Quantum theory of post-collision interaction in inner-shell photoionization: Final-state interaction between two continuum electrons

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In inner-shell photoionization followed by Auger decay, the Auger electron initially screens the ionic Coulomb field "seen" by the photoelectron. This screening phenomenon affects the post-collision interaction that shifts the Auger energy and distorts the line shape. The analytical Auger electron line-shape formula which we derived previously on the basis of asymptotic Coulomb wave functions is now modified to account for the screening effect. The ionic charge seen by the photoelectron is reinterpreted on the basis of asymptotic properties of the continuum wave function pertaining to two outgoing electrons. It is shown that this procedure is consistent with semiclassical models which account for the time required for the Auger electron to overtake the photoelectron. Our modified Coulomb line shapes are found to agree perfectly with the semiclassical line shapes for photon excess energies $E_{\rm exc} \gtrsim (\Gamma_i \varepsilon_A)^{1/2}$, where Γ_i is the width of the initial hole state and ε_A, the Auger electron energy. Agreement between the present theory and recent synchrotron-radiation measurements consequently becomes excellent in this range of photon energies as well.

I. INTRODUCTION

In the radiationless decay of an atom that has been photoionized near an inner-shell threshold, the Coulomb field of the receding photoelectron perturbs the Auger electron energy and line shape.[1] We have treated this *post-collision interaction* (PCI) phenomenon in a previous paper[1] (hereafter referred to as I) from the point of view of resonant scattering theory.[2–4] It was shown in I how the lowest-order line-shape formula, corresponding to the "shake-down" mechanism,[5] emerges from approximations of the general multichannel transition matrix element. The PCI phenomenon was thus treated as a consequence of a resonant rearrangement collision in which a photon and an atom in the initial channel turn into an ion and *two* electrons (one of which has a nearly characteristic energy) in the final channel. With the lowest-order formula we performed fully quantum-mechanical and relativistic calculations of the PCI effect in x-ray-induced argon K-L_2L_3 (^1D) Auger and xenon L_2-L_3N_4 ($J=3$) Coster-Kronig electron emission and attained excellent agreement with measured PCI shifts in the near-threshold region. These calculations confirmed the results of an earlier nonrelativistic prediction of the shift of the xenon L_3-M_4M_5 ($^1G_4$) line.[6]

All these studies were restricted to photon excess energies $E_{\rm exc}$ that are small compared with the Auger electron energy. As pointed out by Ogurtsov[7] and by Russek and Mehlhorn,[8] however, the lowest-order theory in its semiclassical form[9,10] does not take into account the time it takes for the Auger electron to pass the previously emitted slow photoelectron, whence the PCI shift is overestimated when $E_{\rm exc}$ approaches ε_A. Indeed the predictions of the semiclassical PCI model of Russek and Mehlhorn[8] agree extremely well in such a case, that of the xenon N_5-$O_{2,3}O_{2,3}$ (^1S) line, with measurements of both shift and line shape recently performed by Borst and Schmidt.[11] On the other hand, the lowest-order quantum-mechanical calculations[1] do not agree with the results of Refs. 8 and 11. This discrepancy arises because the shake-down model, even in its exact quantum-mechanical form, does not account for the interaction between the photoelectron and the Auger electron in the final state.[1] The only effect considered in the shake-down model is the response of the photoelectron to the change of the ionic core potential produced by the Auger decay.

A consistent description of threshold phenomena in inner-shell ionization, including discrete excitations, requires the use of quantum theory; it is therefore of interest to generalize the lowest-order theory so as to incorporate the "no-passing" effect.[8,11] From a fundamental point of view, this requires a generalization of the K-matrix theory of single-electron photoionization.[12] However, a simplifying factor in the present problem is that, as shown in I, the lowest-order PCI results can be interpreted in terms of an analytical line-shape formula based on asymptotic Coulomb wave functions. The Coulomb line shape depends solely on the excess photon energy $E_{\rm exc}$, the lifetime Γ_i^{-1} of the initial state of the Auger process, and the change Q of the ionic charge during

Auger electron emission.[1] Thus, there is only one quantity which is exposed to the final-state interaction between the photoelectron and the Auger electron, namely Q. In Sec. II we show that Q can indeed be determined uniquely by examining the asymptotic behavior[13,14] of the exact two-electron continuum wave function.

In Sec. III we show that the semiclassical treatment of the no-passing effect[8,11] results in the same choice of Q. On the basis of recent work by Kuchiev and Sheinerman,[15] we derive an analytical semiclassical line-shape formula which depends on Q and for $E_{\rm exc} \gtrsim (\Gamma_i \varepsilon_A)^{1/2}$ essentially coincides with our Coulomb line-shape formula.

Section IV contains a comparison between shifts and line shapes predicted by our modified Coulomb theory and the semiclassical theories.[8,15] We also compare the present results with measured PCI shifts for N_5-$O_{2,3}O_{2,3}$ (^1S) Auger transitions[11] and L_2-L_3N_4 ($J=3$) Coster-Kronig transitions in xenon.[16] The L_2 widths $\Gamma(L_2)$ are approximately 30 times greater than the N_5 widths $\Gamma(N_5)$, therefore the N_5-OO initial states are very long lived compared with those of the L_2-LN transitions. This paper ends with a discussion of the dependence of the Auger line shape on the angle between the directions of emission of the Auger electron and the photoelectron, and of the effective-charge concept within the context of the general theory of final-state interactions in double photoionization.

II. FINAL-STATE INTERACTION BETWEEN TWO CONTINUUM ELECTRONS

A. The Coulomb line-shape formula

In I we have shown, by systematic simplifications of a general multichannel transition matrix element, that the cross section for observing either photoelectrons or Auger electrons in a noncoincidence experiment is

$$\frac{d\sigma}{d\varepsilon} = \frac{2\pi\alpha}{3}\omega \sum_{l,l_A} [\Gamma_{l_A}(E'-\varepsilon)\,|\,\langle \varepsilon l \,|\, \tau' \rangle\,|^2 + \Gamma_{l_A}(\varepsilon)\,|\,\langle (E'-\varepsilon) l \,|\, \tau' \rangle\,|^2] \quad (1)$$

for the Auger multiplet

$$[n_i l_i]^2 L_i \rightarrow [n_f l_f, n_{f'} l_{f'}]^{1,3} L_f \varepsilon_A l_A \, {}^2L_i$$

