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Characterization of high-energy photoionization in terms of the singularities of the atomic potential. II. Beyond *K*-shell ionization in a many-electron atom, using the example of a two-electron atom in an excited state

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We describe single photoionization of excited states of two-electron atoms by photoabsorption at high incident photon energies ω (but still $\omega \ll m$). Our description of photoionization from excited states of the simplest many-body system is also, however, applicable for the characterization of high-energy photoionization of a many-electron atom from any subshell. We are using an approach [Surić *et al.*, Phys. Rev. A **67**, 022709 (2003)] based on asymptotic Fourier-transform (AFT) theory, in which the matrix elements for photoabsorption processes at high energies are understood in terms of the singularities of the many-body Coulomb potential. We obtain the dependence of the total cross section for single ionization of a two-electron atom in any initial state on photon energy. This energy dependence, for a general initial two-electron state, is generally different from the predictions of independent-particle approximation, and it is in qualitative agreement with recent experimental observations of *L*-shell photoionization in Ne and *M*-shell ionization in Ar. As in ground-state ionization, the energy dependence of the dominant contribution to the matrix element is connected, through AFT, with the e-N singularity; and it is determined by the amplitude of the lowest angular momentum l_{min} with which one electron can approach the e-N singularity. When $l_{min}=0$, as in the cases considered experimentally, this gives a factor for the dominant part of the total cross section, which is the same as for the ground state, $(1/\omega^{7/2})$. The final state interaction reduces this energy dependence by just one additional factor of $1/\omega$.

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In this sequence of papers [1,2] we are exploring 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. In our first paper [1], we introduced the ideas of AFT and explored correlation issues, focussing on photoionization of the ground state of a two-electron atom. In this paper we discuss single ionization from higher states of a two-electron atom, which we also find suitable as a model for a qualitatively good description of photoionization of many-electron atoms at high energies. Our approach to high-energy photoabsorption processes in terms of generalized AFT theory provides a unified description of photoabsorption at high energies.

As noted in Refs. [3,4], it was generally thought that an independent-particle approximation (IPA) picture of single photoionization from any state of any atom is adequate at sufficiently high photon energies. This meant that the cross section σ^+ for photoionization of an nl subshell of a complex atom was believed to behave as

$$\sigma_{nl}^{IPA}=\frac{a_{nl}}{\omega^{l+7/2}}, \tag{1}$$

at sufficiently high photon energies ω, where Z is the nuclear charge, $p \simeq \sqrt{2m\omega}$ is the outgoing electron momentum, and a_{nl} is a factor independent of energy, which contains information on the screening effects included in IPA. However, recent study of single ionization [3–6] shows that the IPA picture is inadequate for any subshell nl of a complex atom for which an $l\neq 0$ electron is ionized. The cross section for ionization of an $l\neq 0$ subshell of a many-electron atom decreases as $1/\omega^{9/2}$ for $\omega\to\infty$ [4], due to interchannel coupling [5] (provided that there is also an $l=0$ electron present in the atom), and not as $1/\omega^{l+7/2}$ as predicted by IPA Eq. (1).

This can already be seen in the photoionization of excited states of two-electron atoms, which we study here. We will show that in these situations, as discussed in Refs. [3–6], the total cross section is

$$\sigma_{nl}^{+}\sim\frac{1}{\omega^{9/2}}e^{-\pi mZ\alpha/p} \quad \text{for} \quad l\neq 0. \tag{2}$$

By including the Stobbe factor $S(p)=\exp(-\pi mZ\alpha/p)$ [7], which we will show can be pulled out, just as in the IPA case, the asymptotic behavior described by Eq. (2) is valid already in the energy region considered experimentally in Ref. [5] and near the energy region considered in Refs. [3,6].

