

Characterization of high energy photoionization in terms of the singularities of the atomic potential: I. Photoionization in independent particle approximation (IPA)

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Abstract

We describe a unified nonrelativistic approach to photoionization of atoms by photoabsorption at high incident photon energies ω (but still $\omega \ll m$). Since photoabsorption at high photon energies requires large outgoing electron momentum, the matrix elements for photoabsorption processes can be understood in terms of asymptotic Fourier transforms (AFT). The behavior of the matrix element is determined by the singularities of the integrand. These singularities, in wave functions and the $e\text{-}\gamma$ interaction, reflect the singularities of the Coulomb potentials. We first illustrate the approach for the case of an electron in a screened central potential, subsequently for the more realistic case in which electron-electron correlations are included. We study how the quality of approximate results depends on the quality of wave functions. We show that, even in the high energy limit, the fast electron can not, in general, be represented by a plane wave. Due to the Coulombic interactions cross sections converge very slowly at high energy to the AFT results. However, this slow convergence is due to one common factor (Stobbe factor) which we

can obtain explicitly; ratios of cross sections converge more rapidly.

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I. INTRODUCTION

In this sequence of papers [1–3] we will explore the understanding of high energy photoionization processes which follows from the theory of asymptotic Fourier transforms (AFT). Basically the AFT of a function is determined by its singularities. In our case this means that the high energy behavior of cross sections follows from the Coulomb singularities of the basic electron-nucleus and electron-electron interactions. While our primary interest is in electron correlation, in this first paper we introduce these ideas for the simpler case of photoionization of an electron bound in a screened Coulombic central potential. In a second paper [2] we explore correlation issues, focusing on photoionization of the ground state of a two electron atom. Finally, in a third paper [3] we examine further issues which arise in the consideration of high energy photoionization of a many-electron atom.

The study of single photon ionization processes resulting in single [4,5] or multiple [6,7] ionization of an atom is of fundamental and practical importance. New experimental possibilities, modern synchrotron sources and experimental methods [8], result in better understanding of electron correlation effects in complex systems and in processes involving these systems [9–11].

Photoabsorption by correlated system, and in particular by the ground state of He, has attracted much attention in recent years. For He system, for example, we have learned that for very large photon energies ($\omega \gg 1$ keV) only certain aspects of the initial state correlation are important for the description of the total cross sections. For double ionization in the shake-off limit the important part of the correlation is the correlation between electrons when one electron is at the nucleus [12]. In more complex systems, involving non-s states, we have learned about aspects of final state correlation effects which lead to modifications of the independent particle approximation (IPA) results for single ionization at high energies [4,5,13]. Such understanding of the aspects of correlation important for the process highly simplifies the theoretical treatment and allows treatment of more complex situations [11] at large energies.

However, there are other correlation effects which persist at very large energies and which are not yet understood, such as correlation effects leading to the quasi-free mechanism of double ionization [14]. Also, as one goes to lower energies, but still large compared to binding energies (*e.g.* around 1 keV for He), our understanding of the dominant correlation effects, leading to double ionization, is not sufficient to extract the dominant contributions. For example, for calculating ionization with excitation and for calculating double ionization total cross sections of He, even in the 0.5–1 keV region, large scale numerical calculations requiring highly correlated wave functions [9,10] are used to reproduce experimental data even for this high energy region. The accuracy is often judged by the comparison of the results obtained using the same wave functions but with different interaction forms (gauges), since exact results must be form (gauge) independent. This however means a lack in our understanding of the aspects of the correlation effects important for the processes and how these important correlation effects emerge for different forms at large energies. Such understanding is needed for making calculations of more complex situations, involving photoabsorption, more feasible.

All these and other issues of the high energy ionization by photoabsorption can be studied from a unified point of view. The idea is based on the close relation between high energy photoabsorption matrix elements and asymptotic Fourier transforms (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 [15,16]. Since photoabsorption at high photon energies requires at least one large outgoing electron momentum, we may generally argue that the analysis is equivalent to the analysis of the asymptotics of Fourier transforms. A slow asymptotic decrease for large p , such as $1/p^n$ in a $1/p$ asymptotic power expansion, of the Fourier transform (FT) of a well localized function, comes only from the singularities of that function.

In this sequence of papers [1–3] we will use the theory of the asymptotics of Fourier transforms to study high energy ionization by photoabsorption. By high energy we mean that $\omega \gg E_B$ (where the E_B is binding energy of the state which is ionized), but still $\omega \ll m$

(to stay with a nonrelativistic description of electrons). In this paper we will begin with the discussion of high energy photoionization of an electron bound in a central potential. Then, in [2] we will study the high energy cross sections of a two electron atom in its ground state, particularly the total cross section, for single ionization and the total cross section and the spectrum for double ionization. In [3] we discuss more general cases, such as are relevant, for example, in the discussion of persistence of correlation in single ionization by photoabsorption of the $2p$ shell of Ne [4].

In this paper we describe our general approach to photoabsorption (and perhaps other related) processes at high but nonrelativistic energies, using the example of single ionization within a central field independent particle approximation (IPA) model and assuming the IPA potential near the nucleus is point Coulombic [17]. We use this simple and familiar model in order to explain the main points of our general approach in the context of a relatively simple and familiar situation. We will show that the energy dependence of the photoabsorption matrix element at high energies follows from the singularities of the wave functions and $e-\gamma$ interaction operators, which in turn follow from the singularity of the nuclear Coulombic potential at the electron-nucleus coalescence. We will be able to understand the adequacy of the use of various forms of matrix elements [length (L), velocity (V) or acceleration (A) forms] when using approximate wave functions of various qualities. We will demonstrate that nonrelativistic IPA high energy photoabsorption is determined [up to corrections $O(1/p^2)$, p being outgoing electron momentum, also taken as large, *i.e.* $p \gg mZ\alpha \equiv a$ where Z is the nuclear charge and α is the fine structure constant [18]] by the initial state normalization and the point Coulomb singularity. This, as we demonstrate, is form independent, but whether information about the singularity comes from the interaction (as in A-form) or from the initial and final state (as in L- and V-form) is form dependent. In such a way we are able to identify necessary conditions for all three forms to give correct the high energy result in the IPA case. We also explicitly obtain the leading corrections to the high energy limit.

We begin in Sec. II by giving a general discussion of AFT of singular functions. We discuss the connection with the photoabsorption matrix element, as well as differences (modifications

of the asymptotic AFT) required due to the presence of Coulomb functions. In Sec. III we begin the discussion of the behavior of the photoeffect matrix element in an IPA potential. Then in Sec. IV we consider the simplest case, photoabsorption from an s-state in a pure Coulombic potential, neglecting retardation. There we develop our AFT approach in detail. In Sections V, VI, VII, VIII, we remove the constraints of the simplest case, identifying the resulting additional features. We show how the approach works for non-s states (V) and for a general IPA potential with a point Coulomb singularity (VI). We discuss relativistic and retardation contributions (VII). In Sec. VIII we discuss the convergence with increasing energy to asymptotic forms. We explicitly obtain a common factor (Stobbe factor) which contains all the slowly convergent behavior. This is why ratios of cross sections converge much more rapidly to asymptotic forms than the cross sections themselves. In Sec. IX we summarize our conclusions.

II. 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} represents the large momentum of one ejected electron (there must be at least one) and λ represents quantum numbers of other electrons in the final state. Since at large distances an outgoing electron wave function will be described by a plane wave and incoming spherical waves (with appropriate long range Coulombic logarithmic factors), these oscillations limit the range in \mathbf{r}_1 which contributes to the matrix element integral, which in \mathbf{r}_1 can be viewed as a Fourier transform in electron momentum \mathbf{p} of slowly varying functions. (Since we have assumed non-relativistic energies, there will be no oscillations of any retardation factor in the interaction in this range.) We will discuss the remaining p -dependence in the Coulomb wave function in this range below. Due to the fact that large ω necessarily means large \mathbf{p} the study of the photoabsorption matrix element at large energies is equivalent to the study of the asymptotics of Fourier transforms.

