustrate the meaning of Eq. (33), we apply it to the calculation of high-energy photoabsorption and compare the result with those obtained within the full Fock–Slater IPA calculations. Our comparison with relativistic calculations is fully justified for low-Z atoms and for s-shells of higher-Z atoms, for which retardation and relativistic contributions cancel to a high degree even at higher energies. However, for our illustrative purposes, we also show p-state results for Ne, for relatively small photon energies.

In Table 1, we show the total cross section for K-shell ionization obtained from Eq. (33) for $Z = 2$ using $(N_i/N_i^C)^2 = 0.7358$ (which indicates large screening) [33] and compare it with the results of the full IPA calculations from [33]. As we see from Table 1, the agreement between the high-energy result in Eq. (33) and the full IPA calculations is already very good at 1 keV, despite the large screening; in the energy range 1–2 keV, the disagreement is around 1–2 %. This is to be compared with the lowest-order result, which gives about 50 % disagreement in the same energy range, as indicated in Table 1 by the value of the factor $\exp(-a\pi/p)$ (see the explanation for this factor below).

Table 1. The total cross sections σ_K for photoabsorption from the K-shell of He ($Z = 2$) obtained using Eq. (33) in comparison with the full IPA calculations σ^K_{Sc}; $\exp(-a\pi/p)$ is the Stobbe factor

ω, keV	σ_{1s}, b Eq. (33)	σ^K_{Sc}, b Ref. [33]	$\exp\left(-\frac{a\pi}{p}\right)$
1	396	402	0.542
1.5	107	109	0.596
2	41.7	43.2	0.633
3	10.9	11.2	0.682
4	4.20	4.23	0.715
5	1.99	2.03	0.739
6	1.08	1.10	0.757
8	0.408	0.411	0.784

For the L-state of Ne, screening is even larger ($(N_i/N_i^C)^2 = 0.4386$ for $2s$ state and $(N_i/N_i^C)^2 = 0.2277$ for $2p$). In Table 2, we show the total cross section for the $2s$ and $2p$ states of Ne and compare them with the full relativistic IPA calculations. For the $2s$ state, Eq. (33) gives results that converge to the full IPA result very fast; the disagreement is around 6 % at 1 keV and is less than 1 % at 4 keV. Similarly, the results in Eq. (33) for the $2p$ state converge rapidly to IPA results in the same energy range. This very good agreement between the results in Eq. (33) and the full IPA results already at relatively small energies, even for Ne, can be explained by the properties of IPA wave functions in the vicinity of the Coulomb e–N singularity. Namely, at the photon energy region 1–2 keV, the distances involved (distances around the singularity at which the momentum is transfered between the electron and the nucleus) are within the K-shell orbit for Ne, and well within the K-shell orbit for He, where the screening is small. Therefore, the shapes of the wave functions at these distances are basically Coulomb. This is a very important point that we use and generalize in our approach. The high-energy photoabsorption is essentially of the Coulomb type. This means that the high-energy behavior of cross sections (we here mean the keV range, as in our examples) is de-

Table 2. The total cross sections σ_{2s} and σ_{2p} for photoabsorption from the respective subshells $2s$ and $2p$ of Ne ($Z = 10$) obtained using Eq. (33) in comparison with the full IPA calculations σ_{Sc}^{2s} and σ_{Sc}^{2p}; $\exp(-\pi a/p)$ is the Stobbe factor

ω, keV	σ_{2s}, b Eq. (33)	σ_{Sc}^{2s}, b Ref. [33]	σ_{2p}, b Eq. (33)	σ_{Sc}^{2p}, b Ref. [33]	$\exp\left(-\frac{a\pi}{p}\right)$
1	11276	10600	5629	5416	0.039
2	1932	1895	492	495	0.090
4	289	290	37.4	38.9	0.174
8	38.5	39.1	2.51	2.65	0.286
10	19.7	20.0	1.030	1.092	0.325
15	5.67	5.77	0.1987	0.2144	0.398
20	2.309	2.353	0.0607	0.0669	0.449
30	0.637	0.651	0.0112	0.0128	0.519
50	0.122	0.125	0.00129	0.00159	0.600

termined by the properties of functions near the singularity, which is of the Coulomb type. The screening effects enter these IPA examples, of course, but in a simple way as a constant factor. By straightforward generalization of these findings in high-energy many-body calculations, we can significantly simplify calculations involving e–e correlation, as shown in [1].