of an initially closed-shell atom. Equation (1) attributes the emission of Auger electrons of this particular multiplet to a resonance in the double photoionization process, leading to final $[n_f l_f, n_{f'} l_{f'}]^{1,3} L_f \varepsilon_S l \varepsilon_A l_A \, {}^1P$ states.[1] It thus only accounts for photoelectrons which are emitted in association with a given Auger multiplet. In Eq. (1), α is the fine-structure constant, ω is the energy of the incident radiation, and we have $E'=\omega - I_{ff'}$, where $I_{ff'}$ is the ionization energy of the final double-hole state. The Auger electron emission rate is Γ_{l_A}, for which explicit expressions can be found in the literature.[17] In Eq. (1), we have $l = l_i \pm 1$ ($l_i > 0$), and l_A satisfies the triangular rule $L_f + l_A \geq L_i \geq |\, L_f - l_A \,|$. The function $|\,\tau'\rangle$ is given by

$$|\,\tau'\rangle = \int_0^\infty \frac{|\,\tau l\rangle \langle [n_i l_i]\tau l \, {}^1P \| D^{(1)} \| {}^1S \rangle d\tau}{E_{\rm exc} - \tau + i\Gamma_i/2}\,, \quad (2)$$

where the integration includes the summation over discrete $|\,\tau\rangle$ states and where the reduced electric dipole matrix element, in the central-field frozen-core approximation, is

$$\langle [n_i l_i]\tau l \, {}^1P \| D^{(1)} \| {}^1S \rangle = (-1)^{l_{\max}-1} \sqrt{2l_{\max}} D_1(\tau l, n_i l_i)\,. \quad (3)$$

Here, we have $l_{\max} = \max(l_i, l)$, and D_1 is the dipole radial matrix element. The photon excess energy in Eq. (2) is $E_{\rm exc} = \omega - I_i$, where I_i is the ionization energy of the $n_i l_i$ hole state with lifetime Γ_i^{-1}.

If $|\,\varepsilon l\rangle$ and $|\,\tau l\rangle$ were to correspond to electrons moving in the same ionic field, we would have $\langle \varepsilon l \,|\, \tau l \rangle = \delta(\varepsilon - \tau)$. Since $\tau \cong E_{\rm exc}$ according to Eq. (2), this shows that the first term in Eq. (1) peaks at approximately $\varepsilon_S = E_{\rm exc}$, and the second term at $\varepsilon \cong \varepsilon_A = I_i - I_{ff'}$. As long as $E_{\rm exc} < \varepsilon_A$, the photopeak is thus situated below the stationary Auger peak in energy. If $E_{\rm exc}$ is increased, the photopeak moves towards the Auger peak and will eventually cross it at $E_{\rm exc} = \varepsilon_A$. According to Eqs. (1) and (2), both peaks have distorted non-Lorentzian shapes such that the maximum of the photopeak occurs at $\varepsilon = E_{\rm exc} - \Delta$ and the Auger peak occurs at $\varepsilon = \varepsilon_A + \Delta$, where Δ is a positive PCI shift.[1] The distortion changes as a function of $E_{\rm exc}$; it is predicted to vanish at $E_{\rm exc} = \varepsilon_A$ on the basis of semiclassical considerations.[8,11]

In Eq. (1) the PCI effect is attributed to the change of the ionic core potential produced by the Auger decay. This corresponds to a model in which both final-state electrons move in a potential of $+2/r$ without interacting with each other. In the following, we take their mutual interaction into account by modifying the matrix element $\langle \varepsilon l \,|\, \tau' \rangle$ in Eq. (1).

We limit ourselves to a description of the line shape by excluding all irrelevant factors from Eq. (1). As in I (Sec. 5), we thus examine the normalized Coulomb line shape

$$P_Q(\varepsilon) = \frac{\Gamma_i}{2\pi}\,|\,\langle \varepsilon \,|\, \tau' \rangle\,|^2\,, \quad (4)$$

where

$$\langle \varepsilon \,|\, \tau' \rangle = \int_0^\infty \frac{\langle \varepsilon \,|\, \tau \rangle d\tau}{E_{\rm exc} - \tau + i\Gamma_i/2} \quad (5)$$

does not contain the slowly varying dipole matrix element (3). Here

$$|\,\varepsilon\rangle = r^{-1}(2/\pi\kappa)^{1/2} \sin\left[\kappa r + \frac{Q}{\kappa}\ln 2\kappa r + \arg\Gamma(1 - iQ/\kappa)\right] \quad (6)$$

and

$$|\tau\rangle = r^{-1}(2/\pi\kappa')^{1/2}\sin(k'r) \tag{7}$$

are asymptotic wave functions corresponding to $l=0$, without a short-range phase shift. In Eq. (6), we have $\varepsilon=\frac{1}{2}\kappa^2$, and in Eq. (7), $\tau=\frac{1}{2}\kappa'^2$. According to Eq. (1), one should replace ε by $E'-\varepsilon$ in order to examine the Auger electron line shape in the vicinity of $\varepsilon\approx\varepsilon_A$. For the sake of completeness, the line-shape formula is briefly reviewed in the Appendix.

It was shown in I that Eq. (4), with the choice $Q=Q_f-Q_i=1$ in Eq. (6), reproduces the line shape predicted by fully quantum-mechanical calculations of the cross section (1) in the limit of high excess energies for a number of Auger and Coster-Kronig transitions. It was hence suggested that Eq. (4) could be modified to account for the no-passing effect[8,11] by introducing an $E_{\rm exc}$-dependent Q which will be the only parameter in the theory other than $E_{\rm exc}$ and Γ_i.

In the derivation of the Coulomb line-shape formula (4), the effective charge Q is set equal to the final-state ionic charge Q_f (Q_i is assumed to be zero). It therefore seems clear that the no-passing effect is a consequence of the interaction between photoelectron and Auger electron in the *final* state. The effect can be expected to be present *whenever* two electrons are ejected into the continuum, either resonantly or nonresonantly. This can be seem more clearly if Eq. (4) is interpreted in terms of an expansion of the final-state Coulomb wave function $|\varepsilon\rangle$ in energy-normalized free spherical waves. As in the Appendix, we assume an s-wave final state ($l=0$) with phase shift $\delta_f(\kappa)=0$. The expansion of $P_f(r)=r\,|\varepsilon\rangle$ then is

$$P_f(r)=\sqrt{2/\pi\kappa}\int_0^\infty A(\kappa,\kappa')\sin(\kappa' r)d\kappa' , \tag{8}$$

where we have $\kappa=\sqrt{2\varepsilon}$, and $A(\kappa,\kappa')$ is given by

$$A(\kappa,\kappa')=\lim_{\nu\to 0}\frac{1}{2\pi i}e^{-\pi Q/2\kappa} \times\{c_+[(\kappa+\kappa'+i\nu)^{\alpha_+}-(\kappa-\kappa'+i\nu)^{\alpha_+}] -c_-[(\kappa+\kappa'-i\nu)^{\alpha_-}-(\kappa-\kappa'-i\nu)^{\alpha_-}]\}. \tag{9}$$

The coefficients $c_\pm$ and $\alpha_\pm$ are defined in Eqs. (A5) and (A6), respectively. The limit $\nu\to 0$ ensures that $A(\kappa,\kappa')$ becomes the Dirac δ function for $Q=0$. Equation (9) is singular at $\kappa=\kappa'$ even for $Q\neq 0$. The integral (8), however, remains finite.