The study of the asymptotics of the Fourier transforms which arise in our problems is

based on the theory of generalized functions [15]. By definition [16], $f(x_1, \dots, x_n)$, a function of n variables infinitely differentiable and such that

$$R^l \frac{\partial^m f}{\partial x^{\alpha_1} \partial x^{\alpha_2} \dots \partial x^{\alpha_n}} \rightarrow 0 \quad R \rightarrow \infty, \quad (1)$$

for any l, m and any choice of the indices $\alpha_1, \alpha_2, \dots, \alpha_n$ ($\alpha_1 + \alpha_2 + \dots + \alpha_n = m$), where $R \equiv (x_1^2 + x_2^2 + \dots + x_n^2)^{1/2}$, is called a good function. [In the terminology of [16] these are called χ functions]. The theorem ([15], Theorem 2, page 15) says that the FT of a good function is a good function [15,16]. We will call this the AFT theorem.

An example of such a function, in 3D, is the function $f_1(\mathbf{r}) = \exp(-\lambda r^2)$. The Fourier transform of this function can be obtained analytically and it is

$$F_1(\mathbf{p}) = \int e^{-i\mathbf{p}\cdot\mathbf{r}} e^{-\lambda r^2} d^3r = \left(\frac{\pi}{\lambda}\right)^{3/2} e^{-\frac{p^2}{4\lambda}}. \quad (2)$$

We see that for large p the FT decreases exponentially, *i.e.* faster than any power of $1/p$, in accordance with the FT theorem.

The functions which appear in our photoionization matrix elements, even considering photoionization of a particle in a potential, are not like Eq. (2). They are well localized (due to the fact that the bound state is localized), but they are not differentiable everywhere. Namely, they are differentiable everywhere except at coalescence points, where they are singular [19], *i.e.* non-differentiable. The wave functions, being eigenstates of a many-body Hamiltonian with Coulombic interactions, have singularities at the singularities of the Hamiltonian, which are located at points where the particles coalesce. We will use the term coalescence points for the locations of these singularities. There are double coalescence points when two particles meet: both electron-nucleus (e-N) coalescences, when one electron is at the nucleus, and also an electron-electron (e-e) coalescence, when the two electron positions coincide. There are also multiple coalescence points, when more than two particles coincide. The properties of wave functions in the near vicinity of these singularities, which for bound states (and for double coalescence points, which are of primary importance for the dominant contributions we are studying) are well understood [19,20], can be extracted

from the Schrödinger equation. They are known as coalescence properties, and in the case of s-states they are often called Kato cusp conditions. We are using this term, Kato cusp conditions, more generally, denoting exact behavior of the wave functions at a two-particle singularity. (There would also be singularities in the $e-\gamma$ interaction operator, depending on the form which we take.)

In the vicinity of any two particle coalescence (singularity) the functions which appear in our matrix element may be written in terms of simpler functions, whose FT we know, and a remainder whose FT is asymptotically negligible. These simpler functions are restricted by the Kato conditions to have a Coulombic behavior, as explained later, in the vicinity of a two particle singularity. For these simpler functions one can choose therefore pure Coulombic functions or even simpler functions in which Coulombic functions can be expanded. [Coulombic functions can be expanded in polynomials in r (taking the singular point at $r=0$) about the singular points and in spherical harmonics.] Such a choice is sufficient for our purposes; it gives results accurate neglecting the order a^2/p^2 ($a = mZ\alpha$) and allows collecting all Coulombic slowly converging terms in (powers of) $\pi a/p$ (when full Coulombic functions are used). If better accuracy is required one needs to go beyond using functions with Coulombic shape in the vicinity of singularity. The point is that with such a procedure one can achieve arbitrary accuracy (see [15], theorem 19, page 52). The method of expansion of wave functions around the nucleus, in order to obtain the leading contribution for high energy photoabsorption, has been used previously, both in situations of IPA single photoionization [21,22] and in specific kinematics for double ionization (*e.g.* [12,23]). Here and in papers II and III based on the AFT theory, we are generalizing these approaches.

We will proceed in our simple examples (like in our applications to photoabsorption) with the assumption that the functions of which we calculate FT can be expanded in terms of polynomials in r and spherical harmonics [24]. The Fourier transforms of these polynomials and harmonics can be consistently defined using the theory of generalized functions [15]. These Fourier transforms are polynomials in $1/p$. According to the generalized-function theory, the Fourier transform of a generalized function with singularities can be approxi-

mated by the Fourier transforms of polynomials (in terms of which the function is expanded) with arbitrary accuracy. The expansion can be obtained from expansion of the integrand function in powers of r around the singular points. A simple example of such a singular function is the function $f_2(\mathbf{r}) = \exp(-\lambda r)$. This function is singular at the origin $r = 0$, reflecting the fact that r itself is singular, i.e. not differentiable, at $r = 0$, and in fact it has the same type of singularity as bound state functions appearing in photoionization matrix elements. [Taking the singularity at $\mathbf{r} = 0$ in our three dimensional (3D) example does not imply any loss of generality since a singularity can always be translated to the origin.] The Fourier transform of this function is

$$F_2(\mathbf{p}) = \int e^{-i\mathbf{p}\cdot\mathbf{r}} e^{-\lambda r} d^3r = \frac{8\pi\lambda}{[\lambda^2 + p^2]^2}, \quad (3)$$

which indeed decreases as a power of p .

We are interested in asymptotic FT (given our kinematics of large p) of functions expanded about the singular point $\mathbf{r} = 0$. The function Eq. (3) is expandable in powers of $1/p$ for large p . This expansion in $1/p$ of the FT can be obtained starting with the expansion of the function $f_2(\mathbf{r})$ around the singular point, *i.e.* $f_2(\mathbf{r}) = (1 - \lambda r + \frac{1}{2}(\lambda r)^2 + \dots)$. With this approach one needs a convergence procedure; we multiply each term in the expansion with $e^{-\varepsilon r}$ and let $\varepsilon \rightarrow 0$ after the integration is performed. This is consistent with the definition of the FT of generalized functions (see [15] page 33). In this way we obtain that the FT of the powers of r (we assume that $p \neq 0$, and therefore we do not include δ -function terms) are

$$\lim_{\varepsilon \rightarrow 0} \int e^{-(\varepsilon r + i\mathbf{p}\cdot\mathbf{r})} r^n d^3r = \frac{4\pi(n+1)!}{(ip)^{n+3}} \begin{cases} 0, & \text{even } n \geq 0, \\ 1, & \text{odd } n > 0. \end{cases} \quad (4)$$

[Since wave functions have singularities as in the powers of r^n it is helpful, for later use, to remember that AFT of r^n results in $1/p^{n+3}$, if the term is singular.]

We may also apply our FT theorem to see that since the first term, “1”, in the expansion of $f_2(\mathbf{r})$, is regular everywhere, it therefore can not contribute to the series expansion of F_2 in $1/p$. The same is true for all even powers in r . The only contributions to the series

expansion come from the singular terms, which in this example are just the odd powers in r . (In general there could also be angular functions, like $\cos \vartheta$, which are also singular). With the help of Eq. (4) we obtain

$$F_2(\mathbf{p}) = \lim_{\varepsilon \rightarrow 0} \int (1 - \lambda r + \frac{1}{2}(\lambda r)^2 + \dots) e^{-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r} d^3r = \frac{8\pi}{p^3} \left[\frac{\lambda}{p} - 2 \left(\frac{\lambda}{p} \right)^3 + \dots \right]. \quad (5)$$

Eq. (5) is just expansion of the FT of Eq. (3) in powers of $1/p$, in accordance with the theory of Fourier transforms of generalized functions.