We will first recall some relevant results about single ionization and the AFT approach from Paper I, and then we will analyze situations, related to those studied in Refs. [3–6], in a two-electron system, using our approach in terms of singularities. This means that we consider two electron initial states which, in an IPA picture, can be represented as if one electron is in an $l_1=0$ state while the other electron is in an $l_2=L\neq 0$ state. However, since in the actual physical situation l_1 and l_2 (each angular momentum separately) are not good quantum numbers, but rather only total angular momentum L (we are neglecting L-S coupling, as explained below), we will talk about situations in which the total angular momentum is $L\neq 0$ and for which there is a finite (and perhaps significant) probability of finding one electron with angular momentum $l_1=0$ while the other is in a state $l_2=L$. [Note that l_1 and l_2 here are not the usual spectroscopic angular momenta labels of the two electrons. In the usual spectroscopic notation these angular momenta labels are taken as good quantum numbers.] We will also include all other allowed l_1 and l_2. Our approach in terms of singularities shows that, as in ground-state ionization, the energy dependence of the dominant contribution to the matrix element is connected, through AFT, with the e-N singularity: it is determined by the amplitude of the lowest angular momentum l_{min} with which one electron can approach the e-N singularity. When $l_{min}=0$, this gives a factor for the dominant part of the total cross section, which is the same as for the ground state, $(1/\omega^{7/2})$. Final-state interaction can change this energy dependence by just one additional factor of $1/\omega$ in the leading order, as in the cases described by Eq. (2).

The analysis as well as the effect is closely related to the analysis of ionization of the ground state with excitations into $l\neq 0$ states given in Paper I. There we have demonstrated that, after absorption of the photon (determined by the cusp at the e-N coalescence), the remaining bound electron can be moved from an initial s state into a non-s state by the final-state interaction; this final-state interaction adds just one power of $1/p$ (to the power determined by the cusp), independent of l. In the situation we are considering here, we show that, asymptotically, the power of the leading contribution is determined by the cusp, giving a $1/p^3$ power (in an IPA model this would mean that the photon is absorbed by the s electron), and by the final-state interaction, which, in moving the electron from the $l_2\neq 0$ to the final $l=0$ state, adds just one additional power in $1/p$. The final result is that the vacancy is in the $l_2\neq 0$ state, and the matrix element has the leading power $1/p^4$ for any total $L\neq 0$. This is a strong modification of the IPA result, Eq. (1).

The differences between single ionization in a two-electron atom and in the IPA case are the correlations between the two electrons (in both the initial and the final states). In the case of single ionization of a two-electron atom, we have argued in Paper I, using the AFT theorem, that the dominant contribution to the total cross section is associated with the e-N coalescence, as in the one-electron case, whether or not the atom is in its ground state. However, while the dominant contribution to the single-ionization total cross section (summing over all final bound states, i.e., excitations are not distinguished) of the ground state of a two-electron atom does not involve final-state electron-electron interaction (and it involves initial-state correlation only in a normalization factor), regardless of the form used, the dominant contribution in the case of single ionization of a higher state does generally involve final-state electron-electron interaction. This final-state electron-electron interaction leads to predictions of an energy dependence of the cross sections for single ionization, which are different from the IPA predictions, as we will discuss below.

Our unified approach (AFT modified by Coulomb interaction) is based on the close relation between high-energy photoabsorption matrix elements and asymptotic Fourier transforms 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 [8,9]. 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.

We first look at the general behavior of two-electron bound states at coalescences (singularities). The dominant contributions to the high-energy photoabsorption total cross sections and (double-ionization) spectrum are connected with two-particle singularities. The properties of the bound states at these coalescences are understood sufficiently well to permit analysis of the energy dependence of the photoabsorption cross sections at high energies. In general, the singular behavior of a solution of the Schrödinger equation at the coalescence of two particles, of charges q_i and q_j, reduced mass μ_{ij}, and at small interparticle distances r_{ij} is given [10–12] by