Use of the expansion (8) in the shake-down amplitude (5) leads to

$$\langle\varepsilon\,|\,\tau'\rangle=\left[\frac{\Gamma}{2\pi}\right]^{1/2}\int_0^\infty A(\kappa,\kappa')\frac{2}{\kappa'^2-\beta^2}d\kappa' , \tag{10}$$

where β is defined in Eq. (A7). For $Q=0$, i.e., $A(\kappa,\kappa')=\delta(\kappa-\kappa')$, the absolute square of the amplitude (10) is the normalized Lorentzian profile. Equation (10) shows that the distorted profile is a superposition of Lorentz amplitudes, weighted by the coefficients of free spherical waves in the expansion of the final Coulomb wave function. Quite independently of the lifetimes of intermediate states, the mutual screening of the two outgoing electrons thus alters the coefficients $A(\kappa,\kappa')$ only through modification of the effective charge Q. The question therefore is: Does consideration of the mutual asymptotic interaction between the two outgoing electrons lead to a modification of the coefficients $A(\kappa,\kappa')$ such that the no-passing effect is accounted for? As shown in the following section, the answer is affirmative.

B. Mutual screening of the ionic core by two outgoing electrons

We study the boundary conditions on the final-state wave function Ψ that describes two outgoing electrons with wave vectors $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$ in the reaction

$$\omega + A^{Z-1}\to A^{Z+1}+e+e , \tag{11}$$

with $Z\geq 0$. The structure of the ion is neglected so that the problem is reduced to a determination of the asymptotic form of the spatial part of the two-electron wave function $\Psi=\Psi_{\boldsymbol{\kappa}_1\boldsymbol{\kappa}_2}(\mathbf{r}_1,\mathbf{r}_2)$ in the limit $r_1\to\infty$, $r_2\to\infty$, and $r_{12}\to\infty$. According to Peterkop,[14] the phase of the leading term is of the form

$$\Psi_{\boldsymbol{\kappa}_1\boldsymbol{\kappa}_2}(\mathbf{r}_1,\mathbf{r}_2)\sim r^{-5/2}e^{ikr+iW(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)\ln kr} , \tag{12}$$

where we have $k=[2(\varepsilon_1+\varepsilon_2)]^{1/2}$, $r=(r_1^2+r_2^2)^{1/2}$ and

$$W(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)=\frac{Z+1}{\kappa_1}+\frac{Z+1}{\kappa_2}-\frac{1}{|\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_2|} . \tag{13}$$

In order to obtain the asymptotic form of the wave function which is used to describe single-electron ionization by electron impact[13,14] or double photoionization, one needs to multiply Eq. (12) by a factor containing the scattering amplitude. In the present context, however, we only make use of Eq. (12) by requiring that the product of two Coulomb wave functions $\Phi_i(\hat{Z}_i,\boldsymbol{\kappa}_i\,|\,\mathbf{r}_i)$ ($i=1,2$) for the effective charges $\hat{Z}_1$ and $\hat{Z}_2$ of the ionic core has the same asymptotic property (12) as the exact solution. We have

$$\Phi_1(\hat{Z}_1,\boldsymbol{\kappa}_1\,|\,\mathbf{r}_1)\Phi_2(\hat{Z}_2,\boldsymbol{\kappa}_2\,|\,\mathbf{r}_2)\sim r^{-5/2}e^{ikr+iw(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)\ln kr} , \tag{14}$$

where $w(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)=\hat{Z}_1\kappa_1^{-1}+\hat{Z}_2\kappa_2^{-1}$, and where $\hat{Z}_1$ and $\hat{Z}_2$ depend on the angle between $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$.[13,14] If the exact wave function is expanded in products of one-electron wave functions involving $\Phi_1\Phi_2$, then condition (14) ensures that the expansion coefficients have no divergent phase factor. The *necessary* condition for correctly describing the escape of two electrons from an ion with charge $Z+1$, in terms of Coulomb wave functions, is thus

$$\frac{\hat{Z}_1}{\kappa_1}+\frac{\hat{Z}_2}{\kappa_2}=\frac{Z+1}{\kappa_1}+\frac{Z+1}{\kappa_2}-\frac{1}{|\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_2|} . \tag{15}$$

According to Eq. (6), the Coulomb line-shape formula (4) is based on an effective charge Q which is angle in-

dependent. Thus, since Eq. (15) holds for any angle between κ_1 and κ_2, we shall take the spherical average over it. Assuming $\kappa_1 > \kappa_2$, the result is

$$\frac{Z_1}{\kappa_1}+\frac{Z_2}{\kappa_2}=\frac{Z+1}{\kappa_1}+\frac{Z+1}{\kappa_2}-\frac{1}{\kappa_1} , \tag{16}$$

where Z_1 and Z_2 are spherical averages over $\hat{Z}_1$ and $\hat{Z}_2$, respectively. By choosing $Z_1=Z+Q_1$ and $Z_2=Z+1$, we describe the screening of the ionic core by the slower electron. According to Eq. (16), the faster electron sees the charge $Z_1=Z$, i.e., $Q_1=0$. By choosing $Z_1=Z+1$ and $Z_2=Z+Q_2$, we describe the screening of the inner core by the faster electron. According to Eq. (16), the slower electron sees the charge $Z_2=Z+Q_d$, where the *dynamic* charge Q_d is

$$Q_d=1-\frac{\kappa_2}{\kappa_1} . \tag{17}$$

The slower electron is thus partially screened; only when κ_1 equals κ_2 is it fully screened, i.e., $Z_2=Z$.

It should be stressed that the screening described here is a property of the stationary wave function of the final state in reaction (11), and does not depend on whether the process is resonant or nonresonant. These results can therefore be used to determine the effective charge Q in Eq. (4), given by $Q=Q_f-Q_i$; we have $Q_i=Z$ and $Q_f=Z+Q_d$ for the slow electron, but $Q_f=Z$ for the fast electron. Our quantum-mechanical treatment of the PCI effect therefore indicates that the no-passing effect[8,11] is a consequence of the mutual screening of the two electrons in the final state of the resonant double ionization process leading to Auger electron emission. It also suggests that one choose

$$Q=Q_d=1-\frac{\kappa_S}{\kappa_A}=1-(E_{\rm exc}/\varepsilon_A)^{1/2} \tag{18}$$

in the line-shape formula (4) as long as the photoelectron is slower than the Auger electron, and $Q=0$ if the opposite is true. In the latter case, the Lorentzian form of the profile is recovered. This result is independent of Z, consistent with the choice $Q_i=0$ in the derivation of Eq. (18). As shown below, these findings are also in accord with the semiclassical treatment of the no-passing effect and with recent experiments.