However, in more general situations (as we will have in papers II and III with more electrons involved) we may not assume that singular functions are expandable in infinite series of r (interparticle distance) in the vicinity of any singularity. In such cases, as we show in papers II and III, we can still partition singular function in the vicinity of a singularity into a simple function (perhaps a polynomial) and a remainder which may not be necessarily expandable but vanishes faster than the polynomial as r approaches the singularity. Then the AFT theory tells us that AFT of such function is given with the AFT of a polynomial in $1/p$ and a remainder (a function in $1/p$) which vanishes faster than the polynomial as p increases.

This is an illustration of a general idea. The 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 [21–23]. Here, however, using AFT theory, we may make expansions (or, generally, partitioning) around singular points which, in general, do not have to be at the origin. An important point of this approach is that it clarifies which singularities need to be considered for these expansions (there are in general more than one singularity in many body wave functions and interactions). What singularities need to be considered is determined, as we show, by the kinematics of outgoing electron momenta, identifying situations in which the number of asymptotic FT is minimized. Another important point of our approach is that we start from exact matrix elements (with exact wave functions), and from them extract and collect all contributions in the leading power of $1/p$ which is determining the high energy behavior (and also in some cases the

leading corrections). In such a way we extract the exact energy dependence at high energies. Only afterwards do we make approximations, to calculate the coefficients associated with the terms of leading powers. This is important because, in different forms in which a matrix element may be written, the important singular terms of the integrand may come from different parts of the product of wave functions and interaction. With our approach we identify the dominant terms and avoid losing any of them, and we also avoid uncontrolled introduction of spurious contributions. We will illustrate how both of these problems have arisen in the use of approximate wave functions.

There is however a point of difference between our asymptotic matrix element and asymptotic FT. Namely, after pulling out 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 (pr) dependence (as for example in confluent hypergeometric functions in Coulomb case). For this reason it might be more appropriate to talk about a generalization of FT. However, in the large p limit the Coulomb functions which depend on pr are expandable in uniformly convergent series in powers of pr . Although all these powers of pr must be included, as we discuss, we are able to argue that FT theorems apply to each power separately (a power of p is pulled out from each integral and no p 's appear any more), and due to uniform convergence, also to the full function [25]. (When the final state can not be explicitly determined, this argument relies on the convergence of a distorted wave Coulomb Born expansion for the state, as we will note subsequently.) The Coulombic modification of the FT results, as we demonstrate in Sec. VIII, in a slowly converging factor, the Stobbe factor.

Accurate evaluation of the matrix element at high energies requires knowledge of (in general) both initial and final state electron wave functions at the singular point, or in general at all singular points, if one goes beyond IPA. However, how much of this knowledge is actually needed in a given calculation depends on the form of matrix element used for that calculation. As we will demonstrate here in this IPA case, with A-form we only need knowledge about the normalization of the initial wave function at the e-N coalescence. With

other forms (V and L) we generally need further information about both the initial and final state. The exception is for s-state ionization using 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 in the $1/p$ expansion of the high energy matrix element, which is generally accurate to relative order $O(\pi m Z \alpha / p)$.

III. SINGULARITIES OF THE IPA MATRIX ELEMENT INTEGRAND

For a single electron in a potential the matrix element for photoionization by photoabsorption, in the lowest order of the quantum electrodynamic electron-photon interaction, is [18]

$$M = \int \Psi_{\mathbf{p}}^{(-)*}(\mathbf{r}) I(\mathbf{r}) \Psi_i(\mathbf{r}) d^3r, \quad (6)$$

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, $\Psi_{\mathbf{p}}(\mathbf{r}) = e^{i\mathbf{p}\cdot\mathbf{r}} \Phi_{\mathbf{p}}^{(-)}(\mathbf{r})$ is the final electron continuum state, normalized on the momentum scale (to asymptotically approach a $1/(2\pi)^{3/2}$ amplitude distorted plane wave of momentum \mathbf{p}), and $I(\mathbf{r})$ is the interaction operator, given in the three commonly used forms (keeping retardation to all orders) as

$$I_V = -i \left[e^{i\mathbf{k}\cdot\mathbf{r}} \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} \right], \quad (7a)$$

$$I_L = im \left(\omega - \frac{k^2}{2m} \right) \boldsymbol{\epsilon} \cdot \mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} - e^{i\mathbf{k}\cdot\mathbf{r}} \boldsymbol{\epsilon} \cdot \mathbf{r} \mathbf{k} \cdot \boldsymbol{\nabla}, \quad (7b)$$

$$I_A = \frac{1}{\omega - \frac{k^2}{2m}} \left[i e^{i\mathbf{k}\cdot\mathbf{r}} \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} V(r) - \frac{1}{m} e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{k} \cdot \boldsymbol{\nabla} \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} \right]. \quad (7c)$$

$V(r)$ is an IPA potential energy of the type $V(r) = -(Z\alpha/r)S(r)$, where $S(r)$ is a screening function which for small r we assume to be expandable in integral powers of r [24], $S(r) = (1 + s_1 r + s_2 r^2 + \dots)$, *i.e.* the potential has only a Coulombic 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 $e-\gamma$ interaction

operator in the L- and V-form is, in this sense regular, while in A-form it is singular due to the presence in it of the singular $V(\mathbf{r})$, Eq. (7). The large p expansion in $1/p$ of the Fourier transform of a slowly varying function of r picks out its behavior near the coalescence point (since $pr \sim 1$, large p corresponds to small r) and it only depends on the singular parts of the function. Thus we begin by expanding [or partitioning; see the discussion below Eq. (5) regarding the general situation] 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 expansion of these slowly varying portions of the integrand will lead to a corresponding inverse p expansion of the Fourier transform.

The series expansion of the initial (bound) state of quantum numbers (n, l, m) in an IPA potential with Coulombic singularity is

$$\Psi_i(\mathbf{r}) = N_i^{IPA} r^l (1 - \frac{a}{l+1} r + \lambda_2 r^2 + \lambda_3 r^3 + \dots) Y_l^m(\hat{\mathbf{r}}), \quad (8)$$

where $a = mZ\alpha$. In this expansion [in which terms are alternately regular and singular, with the first, $r^l Y_l^m(\hat{\mathbf{r}})$, being regular], the first two terms are determined solely by the Coulomb singularity of the potential, and therefore are known independent of screening, except for the overall normalization factor N_i^{IPA} (which depend on the choice of IPA potential). Higher order terms in the expansion Eq. (8) do depend on coefficients in the polynomial expansion of the IPA potential, which determine the λ_i coefficients. This fact, that the two first terms in the parenthesis of Eq. (8) are determined by the Coulomb singularity, is well known, and it is a special case of the general behavior of wave functions at coalescence points of many-electron atoms [19,20]. Namely, in the expansion 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 two coalescing particles, the first two terms of the expansion are determined by the singularity of the corresponding part of the Coulomb potential, up to an overall factor. (This factor is generally a function of all the coordinates describing the atomic system, except the relative coordinate describing the coalescence. In IPA this factor is just a constant, dependent on screening). (This viewpoint will be considered in more

detail in [2], where we discuss ionization of a two-electron atom.) These two terms in the expansion, 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 to high energy photoabsorption in any form.