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots)=\sum_{\lambda,m}\left(r_{ij}^{\lambda}\left[1+\frac{q_iq_j\mu_{ij}}{\lambda+1}r_{ij}\right]Y_{\lambda}^{m}(\hat{\mathbf{r}}_{ij})\phi_{\lambda,m}+O_{\lambda,m}(r_{ij}^{\lambda+2};\mathbf{r}_1,\mathbf{r}_2,\ldots)\right), \tag{3}$$

where $\phi_{\lambda,m}$ is a function of all other interparticle coordinates (all except the r_{ij} in which the function is expanded) and $O_{\lambda,m}(r_{ij}^{\lambda+2};\ldots)$ denotes a remainder, a function which depends on all coordinates and which in the vicinity of the $r_{ij}=0$ singularity vanishes faster than $r_{ij}^{\lambda+1}$ for $r_{ij}\to 0$. The lowest nonvanishing $\phi_{\lambda,m}$ depends on the state of the system. For the ground state of He (a spin singlet), for example, the lowest nonvanishing ϕ is $\phi_{0,0}$ for both the e-e and e-N coalescence. Expansion (3) is valid if all other interparticle distances are large compared to r_{ij}. This is sufficient for our purposes, as discussed in Paper I and also further below.

The matrix element for single ionization from the initial two-electron state $\Psi_{LM}(\mathbf{r}_1,\mathbf{r}_2)$ with total momentum L, resulting in a bound electron with quantum numbers (n,l,m), is

$$M^{(+)}=\sqrt{2}\int e^{-i\mathbf{p}\cdot\mathbf{r}_1}\Phi_{\mathbf{p}}^{(-)*}(\mathbf{r}_1)\Psi_{nlm}^{*}(\mathbf{r}_2)D_{\mathbf{p},nlm}^{(-)*}\times(\mathbf{r}_1,\mathbf{r}_2)I^{2e}(\mathbf{r}_1,\mathbf{r}_2)\Psi_{LM}(\mathbf{r}_1,\mathbf{r}_2)d^3r_1d^3r_2, \tag{4}$$

where $I^{2e}(\mathbf{r}_1,\mathbf{r}_2)$ is the e-γ interaction. As in Paper I, in Eq. (4) we have written the final-state wave function $\Psi_f(\mathbf{r}_1,\mathbf{r}_2)$ as a product of a continuum Coulombic wave function exp $(-i\mathbf{p}\cdot\mathbf{r}_1)\Phi_{\mathbf{p}}^{(-)}(\mathbf{r}_1)$ representing the outgoing electron, a bound-electron wave function $\Psi_{nlm}^{*}(\mathbf{r}_2)$, and a factor

$D^{(-)}_{\mathbf{p},nlm}(\mathbf{r}_1,\mathbf{r}_2)$ that contains everything else. This factorization is formal but convenient for our purpose, as will be clear later. In Eq. (4) we are neglecting L-S coupling. This means that we factorize the two-electron wave functions into a spin part (which, in a two-electron system, can be a symmetric triplet or an antisymmetric singlet) and a coordinate part. Further, since $\omega \ll m$, we neglect the interaction of radiation with electron spin. This means that the initial state and final state are either both spin singlets (symmetric coordinate part) or both spin triplets (antisymmetric coordinate part). The asymmetric form, Eq. (4) (the outgoing electron is in $\mathbf{r}_1$, while the bound electron is in $\mathbf{r}_2$), is obtained after employing the symmetry properties of the wave functions (both are either symmetric or antisymmetric in coordinates) and the interaction.

Our approach is to represent the integrand in terms of the simpler functions that describe it in the vicinity of the coalescence. As in our previous cases, we use Coulombic functions that satisfy e-N Kato cusp conditions.

$$\Psi_{LM}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{l_1m_1}\sum_{l_2m_2}\left[\frac{1}{N^C_{n_1,l_1}}\Psi^C_{n_1l_1m_1}(\mathbf{r}_1)\,\phi^{l_1m_1}_{l_2m_2}(\mathbf{r}_2)\right.$$
$$\left.+O_{l_1m_1}(r_1^{l_1+2};\mathbf{r}_1,\mathbf{r}_2)\right], \tag{5}$$

where $\Psi^C_{n_1l_1m_1}(\mathbf{r}_1)$ are hydrogenlike bound-state wave functions. In $\Psi^C_{n_1l_1m_1}(\mathbf{r}_1)$, we do not specify the principal quantum number n because we may take any particular n (for which l_1 exists) in Eq. (5) to the order we are considering. (A specific choice of n might be justified by specific physical reasons, but we do not discuss this point further.)