III. SEMICLASSICAL TREATMENT OF THE NO-PASSING EFFECT

In Sec. II we have discussed the no-passing effect in terms of the angle-integrated double photoionization cross section. In the semiclassical picture this involves consideration of the escape of the photoelectron and Auger electron in terms of only their radial distances from the nucleus.

The essential point in the model of Russek and Mehlhorn[8] is that in Auger decay of a hole state produced by photoionization, the Auger electron does not catch up at once with the photoelectron, but only after an interval that is determined by the time at which the Auger electron is emitted and by the velocities of the two electrons. If the photoelectron starts from a distance $r=R_S$ from the nucleus at $t=0$, and the Auger electron from $r=R_A$ at a later time $t=t_A$, we have

$$\int_{R_S}^{\rho}\frac{dr}{v_S}=\int_{R_A}^{\rho}\frac{dr}{v_A}+t_A , \tag{19}$$

where the velocities v_S of the photoelectron and v_A of the Auger electron depend on r. In the classical approximation, they fulfill the relation

$$\tfrac{1}{2}v^2-\frac{Z'}{r}=E , \tag{20}$$

where we have, for $v=v_S$, $Z'=Z$ and $E=\varepsilon_S$, and for $v=v_A$, $Z'=Z+1$ and $E=\varepsilon_A$. The energies ε_S and ε_A are the *unshifted* energies, i.e., the photoelectron energy distribution has a maximum at $\varepsilon=\varepsilon_S-\Delta$ and the Auger peak at $\varepsilon=\varepsilon_A+\Delta$, where Δ is the PCI shift. In Eq. (19), $\rho=\rho(t_A)$ is the radius at which the Auger electron passes the photoelectron. While it is possible that v_S could be larger than v_A, we consider in the following the photoelectron to be the slower one, i.e., $v_S \le v_A$. Hence one can always from Eq. (19) determine $\rho=\rho(t_A)$.

At the moment when the two electrons are at the same distance $r=\rho$ from the nucleus, they exchange energy which, according to Eq. (20), is equal to ρ^{-1}, because the ionic charge Z' as seen by the photoelectron suddenly changes from Z to $Z+1$. The photoelectron loses the same amount of energy that the Auger electron gains. The PCI shift Δ consequently is a positive quantity as defined above. If we denote the instantaneous Auger electron energy at $t=t_A$ by $\varepsilon'=\varepsilon'(t_A)$, then the *observed* Auger electron energies fulfill the relation[8]

$$\varepsilon=\varepsilon'+\rho^{-1}(t_A) . \tag{21}$$

The observed energies correspond to the probability $P(\varepsilon)d\varepsilon$ that an Auger electron is observed in the interval $(\varepsilon,\varepsilon+d\varepsilon)$. If ε' is independent of the time and ρ infinite, then $P(\varepsilon)$ must coincide with the normalized Lorentzian line shape. Otherwise, there is a distortion which can be determined by squaring the absolute value of the amplitude

$$a(\varepsilon)=\left[\frac{\Gamma}{2\pi}\right]^{1/2}\int_0^{\infty}dt\exp\left[-i\int_0^{t}\left[\varepsilon'-i\frac{\Gamma}{2}-\varepsilon_A\right]dt_A\right] , \tag{22}$$

where $\varepsilon'=\varepsilon-\rho^{-1}$ is obtained from Eqs. (19) and (20) as a function of t_A.[8] Clearly, the Lorentzian line shape is recovered if ε' is taken to be time independent in Eq. (22). As Russek and Mehlhorn have indicated,[8] one can justify the use of the amplitude (22) by considering the solution of the Schrödinger equation for the Auger electron in the slowly varying electric field of the slow photoelectron. Alternatively, one can derive Eq. (22) by approximating the WKB amplitude for a shake-down transition[9] and transforming from the variable r to t with the aid of Eq. (20) for v_S.[8]

The derivation of Russek and Mehlhorn[8] blends classi-

cal arguments involving time with a quantum-mechanical description of the Auger decay. It is therefore of interest to examine whether the approach of Ref. 8 also leads to the concept of a dynamical charge, introduced in Eq. (17). In demonstrating this fact, we examine the condition (19) more closely and also derive the asymptotic PCI-shift formulas of Niehaus[10] and Ogurtsov.[7]

Let the slow electron reach the radial distance r_S at time t_A. Since r_S depends implicitly on ρ, we have

$$\int_{R_S}^{\rho}\frac{dr}{v_S}=\int_{R_A}^{\rho}\frac{dr}{v_A}+\int_{R_S}^{r_S(\rho)}\frac{dr}{v_S}\ , \tag{23}$$

according to Eq. (19). Taking the derivative with respect to ρ on both sides of Eq. (23) yields

$$\frac{1}{v_S(\rho)}=\frac{1}{v_A(\rho)}+\frac{Q}{v_S(r_S(\rho))}\ , \tag{24}$$

where we have defined an effective screening charge Q such that $Q=dr_S/d\rho$. Consequently, we have

$$Q=\frac{v_S(r_S)}{v_S(\rho)}\left[1-\frac{v_S(\rho)}{v_A(\rho)}\right]\ . \tag{25}$$

For large ρ, Eq. (25) reduces to Eq. (18), since we have $v_S(r_S)\cong v_S(\rho)\cong\sqrt{2E_{\rm exc}}$ and $v_A(\rho)\cong\sqrt{2\varepsilon_A}$ in this limit. Thus $Q\cong Q_d$ becomes independent of ρ, and we have $Q_d\cong r_S/\rho$.

At $r=\rho$ the exchange of energy amounts to $\Delta=\rho^{-1}$, where Δ is the positive PCI shift. Since $r_S\cong t_A\sqrt{2E_{\rm exc}}$ and $t_A\cong 2/\Gamma_i$, it follows from Eq. (25) and the definition (18) of Q_d that

$$\Delta\cong\frac{Q_d\Gamma_i}{2\sqrt{2E_{\rm exc}}}=\Delta_0\left[1-\left[\frac{E_{\rm exc}}{\varepsilon_A}\right]^{1/2}\right]\ , \tag{26}$$

where Δ_0 is the shift originally derived by Barker and Berry.[18] The quantity Δ_0 as defined in Eq. (26), which was first given by Ogurtsov,[7] also follows from the formula of Niehaus[10] for $E_{\rm exc}\gg\Delta$.