In the final state electron wave function the situation is very similar, except that in the limit of high momenta the normalization is not affected by screening. Namely, according to [26–29], 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 Coulombic. As shown in [29], using analytic perturbation theory, the corrections to the Coulombic wave function in the vicinity of the nucleus ($r \ll 1/a$, where $a = mZ\alpha$ characterizes the unscreened nuclear charge), due to screening, decrease with 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 (which we need) of momentum $p \gg a$ can be written, following [27,29], as a Coulomb solution plus a remainder,

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C e^{i\mathbf{p}\cdot\mathbf{r}} \left[{}_1F_1\left[-i\frac{a}{p}, 1, -ipr(1 + \cos\vartheta)\right] + O\left(\frac{1}{p^2}; pr, \cos\vartheta, s_i\right) \right], \quad (9)$$

where $O(1/p^2; pr, \cos\vartheta, s_i)$ denotes the remainder, which vanishes faster than $1/p$ (denoted in O by $1/p^2$). Functional dependence of O is also shown; the remainder contains all information on screening, symbolized by the coefficients s_i characterizing a small distance expansion of the screened potential. According to analytic perturbation theory [27,29], an even more accurate continuum wave function of Coulombic shape, in the region $r \ll 1/a$, is obtained by shifting the electron momentum in Eq. (9) from momentum p to p_C , by an amount determined by the parameters of the screened potential, and by replacing normalization N_p^C (if momentum scale normalization is used) by $\sqrt{p_C/p}N_{p_C}^C$. However, although such Coulombic function is more accurate its error still decreases as $1/p^2$ with large momentum p . Therefore we do not need it at this moment here, but we will use it in Sec. VIII.

This result, Eq. (9), is important for our approach because it means, as we show below, that the terms in the expansion of the final state around the coalescence which contribute

to the high energy matrix element are not affected by screening. We show this by expanding the function Eq. (9). Due to the fact that distances involved in the process are $r \sim 1/p$, and since we are considering high energies for which $p \gg (mZ\alpha)$, when we write our wave functions in terms of the scaled variable pr , the terms which will be important for our discussion here involve terms up to linear in the parameter $a/p = mZ\alpha/p$, with further terms contributing in higher orders in $1/p$. We write

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C e^{i\mathbf{p}\cdot\mathbf{r}} \left[1 - i\frac{a}{p}g^{(-)}[i(pr + \mathbf{p}\cdot\mathbf{r})] + O\left(\frac{1}{p^2}; pr, \cos\vartheta, s_i\right) \right], \quad (10)$$

where $\cos\vartheta = \hat{\mathbf{p}}\cdot\hat{\mathbf{r}}$, O includes all contributions of order a^2/p^2 and higher from the full Coulomb function of Eq. (9), and

$$g^{(-)}(i\xi) = -\frac{1}{2\pi i} \oint_{\Gamma} e^{-i\xi t} \ln\left(\frac{t-1}{t}\right) \frac{dt}{t} = \int_0^1 [e^{-i\xi t} - 1] \frac{dt}{t}. \quad (11)$$

The contour Γ is a counterclockwise oriented closed contour encircling the cut $[0, 1]$. By inserting Eq. (10) and Eq. (8) in Eq. (6), using the series expansion form of Eq. (11) for $g^{(-)}(i\xi)$, $\xi = pr + \mathbf{p}\cdot\mathbf{r}$, we obtain a series of integrals of functions which contain powers of r and angular functions.

The function $g^{(-)}(i\xi)$, Eq. (11), determines all contributions of order a/p to the full Coulombic wave function for $pr \sim 1$. It is therefore equivalent to the first Born term in the perturbation expansion of the Coulomb continuum state. Although the function $g^{(-)}(i\xi)$, obtained in the expansion a/p , gives important contributions only for $pr \sim 1$, we note that in the asymptotic region $pr(1 + \cos\vartheta) \gg 1$, this function gives the spherical wave to the leading order in a , as does the first Coulomb–Born term, and it also reproduces the logarithmic phase (to the first order in a) of the distorted plane wave. However, this large r region is not important for our discussion here in the IPA case.

The function $g^{(-)}(i\xi)$ is, generally, needed in calculating the leading contribution to the high energy matrix element. However, it contains \mathbf{p} dependence through pr which, at first sight, may not look welcome, if one wants to view this high energy matrix element as a FT. However, we can expand this function in powers of pr [by expanding the exponential

function in the integral representation, Eq. (11)], and apply the FT theorem to each term, and then sum the series. Since these series are uniformly convergent this is the same as integrating without expansion (see *e.g.* [30] page 158), which we do.

To achieve a convergent integration of each term in the series (which will then separately satisfy the requirements of the FT theorem) a factor $e^{-\varepsilon r}$ is introduced; after the integration is performed the limit $\varepsilon \rightarrow 0$ is taken. This procedure, as pointed in Sec. II, is consistent with the definition of the FT of generalized functions [15]. (This is also necessary since, in our small distance expansion of the bound state wave function, we have lost the boundedness it provides.) For the AFT theorem 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. (Note also that $r^l Y_l^m$ is regular).

We will see that the leading contribution in any form to the high energy matrix element can be obtained, using only the first two terms in the expansion of initial and final state in r , 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 subsections IV and V. Therefore the form independent high energy matrix element (to the leading order in $1/p$) for photoabsorption in an IPA model is obtained from

$$M = N_i^{IPA} N_p^{C*} \lim_{\varepsilon \rightarrow 0} \int e^{-i\mathbf{p} \cdot \mathbf{r} - \varepsilon r} \left[1 + i \frac{a}{p} g^{(-)*} [i(pr + \mathbf{p} \cdot \mathbf{r})] \right] I(\mathbf{r}) r^l \left[1 - \frac{a}{l+1} r \right] Y_l^m d^3 r, \quad (12)$$

where $I(\mathbf{r})$ may take forms like Eqs. (7), which also contains different powers of r and angular functions.

The expression Eq. (12) gives the leading term in the expansion of the matrix element in powers $1/p$ for large p and this term is form independent. We may look at this expression and compare it with a pure Coulombic potential case to see what determines high energy photoabsorption in an IPA model with a Coulombic singularity. We see from Eq. (12) that

the only difference from the pure Coulombic case is in the initial state normalization, which depends on the IPA potential. All other terms are determined by the Coulomb singularity. Therefore at high energies information about screening persists only in the initial state normalization. This behavior for high energy photoabsorption in an IPA potential is known [28], but it is just one aspect of the persistence of electron–electron interaction in high energy photoabsorption, which we discuss within our form–independent approach for two–electron atoms in [2].

In a matrix element form in which the interaction operator is regular (such as V–form and L–form, and we denote it as I_V^R and I_L^R) rather than singular (as in A–form, I_A^S), the contribution from the term in the integrand which involves the first terms both in the expansions of Ψ_i and $\Phi^{(-)}$ vanishes for any l (while in A form this term gives the leading non-vanishing contribution). The leading nonvanishing contributions in such forms (L or V) involve the product of the first term from $\Phi^{(-)}$ (which is regular and we denote as R_f) with the second term in Ψ_i (singular, S_i) and the product of the second term from Φ^- (singular, S_f) with the first term in Ψ (regular, R_i). These two contributions are of the same order in $1/p$. In summary, in leading order in $1/p$ one obtains the leading nonvanishing contribution from:

$$M = \int e^{-i\mathbf{p}\cdot\mathbf{r}-\varepsilon r} [R_f + S_f] \begin{bmatrix} I_L^R \\ I_V^R \\ I_A^S \end{bmatrix} [R_i + S_i] \Rightarrow \int e^{-i\mathbf{p}\cdot\mathbf{r}-\varepsilon r} \begin{bmatrix} R_f I_L^R S_i + S_f I_L^R R_i \\ R_f I_V^R S_i + S_f I_V^R R_i \\ R_f I_A^S R_i \end{bmatrix}. \quad (13)$$