The partitioning [Eq. (5)] of the exact two-electron wave function in the vicinity of the e-N singularity is obtained following the arguments of Paper I. When one electron approaches the nucleus [$r_1 \ll r_0$, where r_0 is the size of the atom, $r_0=1/(mZ\alpha)$], while the other is at large distances [$r_2 \gg r_1$, and r_2 is not much smaller than r_0], then the wave function has an expansion in terms of angular momenta, and a partitioning due to the Kato condition as in Eq. (3). We have then just replaced terms from Eq. (3) with the corresponding (same angular momentum) Coulombic wave functions $\Psi^C_{n_1l_1m_1}/N_{n_1l_1}$, which for small r_1 have the same behavior as those terms. As explained in Paper I, we will use partition (5) in integrations over all distances r_2 [and therefore also for $r_2 \lesssim r_1$, for which partition (5), and also Eq. (3), is not correct]. However, the region $r_2 \lesssim r_1$ for $r_1 \ll r_0$ of the function $\Psi_{LM}(\mathbf{r}_1,\mathbf{r}_2)$ corresponds to the triple-coalescence point, which gives a negligible contribution to the total cross section. The terms in the angular-momentum expansion in Eq. (5) represent one electron approaching the nucleus with angular momentum quantum numbers (l_1, m_1), while the other (distant) electron is in any state (l_2, m_2), which, together with L, M and l_1, m_1, satisfies the angular-momentum algebra. Summation over all such terms is taken.

For the final state, the same procedure, as explained in Paper I, leads to

$$\Psi_f(\mathbf{r}_1,\mathbf{r}_2)=\Psi_f(0,\mathbf{r}_2)\Psi^C_{\mathbf{p}}(\mathbf{r}_1)+O\left(\frac{1}{p_1^2};\mathbf{r}_1,\mathbf{r}_2\right)$$
$$=e^{i\mathbf{p}\cdot\mathbf{r}_1}\Phi^{(-)}_{\mathbf{p}}(\mathbf{r}_1)\Psi_{n0}(\mathbf{r}_2)D^{(-)*}_{\mathbf{p},n0}(0,\mathbf{r}_2)$$
$$+O\left(\frac{1}{p_1^2};\mathbf{r}_1,\mathbf{r}_2\right), \tag{6}$$

where $O(1/p_1^2;\ldots)$ denotes the order of the terms (remainder) that we are neglecting within such a procedure.

By substituting Eqs. (5) and (6) into Eq. (4), the matrix element can be represented as a sum of terms, each of which factorizes into an absorption part and a correlation part,

$$M^{(+)}_L=\sum_{l_1m_1}\sum_{l_2m_2}M^{l_2\to l}_{corr}M^{l_1m_1}_{abs}, \tag{7}$$

where

$$M^{l_1m_1}_{abs}=\int \Psi^{(-)*}_{\mathbf{p}}(\mathbf{r}_1)I^{1e}(\mathbf{r}_1)\Psi^C_{n_1l_1m_1}(\mathbf{r}_1)d^3r_1 \tag{8}$$

is the photoabsorption matrix element for a H-like system [13], and

$$M^{l_2\to l}_{corr}=\frac{\sqrt{2}}{N^C_{n_1l_1}}\int \Psi^*_{nlm}(\mathbf{r}_2)D^{(-)*}_{\mathbf{p},nlm}(0,\mathbf{r}_2)\,\phi^{l_1,m_1}_{l_2,m_2}(\mathbf{r}_2)d^3r_2. \tag{9}$$