In order to evaluate the amplitude (22), ρ^{-1} must be evaluated from Eqs. (19) and (20) as a function of t_A. Due to the nonlinear nature of Eq. (20), this leads to a transcendental equation for $\rho=\rho(t_A)$ which is not very transparent.[8] It is therefore of interest to compare the results of Russek and Mehlhorn[8] with the semiclassical approach of Kuchiev and Sheinerman,[15] in which rectilinear trajectories of the outgoing charged particles are assumed. The latter authors consider arbitrary reactions of the type $X+Y\rightarrow A+D\rightarrow A+B+C$ between any atomic particles such that $A+D$ forms an intermediate complex which breaks up, with a certain lifetime Γ_i^{-1}, into three charged particles, A, B, and C. The assumption of rectilinear motion requires that A, B, and C are far apart, which is consistent with the assumptions underlying our Coulomb line-shape formula (4) for the special case in which X represents a photon and Y, the ion $A^{(Z-1)}$. Kuchiev and Sheinerman[15] also consider Γ_i to be small, but as we shall indicate, this is not a necessary assumption for a reaction in which D is an ion A^{*Z} with an inner-shell hole, C the residual ion Z^{Z+1}, and A and B are electrons.

Kuchiev and Sheinerman[15] consider an amplitude which is similar to Eq. (22). Their method leads, however, to an energy gain of the Auger electron which is of the form

$$\mathcal{A}_{\rm KS}(t)=-\int_0^T\Delta V(t,t_A)dt_A\ , \tag{27}$$

where

$$\Delta V(t,t_A)=\frac{-1}{v_S(t+t_A)}+\frac{1}{|\,\mathbf{v}_S(t+t_A)-\mathbf{v}_A t\,|} \tag{28}$$

is the change in the potential energy of the photoelectron due to the Auger electron emission, and where T is made large before taking the square of the amplitude. In the model of Russek and Mehlhorn,[8] the energy gain is given by

$$\mathcal{A}_{\rm RM}(t)=\int_0^t\rho^{-1}(t_A)dt_A\ , \tag{29}$$

where $\rho=\rho(t_A)$ is determined by Eqs. (19) and (20).

In order to compare with the Coulomb and Russek-Mehlhorn line shapes in detail, we consider the potential spherically averaged over the angle between $\mathbf{v}_S$ and $\mathbf{v}_A$. Instead of Eq. (28), we thus substitute

$$\langle\Delta V(t,t_A)\rangle=\begin{cases}\dfrac{1}{v_A t}-\dfrac{1}{v_S(t+t_A)}, & v_S<v_A\\ 0, & v_S\geq v_A\end{cases} \tag{30}$$

in Eq. (27) and square the amplitude (22) with this energy gain. The result is

$$\bar{P}_Q(\varepsilon)=\frac{\Gamma_i/2\pi}{(\varepsilon_A-\varepsilon)^2+\Gamma_i^2/4}\kappa(\varepsilon)\ , \tag{31}$$

where

$$\kappa(\varepsilon)=\frac{\pi\xi}{\sinh(\pi\xi)}\exp\left[2\xi\arctan\frac{2(\varepsilon_A-\varepsilon)}{\Gamma_i}\right]\ . \tag{32}$$

In the parameter $\xi=-Q_d\kappa_S^{-1}$, the quantity Q_d is the dynamic charge, given by Eq. (18). The result (31) agrees with the general line-shape formula of Kuchiev and Sheinerman.[15] The Auger electron line shape (31) can also be obtained from the Coulomb line-shape formula (4) by assuming that Q/κ is small, and replacing ε by $E'-\varepsilon=E_{\rm exc}+\varepsilon_A-\varepsilon$.

IV. RESULTS OF THE MODIFIED COULOMB LINE-SHAPE FORMULA

In this section we compare our results based on the Coulomb line-shape formula (4) including the dynamic charge [Eq. (18)] with predictions from the semiclassical models of Russek and Mehlhorn[8] and Kuchiev and Sheinerman,[15] and with measured PCI shifts.

First, we tested the formula (18) against the semiclassical equation (25), which gives the effective screening charge as a function of the "passing" radius $\rho=\rho(t_A)$, where t_A is the time of emission of the Auger electron.

Both r_S and ρ in Eq. (25) can be calculated using $t_A = 2/\Gamma_i$ and self-consistent-field values of R_S and R_A. As in the derivation of Eq. (26), we have chosen the average time of Auger electron emission here. No notable differences were found in the range $0.01 < E_{\rm exc}/\varepsilon_A < 1$ for the Ar K-L_2L_3 (^1D) and the Xe L_3-M_4M_5 (^1G), L_2-L_3N_4 ($J=3$), and N_5-$O_{2,3}O_{2,3}$ (^1S) transitions. This result was not affected by changing $t_A = 2/\Gamma_i$ to $t_A = 1/\Gamma_i$, suggesting that it is an excellent approximation in the semiclassical approach to use $r_S = Q\rho$, where Q is time independent and equal to the dynamic charge Q_d.

The second test consisted in constructing a charge $Q_{\rm fit}$ such that our Coulomb line-shape formula produces the same PCI shift as the Russek-Mehlhorn formula for the four transitions indicated above. The result indicates that for $\bar{E} = E_{\rm exc}/\varepsilon_A \gtrsim 0.5$ there is no difference between $Q_{\rm fit}$ and Q_d. Below this limit, there is some spread among the individual $Q_{\rm fit}$ curves, indicating that $Q_{\rm fit}$ is about 15% lower than Q_d for $\bar{E} \cong 0.1$ when $\varepsilon_A/\Gamma \lesssim 10^2$. For $\varepsilon_A/\Gamma \gtrsim 5\times 10^2$, agreement between $Q_{\rm fit}$ and Q_d remains excellent down to $\bar{E} \cong 0.05$. It should be noted that the ratio ε_A/Γ varies between 4×10^3 and 75 for the four transitions considered. The highest value corresponds to the Ar K-L_2L_3 (^1D) Auger transition, and the lowest to the Xe L_2-L_3N_4 ($J=3$) Coster-Kronig transition.

These two tests indicate that, at least asymptotically, the dynamic charge correctly describes the PCI distortion of the Auger line shape—both in the semiclassical and in the Coulomb approximations. In practice, the "asymptotic" condition prevails for $E_{\rm exc}/\sqrt{\Gamma\varepsilon_A} \gtrsim 1$, according to our analysis.