The integrals involved in evaluating Eq. (12) are elementary and they are of two type. The integrals which involve the first term, “1”, from the final state and powers of r and products of spherical harmonics from the $e-\gamma$ interaction and the initial state (these products of spherical harmonics can be combined into just one Y_L^M) are of the type

$$J_1 = \lim_{\varepsilon \rightarrow 0} \int e^{-i\mathbf{p}\cdot\mathbf{r}-\varepsilon r} r^n Y_L^M(\hat{\mathbf{r}}) d^3r = \frac{2\pi(n+2)!}{(ip)^{n+3}} Y_L^M(\hat{\mathbf{p}}) f_{n+3}^L, \quad (14)$$

where

$$f_k^L = \int_{-1}^1 \frac{P_L(x) dx}{(x - i\varepsilon)^k}, \quad (15)$$

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

$$J_2 = \lim_{\varepsilon \rightarrow 0} \int e^{-i\mathbf{p} \cdot \mathbf{r} - \varepsilon r} g^{(-)*}[i(pr + \mathbf{p} \cdot \mathbf{r})] r^n Y_L^M d^3r = \frac{2\pi(n+2)!}{(ip)^{n+3}} Y_L^M(\hat{\mathbf{p}}) h_n^L, \quad (16)$$

where

$$h_n^L = \int_{-1}^1 P_L(x) \left\{ \sum_{j=0}^{n+1} \frac{(-1)^{n-j} (x - i\varepsilon)^{n+2-j} - 1}{(n+2-j)(x - i\varepsilon)^{n+3}} + \frac{i\pi + \ln(x - i\varepsilon)}{(x - i\varepsilon)^{n+3}} \right\}. \quad (17)$$

In performing the radial integration in Eq. (16) we used the integral form, the second form in Eq. (11), of the function $g^{(-)}[i(pr + \mathbf{p} \cdot \mathbf{r})]$. In performing the angular integrations in Eq. (14) and Eq. (16) a rotation of $Y_L^M(\hat{\mathbf{r}})$ is made into the coordinate system in which $\hat{\mathbf{p}} = \hat{z}$ (see *e.g.* [16] page 1074). (Alternatively, we may take $\hat{\mathbf{p}} = \hat{z}$, perform the angular integration, and then make a rotation to fixed coordinates as needed). The integrations in x in Eq. (15) and Eq. (17) are elementary, and we evaluate these types of integrals for specific L in subsections IV and V.

The expressions Eq. (14) and Eq. (16) show how higher powers in r lead to higher powers in $1/p$. It should be pointed out 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 FT theorem. Therefore, depending on the form used, at least one of the two first terms in the expansion 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.

IV. THE SIMPLEST CASE: GROUND STATE IONIZATION OF A H-LIKE ATOM

We now discuss how the leading contribution to the matrix element is obtained in the three forms Eq. (7), considering the simple and familiar case of photoionization of the ground

state of a H-like atom when neglecting retardation.

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

$$I_A = \frac{iZ\alpha}{\omega} \frac{\boldsymbol{\epsilon} \cdot \hat{\mathbf{r}}}{r^2}; \quad I_V = -i\boldsymbol{\epsilon} \cdot \boldsymbol{\nabla}; \quad I_L = im\omega \boldsymbol{\epsilon} \cdot \mathbf{r}, \quad (18)$$

where ω is 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, as it was obtained by taking the gradient of the potential. Note 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 asymptotic large p expansion in $1/p$ of the Fourier transform of a slowly varying function of r picks out its behavior near the coalescence point (small r corresponding to $1/p$ in the large p limit); it only depends on the singular parts of the function in the small r limit. Thus we begin by expanding 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

$$\Psi_i(\mathbf{r}) = N_i(1 - ar + \dots); \quad \Phi_{\mathbf{p}}^{(-)}(\mathbf{r}) = N_p^C(1 - i\frac{a}{p}g^{(-)}[i(pr + \mathbf{p} \cdot \mathbf{r})] + \dots). \quad (19)$$

If we proceed as we have described in the previous section we shall arrive, of course, at the familiar high energy expression, which is usually obtained in V-form by assuming that the energetic outgoing electron can be regarded as free and may be represented by a plane wave [31–33]. But in our procedure we shall be more careful and not make such an assumption, which in general is incorrect (as for non-s states, or in L form even for s-states).

By substituting Eq. (19) and Eq. (18) into the matrix element Eq. (6) 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 so that only functions in $\cos\vartheta$ appear). Applying $\boldsymbol{\epsilon} \cdot \boldsymbol{\nabla}\Psi_i = \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}}(-a + a^2r + \dots)$ we arrive at the two types of integrals written in Eq. (15) and Eq. (17). The integral involving the first term from the expansion of $\Phi_{\mathbf{p}}^{(-)}$ (the “1”) and terms from the expansion of Ψ_i is

$$\int e^{-(\varepsilon+i\mathbf{p}\cdot\mathbf{r})} r^n \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}} d^3r = \frac{2\pi(n+2)!}{(ip)^{n+3}} \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}} C_n; \quad C_n = \begin{cases} \frac{-2}{n+1} & \text{even } n \geq -2, \\ 0 & \text{odd } n > -1, \\ i\pi & n = -1. \end{cases} \quad (20)$$

Note that the zero result for the odd $n > -1$ case 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 expansion of $\Phi_p^{(-)}$ are easily performed using the integral representation Eq. (11). We obtain

$$\int e^{-(\varepsilon+i\mathbf{p}\cdot\mathbf{r})} g^{(-)*}[i(pr + \mathbf{p} \cdot \mathbf{r})] r^n \boldsymbol{\epsilon} \cdot \hat{\mathbf{r}} d^3r = \frac{2\pi \boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}}{(ip)^{n+3}} D_n; \quad D_n = \begin{cases} \frac{2(n+2)! (1-i\pi)}{n+1} & \text{even } n \geq 0, \\ i\pi - 2 & n = -2, \\ 4n! \sum_{k=0}^{\frac{n-1}{2}} \frac{2k+2}{n-2k} & \text{odd } n > 0, \\ -\pi^2/2 - i\pi - 2 & n = -1. \end{cases} \quad (21)$$

In both Eq. (20) and Eq. (21) the p -dependence of the results is seen by inspection, resulting from the nature of the scaling in pr . Eq. (20) shows that higher powers in r lead to higher powers in $1/p$, but nonvanishing contributions come only from singular terms. We will exploit this behavior in identifying the leading contributions in $1/p$ in our calculations. Eq. (21) shows that all terms in the series expansion of $g^{(-)}[i(pr + \mathbf{p} \cdot \mathbf{r})]$ contribute to the same order in $1/p$, as we would expect from scaling in pr . In the expansion of the final state wave function in Eq. (19) the first term (“1”) 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 case but for any state with angular momentum l , for which the first terms in the expansion around $\mathbf{r} = 0$ are $\Psi_i \sim r^l Y_l^m (1 - ar/(l+1) + \dots)$.

We further note that, in the case of an s-state, in V-form the contributions from the first term of Ψ (just a constant for an s-state) vanish, due to the derivative in the interaction operator $\boldsymbol{\epsilon} \cdot \nabla$. For non-s states there will be 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).

Thus, in V form for this s-state case, the leading contribution involves only the first term in Φ and the second term in the expansion of the initial state Ψ , justifying the usual calculation which has made the plane wave approximation for the final state. Using Eq. (5) we obtain the familiar result for s-state ionization neglecting retardation (dipole approximation):

$$M = -A \frac{\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}}{p^3} C_0 = 2A \frac{\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}}{p^3}, \quad (22)$$

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

Now we show that using the same procedure in L-form we get the same result. However, here the singularity of the final state also contributes, and an incorrect result is obtained if one assumes that a plane wave provides an adequate description for the energetic electron. Such an assumption would mean, in terms of our approach, simply taking just the term in the integrand involving the first term “1” from the expansion of Φ and the second term from the expansion of Ψ . This contribution is $6A(\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}/p^3)C_2 = 4A(\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}/p^3)$ [we have put $\omega \rightarrow p^2/(2m)$], which is twice the correct result Eq. (22). However, as we have already explained, we must include all terms contributing to the same power in $1/p$. Therefore we must include the term in the integrand which involves the second term “ $g^{(-)}$ ” from Φ^- and the first term from Ψ_i . This gives a contribution $-(A/4)(\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}/p^3)D_1 = -2A(\boldsymbol{\epsilon} \cdot \hat{\mathbf{p}}/p^3)$. The sum of the two gives the correct high energy limit Eq. (22), showing that L-form and V-form indeed agree.