The correlation factor $M^{l_2\to l}_{corr}$ is the probability amplitude for moving the electron that is in a state l_2, after absorption of an electron in state l_1 occurs, into the final state (n,l,m). $M^{l_2\to l}_{corr}$ depends on all these quantum numbers, but we keep explicit only l_2 and l in order to simplify the notation. [Note the notation that $M^{l_1m_1}_{abs}$ has the angular-momentum quantum numbers l_1m_1 of the electron that absorbs the photon; $M^{l_2\to l}_{corr}$ involves the angular momentum l_2 of the other electron in the initial state, which due to final-state correlation is moved into final state of angular momentum l, indicated as $l_2\to l$.]

We are interested in obtaining cross sections accurate to the leading order in the e-e interaction for large p. For this purpose we may employ, as discussed in Paper I, $3C$ functions [14,15] for the final two-electron states. The $3C$ functions are accurate including the order $mZ\alpha/p^2$ [1]. This means that for $D^{(-)}_{\mathbf{p},nlm}(\mathbf{r}_1,\mathbf{r}_2)$, we use

$$D^{(-)}_{\mathbf{p},nlm}(\mathbf{r}_1,\mathbf{r}_2)=\Gamma\left(1-i\frac{m\alpha}{p}\right)e_1^{-\pi m\alpha/2p}F_1\left[i\frac{m\alpha}{p},1,-\frac{i}{2}\right.$$
$$\left.\times(pr_{12}-\mathbf{p}\cdot\mathbf{r}_{12})\right]+O\left(\frac{1}{p^2}\right), \tag{10}$$

where $O(1/p^2)$ denotes that by employing the $3C$ function the error in calculating the matrix element decreases faster than $1/p$ for large p. With function (10), the leading order of the correlation factor $M^{l_2\to l}_{corr}$ is accurately obtained. When the final state of the remaining bound electron is an s state ($l=0$; the case in which we are interested here), it is

$$M_{corr}^{l_2\to 0}=\frac{\sqrt{2}}{N_{n_1,l_1}^{C}}\begin{cases}\int R_{n0}(r_2)\rho_{l_2}(r_2)r_2^2dr_2, & l_2=0\\ -i\frac{m\alpha}{p}\frac{\sqrt{4\pi}}{l_2(l_2+1)}Y_{l_2}^{m_2}(\hat{\mathbf{p}})\int R_{n0}(r_2)\rho_{l_2}(r_2)r_2^2dr_2, & l_2\neq 0,\end{cases}\tag{11}$$

where $R_{n0}(r_2)$ is the radial component of the final-state bound electron and $\rho_{l_2}(r_2)$ is the radial component of $\phi_{l_2,m_2}^{l_1,m_1}(\mathbf{r}_2)$. [$\rho_{l_2}(r_2)$ depends on l_1, too, but we do not write it explicitly to keep the notation simple.]

In discussing the dominant contributions to the matrix element and to the cross sections, it is useful to recall the leading order in powers of $1/p$ of the $M_{abs}^{l_1}$ for various l_1. Generally, l_1 can have any value $l_1\geqslant 0$, and for large p, the leading order of $M_{abs}^{l_1}$ is [4,16]

$$M_{abs}^{l_1}\sim\frac{1}{p^{l_1+3}}.\tag{12}$$

The leading order of $M_{corr}^{l_2\to 0}$ can be seen from Eq. (11). It is $M_{corr}^{l_2\to 0}\sim 1/p$ whenever the interaction changes angular momentum, and $M_{corr}^{l_2\to 0}\sim 1$ for no change of angular momentum.