Figure 1 contains a plot of PCI shifts which universally displays the no-passing effect. As a function of $\bar{E}$, we plot the semiclassical PCI shifts Δ_0 and Δ, scaled in units of $\Gamma_i' = \Gamma_i(\varepsilon_A)^{-1/2}$. This scaling removes any dependence on particular Auger or Coster-Kronig transitions. According to Eq. (26), Δ_0 does not account for the no-passing effect, whereas Δ does. It should be noted that the difference between the scaled Δ values does not depend on $\bar{E}$ and is equal to $1/\sqrt{8}$, in accordance with Eq. (26). The circles in Fig. 1 correspond to the maxima of the Coulomb line-shape formula (4). The points lying on the Δ_0 curve were calculated from Eq. (4) with $Q=1$, for two sets of ε_A and Γ_i values. The points on the lower curve were calculated similarly, except that $Q = Q_d$ was used. The differences between the calculated Coulomb values and the semiclassical curves are negligible, even though the Coulomb results correspond to entirely different $E_{\rm exc}/\Gamma_i$ values, as shown in Fig. 1. The results displayed in Fig. 1 emphasize the universal character of post-collision interaction, even when the no-passing effect is taken into account. The PCI phenomenon does not depend on the atomic structure but only on the asymptotic properties of the continuum wave functions outside the ionic core.

In Fig. 2 we compare Coulomb line shapes calculated from Eq. (4) including the dynamic Q_d with line shapes derived from the semiclassical model of Ref. 8, for the

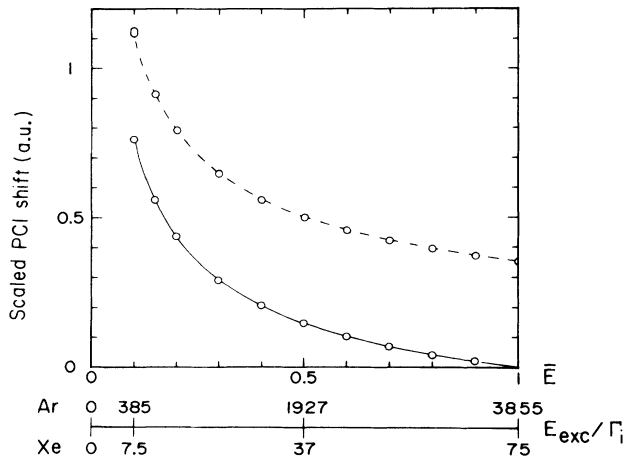

FIG. 1. Comparison between PCI shifts predicted by the Coulomb line-shape formula [Eq. (4)] and by the semiclassical theory of Ref. 8. The PCI shifts, scaled by a factor of $\varepsilon_A^{1/2}\Gamma_i^{-1}$, are plotted as a function of the reduced energy $\bar{E} = E_{\rm exc}/\varepsilon_A$. The dashed curve corresponds to Δ_0, and the solid curve to Δ, both as given in Eq. (26). The circles on the dashed curve were calculated with $Q=1$ in Eq. (4), and the circles on the solid curve with $Q = Q_d$ in the same formula. For each circle shown, two sets of ε_A and Γ_i values were used, corresponding to the Ar K-L_2L_3 (^1D) and the Xe L_2-L_3N_4 ($J=3$) transitions. With the scaling used here, the correspondence between the quantum-mechanical and the semiclassical shifts is applicable to any Auger or Coster-Kronig transition.

Ar K-L_2L_3 and Xe L_2-L_3N_4 transitions discussed above. The smaller $\bar{E}$ values correspond, in each case, to $E_{\rm exc}/\sqrt{\Gamma\varepsilon_A} \cong 1$; at these energies some deviations occur between $Q_{\rm fit}$ and Q_d. It can be seen that asymptotically there is no difference between the modified Coulomb and

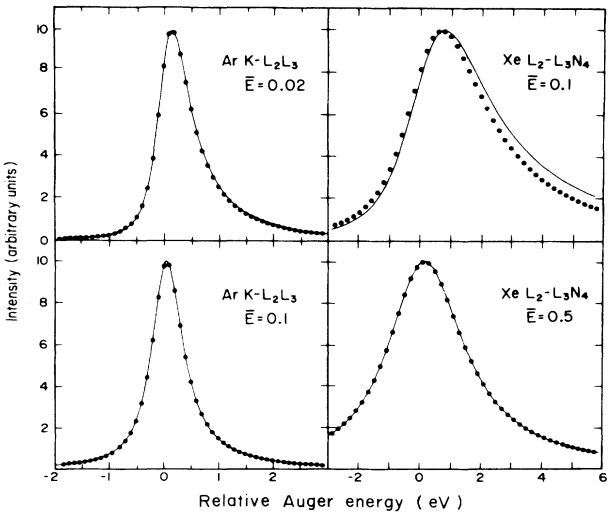

FIG. 2. Comparison between Coulomb line shapes [Eq. (4)] with $Q = Q_d$ (solid curves) and semiclassical line shapes according to Russek and Mehlhorn (Ref. 8) (dots). In both cases, the lesser value of the reduced energy $\bar{E}$ corresponds to $E_{\rm exc}/(\Gamma_i\varepsilon_A)^{1/2} \cong 1$.

the semiclassical line shapes, as anticipated by the theoretical considerations in Secs. and II and III. It can consequently be inferred that the modified Coulomb line-shape formula will also correctly describe the measurements of Xe N_5-$O_{2,3}O_{2,3}$ (^1S) Auger line shapes reported by Borst and Schmidt.[11] In Fig. 3 a similar comparison is carried out between Coulomb line shapes and line shapes derived from Eq. (32). The results show that the spherically averaged Kuchiev-Sheinerman[15] formula is an excellent approximation to the quantum-mechanical result.

In Figs. 4 and 5 we compare PCI shifts predicted by the Coulomb line-shape formula (4) incorporating the dynamic Q_d with experimental results. Two corrections are required before a comparison is possible.[1] First, the calculated line shape must be convoluted with the final-state density function

$$\mathcal{L}_{ff'}(\varepsilon_1,\varepsilon_2)=(\Gamma_{ff'}/2\pi)[(E'-\varepsilon_1-\varepsilon_2)^2+\Gamma_{ff'}^2/4]^{-1}\ , \tag{33}$$

where $\Gamma_{ff'}^{-1}$ is the lifetime of the final double-hole state. For the Xe N_5-$O_{2,3}O_{2,3}$ (^1S) transitions, we have $\Gamma_{ff'}=0$, but for the Xe L_2-L_3N_4 ($J=3$) transitions, $\Gamma_{ff'}=2.82$ eV is comparable to the initial-state width $\Gamma_i=3.05$ eV. Second, the resulting calculated line shape must be convoluted with the spectrometer window function, which is different in the two experiments.[11,16,19]

In Fig. 4, we further compare the experimental PCI shifts with lowest-order Dirac-Fock calculations, carried out by the numerical procedure described in I. The Dirac-Fock predictions do not agree with the experimental results, unlike the predictions from the modified line-shape formula (4) including Q_d. On the other hand, as Fig. 4 shows, the Dirac-Fock predictions coincide with those of the unmodified Coulomb line-shape formula (4) with $Q=1$. This is also true for the line shapes.[1]