Finally, we may calculate the photoeffect matrix element in A-form using the same procedures. As we have already remarked, in this form the electron-photon interaction operator I_A , Eq. (18), is singular at the origin, with a singularity arising from the singularity of the potential. The leading contribution to the matrix element Eq. (6) in A-form comes from the first terms in the expansion of Φ^- and Ψ_i only (a term in the integrand which

did not contribute in L and V form due to its regularity, not just 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 A-form is easily evaluated with the help of Eq. (20) for $n = -2$, again giving the same result Eq. (22). [Note that, in A form, the next to leading term, in $1/p$ expansion, can also be obtained without referring to screening (involves $g^{(-)}$ or ar). This fact we exploit further in VIII when discussing convergence toward the high energy limit.]

Let us summarize what we have learned about the quality of approximate electron wave functions needed to obtain correct results for the high energy limit of non-relativistic photoabsorption. As we have seen in our simple example, the correct high energy result is obtained in all the three matrix element forms if both initial and final state wave functions are correct at coalescences up to linear terms in a/p . The calculation in A-form makes the least demands on the quality of the approximate wave functions: only the ground state normalization at the coalescence and the amplitude of the continuum wave $[1/(2\pi)^3]$ in that variable are needed. The final result is expressed in terms of the value of the initial state wave function at the origin (which is just the normalization factor for the s-state). The result for the s-state in V-form may be obtained in terms of the derivative of the initial state wave function at origin $(d\Psi/dr)_{r=0}$. This is connected with the value of the function at the origin (normalization factor) through the Kato cusp condition $(d\Psi_i/dr)_{r=0} = -a\Psi_i(0) \equiv -aN_i$, which follows from the statement that the small r behavior is $N_i(1 - ar)$ for the $l = 0$ case. The result in L-form requires further knowledge of the final state continuum wave function, beyond the plane wave approximation. The point is that the sources of the dominant contributions to the matrix element have different origins in the different forms of the matrix element, even though the result is the same in all three forms.

V. BEYOND S STATES

Now we discuss non-s states, for now 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 power series expansion about the electron-nucleus coalescence. The needed integrals are those already given in Eqs. (14–15). Now, however, a plane wave does not adequately describe the fast outgoing electron, except in A-form, in which the electron-photon interaction provides the needed singular behavior for the integrand function.

The leading contribution to the high energy photoabsorption matrix element M , Eq. (6), in the expansion in powers $1/p$, which is obtained in A-form by taking the the leading, regular, terms in the expansion of the initial and final electron states is

$$M_0^{l,m} = \frac{-i2mZ\alpha N_i^C l!}{(2\pi)^{3/2}(ip)^{l+3}} \frac{4\pi}{3} \sum_{\mu} Y_1^{\mu*}(\boldsymbol{\epsilon}) \int d\Omega \frac{Y_1^{\mu}(\hat{\mathbf{r}}) Y_l^m(\hat{\mathbf{r}})}{(\cos\vartheta - i\varepsilon)^{l+1}}. \quad (23)$$

The remaining angular integration involves only elementary integrals Eqs. (14). For $l = 1$, the case we discuss below in other forms for illustration, Eq. (23) gives

$$M_0^{1,m} = (-1)^{1-m} \frac{8\pi ia}{p^4} N_i N_p^C Y_1^m(\boldsymbol{\epsilon}) \quad (24)$$

[The expression Eqs. (23) is obtained, for simplicity, taking z -axes in the direction of $\hat{\mathbf{p}}$. One needs to make rotation into fixed coordinates when integrating over electron angles.] Note that the part M_0 of the matrix element M is obtained in A-form using plane waves. In other forms the calculation of M_0 requires higher order (singular) terms, generally, from both initial and final state. For these reasons we do not call M_0 the first (plane wave) Born approximation result, because it is so only in A-form, and in other forms it is, generally, a higher order Born result.

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

$$\begin{aligned} \boldsymbol{\epsilon} \cdot \nabla [R_l(r) Y_l^m(\hat{\mathbf{r}})] &= \frac{\sqrt{4\pi}}{\sqrt{3}} \sum_{\nu=-1}^1 Y_1^{\nu*}(\boldsymbol{\epsilon}) \left[\frac{\sqrt{l+1}}{\sqrt{2l+3}} \langle 1, \nu; l, m | l+1, m+\nu \rangle Y_{l+1}^{m+\nu}(\hat{\mathbf{r}}) \left(\frac{d}{dr} - \frac{l}{r} \right) R_l \right. \\ &\quad \left. - \frac{\sqrt{l}}{\sqrt{2l-1}} \langle 1, \nu; l, m | l-1, m+\nu \rangle Y_{l-1}^{m+\nu}(\hat{\mathbf{r}}) \left(\frac{d}{dr} + \frac{l+1}{r} \right) R_l \right], \quad (25) \end{aligned}$$

where $\langle 1, \nu; l, m | L, M \rangle$ are Clebsch–Gordon coefficients. For $l > 0$ the term with the lowest power in r in the expansion of the function Eq. (25) around the coalescence ($\mathbf{r} = 0$) is regular, and it comes from the second term of Eq. (25). Therefore, as in the case of L–form, the term “ $g^{(-)}$ ” from the final state function Φ^- will also contribute in lowest order. The exception, for V–form, is the s–state, as we saw in the previous subsection, because for $l = 0$ the second term in Eq. (25) is zero and the lowest power in r is singular.

For illustration we consider the initial $l = 1$ case. By inserting expression Eq. (25), for $l = 1$, expanding radial functions around the coalescence $R_1 = N_i r [1 - (a/2)r + \dots]$, keeping, as before, the expansion explicitly through terms linear in ar , including contributions from $g^{(-)}$ term and performing the integration by choosing the direction of \mathbf{p} as the z –axis, we obtain for the matrix element in V–form

$$\begin{aligned} M_V &= ia N_i N_p^C Y_1^m(\boldsymbol{\epsilon}) \int e^{-i\mathbf{p}\cdot\mathbf{r} - \varepsilon r} \left[\frac{(-1)^m}{2^{|m|} \cdot 3} P_2(\cos \vartheta) r + \frac{2}{3} r - \frac{i}{p} g^{(-)*} [i p r (1 + \cos \vartheta)] \right] d^3 r \\ &= (-1)^{1-m} \frac{8\pi i a}{p^4} N_i N_p^C Y_1^m(\boldsymbol{\epsilon}), \end{aligned} \quad (26)$$

which is just the result obtained in A–form, Eq. (23). Here, as before, we show the expansion explicitly through terms linear in ar (and a/p). If one would neglect the contribution from the final state singularity, as one would if assuming a plane wave was an adequate representation of the fast electron wave function, one would get a result different from zero (in the chosen frame where \mathbf{p} is z –axes) only for angular momentum projection $m = 0$, and even that result would be erroneous by factor of two. The contribution to the matrix element Eq. (26) 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 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 get the correct leading contribution.