We will now consider the leading order in the photoabsorption matrix element for single ionization from a general two-electron $L\geqslant 1$ state with a final-state electron bound in an *s* state. The case $L=0$ (in fact, ground-state ionization of He-like system with excitation to any state) has been discussed in detail in Paper I. Other cases (general *L*, with final-state electron in any state) can be discussed along the lines presented here and in Paper I. The only difference is the expression for the leading order of $M_{corr}^{l_2\to l}$, which (for any *l*) can also be obtained using $3C$ functions, following Paper I and our discussion here. The difference is only in the fact that for $l\neq 0$, more terms are involved when the final-state interaction changes l_2 to *l*. The important general result in all these cases is that whenever the final state interaction changes angular momentum we get one additional $1/p$ power.

We first consider the case $L=1$ and then consider $L\geqslant 2$. We will assume that all l_1 and l_2 allowed by angular-momentum algebra are present in expression (5). This is generally true although the amplitude of some contributions can, in some cases, be small. The term with $l_1=0$ and $l_2=1$ gives the leading contribution, of the order $1/p^4$. One electron approaches the nucleus with angular momentum $l_1=0$ and absorbs a photon, giving the factor $1/p^3$, Eq. (12). The other electron is in the state $l_2=1$ and requires final state correlation, Eq. (9), to get into $l=0$, which gives an additional factor $1/p$. Another contribution, from $l_1=1$ and $l_2=0$, is of the same order $1/p^4$. All other terms, which involve $l_1\geqslant 1$ and $l_2\geqslant 0$, give a higher-order contribution. Note that in an IPA model the first term (with $l_1=0$ and $l_2=1$, and which requires final-state interaction) does not exist, while the other term (with $l_1=1$ and $l_2=0$, and which does not require final-state interaction) gives the only contribution. For this reason the first term is referred to as a modification of the IPA result [4].

For $L\geqslant 2$, the leading-order contribution to the matrix element comes from the term with $l_1=0$ and $l_2=L$, and it is of the order of $1/p^4$, as follows from Eqs. (12) and (9). All other terms of the expansion, Eq. (5), give terms of higher order in $1/p$. This can be seen by observing that all other terms, except the terms $l_1=L$ and $l_2=0$ (the only term which would exist in an IPA model, and which we may call the IPA term), contain a $1/p$ factor from the correlation, while the absorption factor is of higher order than $1/p^3$. The IPA terms, $l_1=L$ and $l_2=0$, have, however, an absorption factor of the order $1/p^{3+L}$ which, for $L\geqslant 2$, is of higher order than the leading term ($1/p^4$).

We therefore see that in the general situation the leading contribution to the matrix element is of the order $1/p^4$. In addition, from all terms in expansion (7), we can pull out a factor common to all $M_{abs}^{l_1}$. This, as discussed in Paper I, results in a slowly converging Stobbe factor [$\exp(-\pi a/p)$] in the cross section. It follows that the energy dependence of the single-ionization cross section is given by

$$\sigma\sim\frac{1}{\omega^{7/2}}e^{-\pi a/p}\quad\text{for}\ L=0,\qquad\sigma\sim\frac{1}{\omega^{9/2}}e^{-\pi a/p}\quad\text{for}\ L>0.\tag{13}$$

As discussed in Ref. [1], the terms neglected in Eq. (13) vanish with a factor $1/\omega$ faster. We may say that, asymptotically, the power of the leading contribution is determined both by the cusp, giving a $1/p^3$ power (in the IPA model this would mean that the photon is absorbed by an *s* electron) and by the final-state interaction which, moving the vacancy from the *s* state to the $L\neq 0$ state, adds just one additional power in $1/p$. The final result is that the vacancy is in the $L\neq 0$ state and the matrix element has the leading power $1/p^4$ for any $L\neq 0$. This is a strong modification of the IPA result.

These results are general and apply to many-electron atoms. In more complex systems, the expansions of the wave functions in the vicinity of the e-N coalescence corresponding to Eqs. (5) and (6) will be similar, except that coordinates, spins, and angular momenta of more electrons (not involved in the coalescence) will be involved. In general, each term in this expansion factorizes into a Coulombic function of the electron involved in the coalescence, and a function that describes all other electrons together, including the correlation of these electrons with the electron involved in the coalescence. This follows from the behavior of a general solution of Schrödinger equation in the vicinity of a singularity, Eq. (3). The whole procedure and the conclusions follow from this factorization.