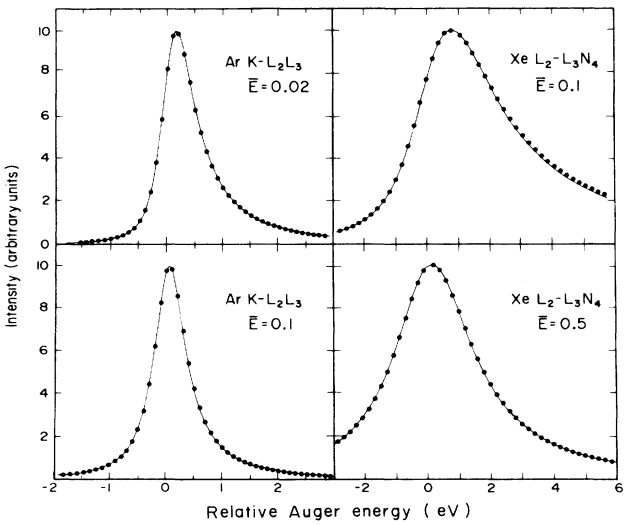

FIG. 3. Comparison between Coulomb line shapes [Eq. (4)] with $Q=Q_d$ (solid curves) and semiclassical line shapes according to Kuchiev and Sheinerman (Ref. 15) (dots).

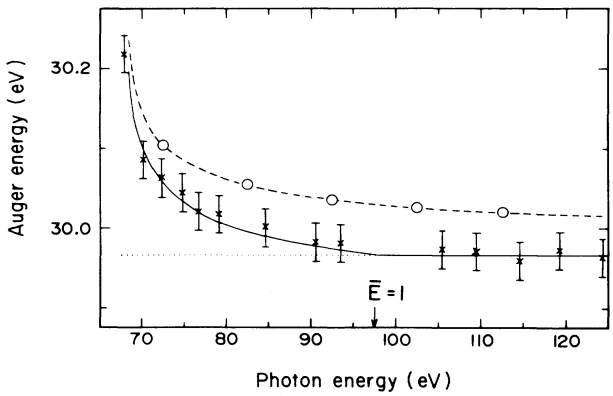

FIG. 4. Measured energies of the Xe N_5-$O_{2,3}O_{2,3}$ (^1S) Auger electron line, from Ref. 19, as a function of incident-photon energy (crosses). The solid curve was calculated by convoluting the modified Coulomb line shape [Eq. (4) with $Q=Q_d$] with the instrumental window function (Ref. 19) and adding the resulting PCI shift to $\varepsilon_A=29.97$ eV, which is the measured asymptotic Auger electron energy (Ref. 11). The dots indicate the results of lowest-order Dirac-Fock calculations of the PCI shift (Ref. 1); the dashed curve represents shifts predicted from the unmodified Coulomb line-shape formula [Eq. (4) with $Q=1$].

Measured[16] and calculated Xe L_2-L_3N_4 Coster-Kronig energies are plotted in Fig. 5. The L_2 hole-state width is much larger than the N_5 width, whence the PCI shifts shown in Fig. 5 are much larger than in the N-OO case of Fig. 4. It was not possible to determine the absolute Coster-Kronig energy scale in these measurements.[16] Consequently, ε_A was used as a fitting parameter in the comparison between theory and experiment. The measured maxima ε_{max} were given in the form

$$\varepsilon_{max}=\Delta+\varepsilon_A\ , \tag{34}$$

where Δ is the PCI shift calculated from Eq. (4) using Q_d with $\varepsilon_A=228$ eV, convoluted with Eq. (33) and the window function. As shown in Fig. 5, it was possible to obtain a very good fit of the experimental data using the least-squares value of ε_A. Replacing Δ with shifts calculated from Eq. (4) with $Q=1$ leads to systematic deviations between theory and experiment. The measured results of Ref. 16 thus confirm the findings of Borst and Schmidt[11] regarding the no-passing effect.

V. CONCLUSIONS

We have demonstrated that introduction of a "dynamical" charge Q_d [Eq. (18)] in the analytical Coulomb line-shape formula [Eq. (4)] takes adequate account of the no-passing effect[8,11] in post-collision interaction during Auger transitions following near-threshold photoionization. The present analysis furthermore shows that the dynamical charge Q_d is associated with the final two-electron continuum state in a resonant scattering process in which a photoelectron and an Auger electron are emitted. It appears that Q_d accounts for the screening by the fast electron of the ionic charge "seen" by the slow

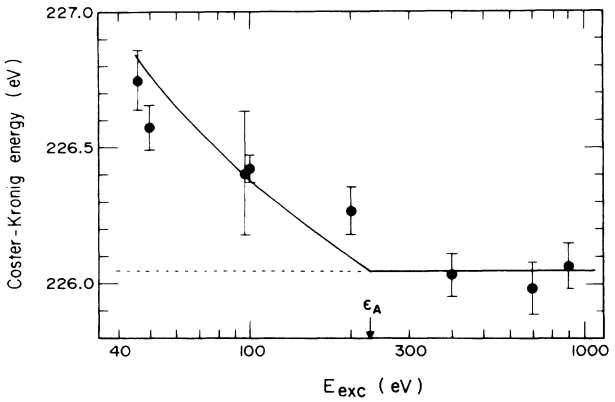

FIG. 5. Measured Xe L_2-L_3N_4 ($J=3$) Coster-Kronig electron energies (Ref. 16) (dots with error bars) as a function of photon excess energy. The solid curve was calculated by convoluting the modified Coulomb line shape [Eq. (4) with $Q=Q_d$] with the final-state density function and the instrumental window function. The energy ϵ_A was derived from the data by least-squares analysis.

electron, whenever two electrons are emitted into the continuum, either resonantly *or* nonresonantly. The influence of Q_d becomes significant at rather high velocities, hence this interaction mode is not directly related to the Wannier effect which prevails between two slow-moving electrons in a Coulomb field.[20,21] In fact, at high photon excess energies the major contribution to the nonresonant double photoionization cross section comes from a final-state phase-space part which corresponds to a *slow*- and a *fast*-moving electron. It is therefore only when the photoionization process becomes resonant that segments of the final phase space are probed in which the two electrons move with *high* and comparable velocities. It is for this reason that this delicate screening effect does not show up in nonresonant double photoionization nor in ordinary electron ionization cross sections.

The conclusions reached above should also follow from a more detailed quantum-mechanical treatment of the quadruply differential cross section of process (11), describing the ejection of the two electrons in specific directions and with given energies. Here we only make a few exploratory remarks regarding the angular and radial correlations of the emitted electrons and their relationship to the dynamic-charge concept.