VI. SCREENED POTENTIALS

Now we demonstrate that the previous results are sufficient to determine the asymptotic behavior of nonretarded photoabsorption in a general central potential. The entire previous discussion, although made for a nuclear point Coulomb potential model, is in fact valid for a general IPA potential which has the singularity of the Coulomb potential at the nucleus. Our discussion relied on the behavior of wave functions and interactions at this singularity. These behaviors, for the leading terms in the expansion which we utilized, are the same for an IPA potential as long as it is Coulombic at the singularity. To see the effects of the difference between an IPA potential (with Coulombic singularity) and a pure Coulombic potential we may assume a potential energy of the type $V(r) = -(Z\alpha/r)S(r)$, where $S(r)$ is a screening function which for small r behaves as $S(r) = (1 + s_1r + s_2r^2 + \dots)$, as assumed in III.

The interaction operators in L and V form are independent of the potential. In A form one obtains I as

$$I_A^{IPA} = \frac{-i}{\omega} [V(r), \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla}] = \frac{i}{\omega} \boldsymbol{\epsilon} \cdot \boldsymbol{\nabla} V(r). \quad (27)$$

The expansion of I_A^{IPA} about the coalescence gives

$$I_A^{IPA} = \frac{iZ\alpha\boldsymbol{\epsilon} \cdot \hat{\mathbf{r}}}{\omega} \left(\frac{1}{r^2} - s_2 - 2s_3r + \dots \right). \quad (28)$$

Note that the term involving s_2 in Eq. (28), 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 (and in Sec. VIII we show that it is in fact true in the first two orders) at high energies one obtains the same expression for photoionization in an IPA potential as in the Coulombic case. However, the normalization factors N_i^{IPA} will be different, and consequently IPA predictions will differ from the pure Coulombic prediction by these factors.

VII. RETARDATION AND RELATIVITY

We now discuss the inclusion of retardation. This changes the forms of the interaction operators. In 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 L-form and A-form, 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 expressions Eq. (7). In evaluating the integrals we need to specify how to deal with the photon retardation oscillating term $e^{i\mathbf{k}\cdot\mathbf{r}}$ in the $e\text{-}\gamma$ interaction $I(\mathbf{r})$. One way, particularly if we are considering retardation to a certain order in \mathbf{k} , is to expand $e^{i\mathbf{k}\cdot\mathbf{r}}$ in powers of $\mathbf{k}\cdot\mathbf{r}$. Another way of dealing with $e^{i\mathbf{k}\cdot\mathbf{r}}$ is to attach it to the fast oscillating term $e^{-i\mathbf{p}\cdot\mathbf{r}}$ and consider a FT in the variable $\Delta = \mathbf{p} - \mathbf{k}$, since in the nonrelativistic region $\mathbf{p} - \mathbf{k}$ is large whenever \mathbf{p} is large and our arguments using the AFT theorem in the asymptotic region apply. We just note here that in IPA single ionization from the ground state, retardation effects give a contribution of relative order $(v/c)^2$ [34,35], where v is velocity of the outgoing electron, which is of the same order as relativistic contribution. We will use this fact in the case of two electron atom to argue that retardation effects have the same relative contribution in single ionization and in double ionization in the SO region, due to factorization of 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 will still be true in certain kinematic situations which, however, at those energies are not dominant for the photoabsorption processes. Namely, at relativistic energies (and as $\omega \rightarrow \infty$) a region around the nucleus of Compton wavelength distances continue to contribute to photoabsorption, no matter how high the energy. This means that, although it is a relatively small region, the final state wave function in the whole region, rather than just at the point of coalescence, is needed, and certain knowledge to all orders in a is required [21]. Assuming analyticity, the region is characterized by an expansion about the origin, and expansion of the matrix element as a

series in a/Δ is still possible. Use of a plane wave approximation is no longer valid in any form.

VIII. CONVERGENCE OF THE CROSS SECTIONS TO THE HIGH ENERGY LIMIT—THE STOBBE FACTOR

Here we discuss the rate of convergence, with increasing energy, toward the exact IPA high energy limit for the cross sections, which we have so far obtained using an asymptotic expansions of the matrix element Eq. (12). The ratio of the first correction to the leading contribution is of the order of $1/p$, 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 K-shell binding energy. 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

$$N_p^C = \frac{1}{(2\pi)^{3/2}} \Gamma(1 + i\frac{a}{p}) e^{\frac{\pi a}{2p}}. \quad (29)$$

But there are also other Coulombic terms with this slow convergence (*e.g.* the first correction, which is unaffected by screening). We therefore collect all Coulombic terms in both initial and final state expansion of the IPA wave functions. Formally, this means that that we simply replace the initial state wave function with

$$\Psi_i^{IPA}(\mathbf{r}) = \frac{N_i^{IPA}}{N_i^C} \Psi_i^C(\mathbf{r}) + O[(\lambda_2^C - \lambda_2)r^{l+2}], \quad (30)$$

where λ_2 (λ_2^C) is the coefficient multiplying the third term in the expansion of the IPA (Coulombic) wave function, Eq. (8), $\Psi_i^C(\mathbf{r})$ is normalized Coulombic 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 Coulombic and screened third term in the expansion 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 Coulombic part of Eq. (9), but with shifted energy and with corrected normalization [27,29]. As already mentioned, according to [27,29], the exact

IPA wave function is Coulombic in the vicinity of the e-N singularity. A fairly accurate function (containing the dominant terms of relative order $1/p^2$) is obtained by using shifted momentum p_C rather than the true momentum p . 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 Coulombic function we should use, according to [27,29], 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, described by

$$\Psi_{\mathbf{p}}^{(-)}(\mathbf{r}) = \sqrt{\frac{p_C}{p}} \Psi_{\mathbf{p}_C}^{(-)}(\mathbf{r}) + O\left(\frac{1}{p^2}\right), \quad (31)$$

where the shifted momentum p_C is given by [27]

$$\frac{p^2}{2m} - \frac{p_C^2}{2m} = |E_B^C| - |E_B^{IPA}|, \quad (32)$$

where E_B^C (E_B^{IPA}) is the Hydrogen-like (IPA) binding energy of the state which is ionized.

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

$$\begin{aligned} M &= \frac{N_i^{IPA}}{N_i^C} \sqrt{\frac{p_C}{p}} \int \Psi_{\mathbf{p}}^{C(-)*}(\mathbf{r}) I_A(\mathbf{r}) \Psi_i^C(\mathbf{r}) d^3r + O\left(\frac{1}{p^2}\right) \\ &= \frac{N_i^{IPA}}{N_i^C} \sqrt{\frac{p_C}{p}} M_i^C + O\left(\frac{1}{p^2}\right). \end{aligned} \quad (33)$$

From Eq. (33) it immediately follows that at high energies

$$d\sigma^{IPA} = \left(\frac{N_i^{IPA}}{N_i^C}\right)^2 d\sigma^C + O\left(\frac{1}{p^2}\right), \quad (34)$$

where $d\sigma^C$ is the differential cross section obtained from Coulombic H-like wave functions calculated at shifted momentum p_C , and where O designates how rapidly the error decreases. [Momentum p from the phase space cancels p from the factor p_C/p leaving only shifted momentum p_C on the right side of Eq. (34).] The error in Eq. (34) is determined by the errors in the wave functions. According to the results presented in [27] the difference between screened and Coulombic functions [when unnormalized functions (the same first coefficient in the expansion is taken) are compared] is very small (and for a potential with a polynomial

expansion for small r decreases as $1/p^2$ [36]. This means that dominant terms of the relative order $1/p^2$ are collected. We will illustrate the fast convergence of this procedure for the cases which involve low Z atoms (He) and outer shells of higher Z atoms (L-state of Ne).