We will now apply this general approach to an example of a two-electron system for the case $L=1$. For simplicity, we ignore *e-e* interaction in the initial state. The purpose of this simple example is to illustrate the size of the modification due to final-state interaction, the dependence of this modification on the nuclear charge *Z*, and how it depends on the symmetry of the coordinate part of the wave functions. We consider both spin-singlet and spin-triplet states (which are differently affected in two-electron system by the final-state interaction when $L=1$, as we shall see). We take one electron to be in a state $n=2$, $l=0$, while the other is in the state $n=2$, $l=1$. Then the uncorrelated wave function is

$$\Psi_{1M}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\Psi_{200}(\mathbf{r}_1)\Psi_{21M}(\mathbf{r}_2)+\zeta\Psi_{200}(\mathbf{r}_2)\Psi_{21M}(\mathbf{r}_1)], \tag{14}$$

where $\zeta=1$ for the spin-singlet and $\zeta=-1$ for the spin-triplet state. These IPA functions have correct *e-N* coalescences. Applying the above procedure, taking for Ψ Coulomb functions, we get that the total cross section per electron (summed over all polarizations of photon and electrons) is

$$\sigma^{+}_{L=1}=\sigma^{C}_{2p}\left(1-\frac{\zeta}{Z}+\frac{3}{4Z^2}\right), \tag{15}$$

where Z is the nuclear charge and σ^{C}_{2p} is the total cross section for photoabsorption from a H-like $2p$ state. We see that the modification depends as $1/Z$ on nuclear charge [17], and the sign of the modification depends on the symmetry of the coordinate part of the wave functions. For He, for example, Eq. (15) means a 50% modification of the IPA result [18]. Note that in situations with a filled *s* subshell and an electron in a *p* subshell (the situations considered experimentally in Refs. [3,5,6]), only the case with $\zeta=-1$ would contribute. This is because the final-state interaction must move an electron with the same spin projection as the ejected electron (the *s* subshell remains filled), and this is possible only for $\zeta=-1$.

In summary, we have described within a unified nonrelativistic approach single photoionization of two-electron atoms by photoabsorption at high photon energies ω (but still $\omega \ll m$). We have demonstrated that at high-energy, single ionization by photoabsorption from any state can be understood in terms of the singularities of the many-body Hamiltonian. We have demonstrated that the dominant contribution to the single-ionization total cross section of a general state involves final-state electron-electron interaction (and involves initial-state correlation through the *e-e* interaction when one electron is in the vicinity of the nucleus). This final-state electron-electron interaction leads to predictions of an energy dependence of the cross sections for single ionization, which are different from the IPA predictions. We have shown using our AFT approach that, due to the final-state interaction, the energy dependence of the dominant contribution to the matrix element is connected, through AFT, with the *e-N* singularity. It is determined by the amplitude of the lowest angular momentum with which one electron can approach the *e-N* singularity. When the lowest angular momentum of the electron approaching the nucleus is $l=0$, as in the cases considered experimentally, the total cross section decreases with large photon energies (but still $\omega \ll m$), not faster than $\exp(-\pi a/p)/\omega^{9/2}$ for any initial total angular momentum *L*.

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[2] We will refer to the previous paper [1] and the present paper as Papers I and II, when convenient.

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[7] We write asymptotic total cross sections including the factor $S(p)=\exp(-\pi a/p)$ (which we call the Stobbe factor [1]) since, as we have shown in Paper I and also here, it appears in total cross sections for single and double ionization. It is a slowly converging factor $[S(p)\rightarrow 1$ as $\omega\rightarrow\infty]$ and generally very high energies are required for it to be close to unity. Comparison with experiments performed even at a few keV, of even light atoms, requires inclusion of this factor, except when ratios of cross sections are being considered (for which it cancels out).

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