According to Eq. (15), one may also introduce a dynamic charge

$$\hat{Q}_d = 1 - \kappa_S / |\kappa_S - \kappa_A| \tag{35}$$

which depends on the angle θ between the directions of the photoelectron and the Auger electron. However, $\hat{Q}_d$ cannot be used in association with the Coulomb line-shape formula (4) because it is based on the angle-integrated noncoincidence double photoionization cross section (1), nor can $\hat{Q}_d$ be incorporated in the semiclassical model of Russek and Mehlhorn.[8] In contrast, the approach of Kuchiev and Sheinerman[15] allows for an estimate of the dependence of the Auger line shape on θ. This follows from using Eq. (28) rather than its spherical average (30) in the evaluation of the line shape.[15] One finds that the parameter ξ in Eq. (32) is replaced by $\hat{\xi} = -\hat{Q}_d/\kappa_s$, which makes the Auger electron line shape angle dependent. According to Eq. (35), $\hat{Q}_d$ is singular for $\kappa_S = \kappa_A$ and $\theta = 0$. When $\bar{E} = E_{exc}/\epsilon_A \cong 1$ and θ is small, the line shapes obtained in coincidence measurements may thus be very different from those observed in noncoincidence experiments.[15] This trend has been confirmed by detailed calculations of the profile (31) as a function of $\bar{E}$ and θ for the Xe N_5-$O_{2,3}O_{2,3}$ (^1S) transition.[22] In this analysis the spherical average over angle-dependent profiles was also obtained and compared with the profile (31) in which the "spherically averaged" charge (18) was used. The two results are not identical except for very low and very high $\bar{E}$ values. This discrepancy may be due to the fact that in the cross section the θ-dependent profile is multiplied by a factor which in general depends on the angles between the incident photon beam and the emitted electrons. More work is clearly needed to clarify this point as well as the significance of the cusp in Eq. (35).

A fully consistent but very elaborate way to account quantum mechanically for the no-passing effect[8,11] in noncoincidence experiments is to evaluate the angle-integrated double photoionization cross section near the Auger electron resonance using a final-state wave function which is a superposition of antisymmetric products of two central-field wave functions, both describing a continuum electron in the field of the ion with the unscreened charge $Z+1$. This procedure in which the Hamiltonian matrix is diagonalized with respect to the unscreened basis requires a generalization of the K-matrix theory of single-electron photoionization.[12] In this theory, the Hamiltonian matrix is diagonalized with respect to a basis which consists of linear combinations of Slater determinants that describe one excited continuum electron coupled to the electrons of the excited core. The new feature that arises when there are two continuum electrons is the electron-electron interaction between doubly ionized states of the same symmetry and parity. This interaction involves matrix elements of the type $\langle \epsilon_1\epsilon_2 | r_{12}^{-1} | \epsilon_3\epsilon_4 \rangle$ with four continuum spin orbitals, labeled ϵ_n ($n=1-4$) which may be evaluated using a recently developed computer program.[23] For example, the treatment of the no-passing effect for the Xe N_5-$O_{2,3}O_{2,3}$ (^1S) transitions would involve the calculation of these electron-electron interaction matrix elements between continuum orbitals of ($5p^{-2}$) (^1S) $\epsilon_1 l_1 \epsilon_2 l_2$ (^1P) states, constructed from bound-state Dirac-Fock wave functions and from the two continuum four-spinors that correspond to $Q_f = +2$, i.e., $Z = +1$ in Eq. (11). It remains also to be seen whether the dynamic charge (17) can be related to the phases of the generalized two-electron K-matrix eigenfunctions in the asymptotic region.

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APPENDIX: DERIVATION OF THE COULOMB LINE-SHAPE FORMULA

In I we considered the process

$$\omega + X^- \rightarrow X^+ + e^- + e^- \tag{A1}$$

and evaluated the cross section with the use of asymptotic wave functions for the continuum states. The cross section was calculated in the shake-down limit by taking into account only the overlap element (5), where the reduced dipole matrix (3) was taken to be constant. The final-state wave function (6) was assumed to be an s wave in an *arbitrary* Coulomb field corresponding to an effective charge Q. The intermediate-state wave function (7) was taken to be a free spherical s wave. Any short-range phase shifts were thus neglected.

The resultant amplitude is of the form

$$\langle \varepsilon \mid \tau' \rangle = -[A_0(\kappa) + A_L(\kappa)] , \tag{A2}$$

where $\kappa = \sqrt{2\varepsilon}$,

$$A_0(\kappa) = \frac{1+i}{2} e^{-\pi Q/2\kappa} (\beta\kappa)^{-1/2} \times \{ c_+ [(\kappa+\beta)^{-\alpha_+} - (\kappa-\beta)^{-\alpha_+}] - c_- [(\kappa+\beta)^{-\alpha_-} - (\kappa-\beta)^{-\alpha_-}] \} , \tag{A3}$$

and

$$A_L(\kappa) = (\sqrt{2}/2\beta) e^{-\pi Q/2\kappa} [c_+ (J_1 - J_2) + c_- (J_3 - J_4)] . \tag{A4}$$

The quantities appearing in Eqs. (A3) and (A4) are defined as follows:

$$c_\pm = \Gamma(\pm iQ/\kappa)(2\kappa)^{\pm iQ/\kappa} \exp[\pm i \arg\Gamma(1 - iQ/\kappa)] , \tag{A5}$$

$$\alpha_\pm = 1 \pm iQ/\kappa , \tag{A6}$$

$$\beta^2 = 2E_{\rm exc} + i\Gamma_i ,$$

$$J_{1,2} = e^{i\pi/4} \frac{\Gamma(\frac{1}{2} + iQ/\kappa)}{\Gamma(\frac{1}{2})\Gamma(1 + iQ/\kappa)} \frac{F(-\frac{1}{2}, -iQ/\kappa; \frac{1}{2}; \pm\beta/\kappa)}{(\kappa \mp \beta)^{\alpha_+}} , \tag{A7}$$

$$J_{3,4} = e^{-i\pi/4} \frac{\Gamma(\frac{1}{2} - iQ/\kappa)}{\Gamma(\frac{1}{2})\Gamma(1 - iQ/\kappa)} \times \frac{F(-\frac{1}{2}, +iQ/\kappa; \frac{1}{2}; \pm\beta/\kappa)}{(\kappa \mp \beta)^{\alpha_-}} . \tag{A8}$$

In Eqs. (A7) and (A8), the upper signs refer to J_1 and J_3, and the lower signs to J_2 and J_4; F is the hypergeometric function.

The Coulomb line shape is given by Eq. (4) for the photoelectron line. In order to obtain the Auger electron line shape, ε in Eq. (4) must be replaced by $E' - \varepsilon = E_{\rm exc} + \varepsilon_A - \varepsilon$. This expression is normalized so that it becomes a normalized Lorentzian profile in the limit $Q \rightarrow 0$. Depending on Q, various line shapes are obtained. The two line shapes discussed in the text correspond to $Q = 1$ and $Q = Q_d$, with the dynamic charge Q_d defined by Eq. (18).

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