For Coulombic states the integrals Eq. (33) can be evaluated analytically and, as illustrative examples, for the cross section per electron for electron ionization from the 1s, 2s and 2p shells we have [37]

$$\sigma_{1s}^C = \frac{32\pi a^5 \alpha p}{3m^3 \omega^3 (p^2 + a^2)} \frac{(2\pi \frac{a}{p}) e^{\frac{a}{p}(\pi - 4 \arctan \frac{2}{a})}}{(e^{\frac{\pi a}{p}} - e^{-\frac{\pi a}{p}})}, \quad (35)$$

$$\sigma_{2s}^C = \frac{4\pi a^5 \alpha p (p^2 + a^2)}{3m^3 \omega^3 (p^2 + (a/2)^2)^2} \frac{(2\pi \frac{a}{p}) e^{\frac{a}{p}(\pi - 4 \arctan \frac{2p}{a})}}{(e^{\frac{\pi a}{p}} - e^{-\frac{\pi a}{p}})}, \quad (36)$$

$$\sigma_{2p}^C = \frac{\pi a^7 \alpha p (p^2 + \frac{11}{12} a^2)}{3m^3 \omega^3 (p^2 + (a/2)^2)^3} \frac{(2\pi \frac{a}{p}) e^{\frac{a}{p}(\pi - 4 \arctan \frac{2p}{a})}}{(e^{\frac{\pi a}{p}} - e^{-\frac{\pi a}{p}})}. \quad (37)$$

As an illustration of what Eq. (34) means we apply it to the calculation of high energy photoabsorption and compare it with the results obtained within 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 show also p–state results for Ne, for relatively small photon energies.

In Table I we show the total cross section for K–shell ionization obtained from Eq. (34) for $Z=2$ using $(N_i/N_i^C)^2 = 0.7358$ (which indicates large screening) [38], and compare with the results of full IPA calculations from [38]. As we see from Table I the agreement between the high energy result of Eq. (34) and full IPA calculations is very good already at 1 keV, despite the large screening, and in the energy range 1–2 keV the disagreement is around 1–2%. This should be compared with the lowest order result, which gives about 50% disagreement in the same energy range, as indicated in Table I by the value of the factor $\exp(-a\pi/p)$ (see the explanation for this factor below).

For the L–state of Ne screening is even larger $[(N_i/N_i^C)^2 = 0.4386$ for the 2s and $(N_i/N_i^C)^2 = 0.2277$ for the 2p]. In Table II we show the total cross section for 2s and

2p states of Ne and compare them also with full relativistic IPA calculations. For the 2s state Eq. (34) gives results which converge very fast to the full IPA result; at 1 keV the disagreement is around 6% and at 4 keV it is less than 1%. Similarly, for the 2p state the results of Eq. (34) converge rapidly to IPA results in the same energy range. This very good agreement between the results of Eq. (34) and 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 Coulombic e-N singularity. Namely, at 1-2 keV photon energy region, the distances involved (distances around the singularity at which the momentum is transferred between electron and nucleus) are within the K-shell orbit, in the case of Ne, and well within the K shell orbit in the case of He, where the screening is small. Thus the shapes of the wave functions at these distances are basically Coulombic. This is a very important point which we employ and generalize in our approach. The high energy photoabsorption is essentially Coulombic. This means that the high energy behavior (we are talking here about keV range as in our examples) of cross sections is determined by the properties of functions near the singularity, which is Coulombic. The screening effects enter, of course, but in a simple way as a constant factor, in these IPA examples. By straightforward generalization of these findings in high energy many-body calculations one can significantly simplify calculations involving e-e correlation, as we show in [2]. We will revisit the He single ionization example in [2], discussing it from the point of view of full correlated initial and final states, and discuss modifications of the cross section due to correlation.

Another important point which we want to make in this subsection, relevant for later discussion, is the relatively fast convergence of the ratios of photoabsorption cross sections to the results predicted by lowest order results (Born results in A-form). First, note that the slowest converging factor in our examples Eqs. (35-37) is $\exp(-\pi a/p)$ [with increasing energy $(a/p)(\pi - 4 \arctan(a/p)) \rightarrow -\pi a/p$]. This factor comes from the final state Coulombic interaction which means that in expanding wave functions around coalescence we get this factor by collecting all Coulombic interaction in the final state for each term in the expansion of the initial state. It 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 L-shell, Eqs. (36, 37). Note, in our examples the ratio

$$\frac{\sigma_{2s}}{\sigma_{2p}} \sim \omega + \frac{a^2}{12m} + O\left(\frac{a^2}{\omega}\right), \quad (38)$$

i.e. it is nearly linear function of photon energy ω in the keV range. If we have used the lowest order result (in the expansion around the coalescence) we would get $\sigma_{2s}/\sigma_{2p} \sim \omega$, *i.e.* a result very similar to the exact result (at keV range for Ne, for example) although the first order results for cross sections differ by order of magnitude from the exact in this energy range, as indicated roughly by the factor $\exp(-\pi a/p)$ in Table II.

IX. CONCLUSIONS

Studying high energy photoionization of an electron bound in a central potential, we have described a unified nonrelativistic approach to photoionization of atoms by photoabsorption at high incident photon energies ω (but still $\omega \ll m$). We have demonstrated, for this case, that high energy ionization by photoabsorption can be understood in terms of the singularities of the Hamiltonian. Our discussion was not dependent on the choice of the form [length (L), velocity (V), acceleration (A) etc.] of the photoionization matrix element.

Since 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 asymptotics of Fourier transforms. Based on Fourier transform theory, we have shown that a slow asymptotic decrease for large momentum p , such as $1/p^n$ in a $1/p$ asymptotic power expansion, of photoabsorption matrix element is connected with the singularities of the e-N potentials. We have demonstrated how this expansion in inverse powers of large momenta can be obtained from the expansion 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 a Coulombic e-N singularity. We have demonstrated that the approach, as well as final results, are gauge and form independent. However the dependence of the final results on the quality of initial and final state wave functions varies with gauge and form. We have found that 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 the leading contribution to the matrix element for photoabsorption is, in A-form, the lowest order Born result. In L- and V-form it is generally a higher order Born result, with the exception of V-form in ground state ionization where it is also the lowest order Born result. This means that the fast electron can not, in general (except in A-form), 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-form require knowledge of both 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 case of ionization of an electron in a screened potential. We have demonstrated that, by collecting all Coulombic terms in the vicinity of the e-N singularity we also collect the dominant terms up to the relative $1/p^2$ order and provide fast convergence of the cross sections. Although the neglected terms in the matrix element are still of relative order $1/p^2$ they were negligible. In such a way we have demonstrated that the high energy behavior (keV range as in our examples) of cross sections is determined by the properties of functions near a singularity which is Coulombic. 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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can apply the AFT approach to functions which have additional \mathbf{p} dependence (after pulling out the plane wave oscillations). This additional \mathbf{p} dependence does not cause any problem (and our Coulombic functions are an example of that) as long as it does not imply oscillations which would cancel the plane wave oscillations.

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TABLES

TABLE I. Total cross sections (in barns) for photoabsorption from the K-shell of He , $Z=2$, obtained using Eq. (34), σ_K , are compared with full IPA calculations, $\sigma_{S_c}^K$.

ω (keV)	σ_{1s} Eq. (34)	$\sigma_{S_c}^K$ Ref. [38]	$e^{-\frac{\alpha\pi}{p}}$
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

TABLE II. Total cross sections (in barns) for photoabsorption from the $2s$, σ_{2s} , and from the $2p$, σ_{2p} , subshell of Ne, $Z=10$, obtained using Eq. (34) are compared with full IPA calculations, σ_{Sc}^{2s} and σ_{Sc}^{2p} . The Stobbe factor $\exp(-\pi a/p)$ is also given.

ω (keV)	σ_{2s} Eq. (34)	σ_{Sc}^{2s} Ref. [38]	σ_{2p} Eq. (34)	σ_{Sc}^{2p} Ref. [38]	$e^{-\frac{\pi a}{p}}$
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