Another important point that we want to make in this subsection, relevant for more complex systems [1, 34], is the relatively fast convergence of the ratios of photoabsorption cross sections to the results predicted by lowest-order results (the Born approximation results in the A-form). We first note that the slowest converging factor in our examples in Eqs. (34)–(36) is $\exp(-\pi a/p)$. In partitioning wave functions around the coalescence, we obtain this factor by collecting all Coulomb interaction in the final state for each term in the partitioning of the initial state. The factor is therefore present for any state. The existence of a common slowly converging factor provides fast converging ratios of the cross sections. Further, the ratios of the cross sections for ionization from subshells of the same shell converge particularly fast, as we illustrate using our examples for the L-shell, Eqs. (35) and (36). In our examples, the ratio

$$\frac{\sigma_{2s}}{\sigma_{2p}} \sim \omega + \frac{a^2}{12m} + O\left(\frac{a^2}{\omega}\right) \tag{37}$$

is a nearly linear function of the photon energy ω in the keV range. If we had used the lowest-order result in $1/p$, we would obtain $\sigma_{2s}/\sigma_{2p} \sim \omega$, which is very similar to the exact result (in the keV range for Ne, for example), although the first-order results for cross sections differ by an order of magnitude from the exact results in this energy range, as indicated roughly by the factor $\exp(-\pi a/p)$ in Table 2.

9. CONCLUSIONS

We have illustrated the AFT nonrelativistic approach to atomic processes by studying high-energy photoionization (with incident photon energies $\omega \ll m$) of an electron bound in a central potential. We have demonstrated that in this case, high-energy ionization by photoabsorption can be understood in terms of the singularities of the Hamiltonian, which also illustrates more general situations. Our discussion did not depend on the choice of the form [length (L), velocity (V), acceleration (A), etc.] of the photoionization matrix element.

Because photoabsorption at high photon energies requires at least one large outgoing electron momentum, we have argued that the analysis is equivalent to the analysis of the asymptotic form of the FT. Based on the Fourier transform theory, we have shown that a slow asymptotic decrease of the photoabsorption matrix element for large momentum p (such as $1/p^n$) is related to singularities of the e–N potentials. We have demonstrated how this large-momentum behavior can be obtained from the behavior of wave functions and interactions around singularities. With this approach, we can identify the dominant terms and avoid omitting any of them.

We have applied our approach to study the high-energy total cross section for ionization in a central potential with the Coulomb e–N singularity. We have demonstrated that the approach and the final results are form («gauge») independent. However, the dependence of the final results on the quality of the initial and final state wave functions in the vicinity of a singularity varies with form («gauge»). We have found that the acceleration form, which places the singularities of the Hamiltonian in the e–γ interaction, has the least requirement on the quality of wave functions at the singularity, in situations considered. We have shown that in the A-form, the leading contribution to the photoabsorption matrix element is the lowest-order Born result. In the L- and V-forms, it is generally a higher-order Born result, with the exception of the V-form in the ground state ionization, where it is also the lowest-order Born result. This means that in general (except in the A-form), the fast electron cannot be represented by a plane wave, even in the high-energy limit. For this leading contribution to the matrix element, the A-form requires only the proper normalization of the initial state at the e–N singularity. In contrast, the L- and V-forms require knowledge of both the normalization and slope of the wave functions at the singularities.

We have discussed slow convergence of the cross sections to the high-energy limit, considering the ionization of an electron in a screened potential. We have demonstrated that by collecting all Coulomb terms in the vicinity of the e–N singularity, we also collect the dominant terms up to the relative order $1/p^2$ and provide fast convergence of the cross sections. Although the neglected terms in the matrix element are still of the relative order $1/p^2$, they are negligible. Thus, we have demonstrated that the high-energy behavior of cross sections (in the keV range, as in our examples) is determined by the properties of functions near the singularity, which is of the Coulomb type. The screening effects enter through normalization factors in the IPA cases. We have also demonstrated that the only slowly converging factor (the Stobbe factor $\exp(-\pi a/p)$, which converges as $1/p$, while all other terms converge faster) is common for ionization from all states. The existence of a common slowly converging factor provides fast converging ratios of the cross sections.

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