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QUANTUM THEORY OF POST COLLISION INTERACTION IN INNER-SHELL PHOTOIONIZATION

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**Abstract** The angle-averaged PCI effect is interpreted in terms of a line shape formula which is based on asymptotic Coulomb wave functions and which accounts for the mutual screening of the Auger electron and photoelectron in the final state. The angle-dependent PCI line shape is analyzed using the related semiclassical approach by Kuchiev and Sheinerman.

Inner-shell photoionization followed by Auger decay is an example of a resonant rearrangement collision in which three charged particles, an ion and two electrons, are formed. Their mutual Coulomb interaction affects the cross section which results in deviations from predictions of the usual two step model in which ionization and decay are treated as distinct process. The semiclassical approach introduced by Niehaus,<sup>1</sup> has been very powerful for the description of this post-collision interaction (PCI) phenomenon.<sup>2-4</sup> However, a consistent treatment of threshold phenomena in inner-shell ionization, including both discrete excitations and PCI requires use of scattering theory in its quantal form.<sup>5,6</sup>

In this note we shall review some aspects of our work on PCI.<sup>5-9</sup> It is shown that time-independent quantum mechanical considerations based on asymptotic Coulomb wave functions<sup>7</sup> in association with an effective charge concept<sup>8</sup> account for the most salient features of the PCI effect in non-coincidence experiments. Our approach<sup>7,8</sup> is related to the semiclassical model of Kuchiev and Sheinerman.<sup>3</sup> Their angle dependent PCI line shape formula is used for qualitative predictions of the Auger electron line shape in the case where the Auger electron and photoelectron are observed in coincidence.<sup>8,9</sup>

The Auger process is treated as a resonance in double photoionization. Our starting point is thus a generalization of the conventional resonant multichannel scattering theory to allow for two electrons, the photoelectron and the Auger electron, in the outgoing channel.<sup>5</sup> As a consequence the influence of the lifetime of the initial inner-shell hole state on the PCI effect is correctly taken into account. If we exclude all irrelevant factors and limit ourselves to a description of the angle-averaged Auger electron line shape  $P_Q(\epsilon)$  we have

$$P_Q(\epsilon) = (\Gamma_i/2\pi)|\langle E - \epsilon | \tau' \rangle|^2 \quad (1)$$

where

$$|\tau'\rangle = \int_0^\infty |\tau\rangle (E_{exc} - \tau + i\Gamma_i/2)^{-1} d\tau \quad (2)$$

In Eqs. (1) and (2)

$$|E - \epsilon\rangle = (2/\pi\kappa)^{1/2} \sin[\kappa r + \frac{Q}{\kappa} \log 2\kappa r + \arg \Gamma(1 - iQ/\kappa)] \tag{3}$$

and

$$|\tau\rangle = (2/\pi\kappa')^{1/2} \sin \kappa' r \tag{4}$$

are asymptotic s-waves, without a short range phaseshift.<sup>7,8</sup> In the non-Lorentzian Coulomb line shape  $P_Q(\epsilon)$  which can be expressed in closed form<sup>7</sup>  $E = E_{exc} + \epsilon_A$ , where  $E_{exc} = \omega - I_i$  and  $\epsilon_A = I_i - I_{ff'}$ . Here  $\omega$  is the incident photon energy and  $\epsilon_A$  the Auger electron energy for the transition from an initial one-hole state  $|i\rangle$  with the lifetime  $T_i = \Gamma_i^{-1}$  to a final double-hole state  $|ff'\rangle$ . In Eq.(3)  $E - \epsilon = \frac{1}{2}\kappa^2$ , and in Eq.(4)  $\tau = \frac{1}{2}\kappa'^2$ . Besides the excess energy  $E_{exc}$  and the width  $\Gamma_i$ ,  $P_Q(\epsilon)$  depends according to Eq.(3) only on one additional parameter, namely, the effective charge  $Q$ , which may depend on  $\kappa$ . If  $P_Q(\epsilon)$  is expressed as a function of  $\epsilon_p = E - \epsilon$  rather than  $\epsilon$  it describes the shape of the corresponding photoelectron line. Since  $Q$  only appears in the final-state wave function (3) it implicitly implies that the photoelectron sees the charge  $Q_i = 0$  rather than  $Q_i = 1$  prior to the Auger decay. As shown below this assumption is justified by a proper choice of  $Q$ .

The overlap amplitude  $\langle \epsilon_p | r' \rangle$  may be expressed as a superposition of Lorentz amplitudes, weighted by the coefficients  $A(\kappa, \kappa')$  of the free spherical waves (4) in the expansion of the final-state Coulomb wave function (3).<sup>8</sup> The result

$$\langle \epsilon_p | r' \rangle = (\Gamma_i/2\pi)^{1/2} \int_0^\infty A(\kappa, \kappa') \frac{2}{\kappa'^2 - \beta^2} d\kappa' \tag{5}$$

where  $\beta^2 = 2E_{exc} + i\Gamma_i$ , shows that independently of the magnitude of the lifetime  $T_i$  the photoelectron "shakes down" during the Auger decay into various final states corresponding to a given  $Q$ . As Fig.1 shows for the xenon  $N_5 - O_{2,3}O_{2,3}^1S$  transition the influence of  $T_i$  is embedded in

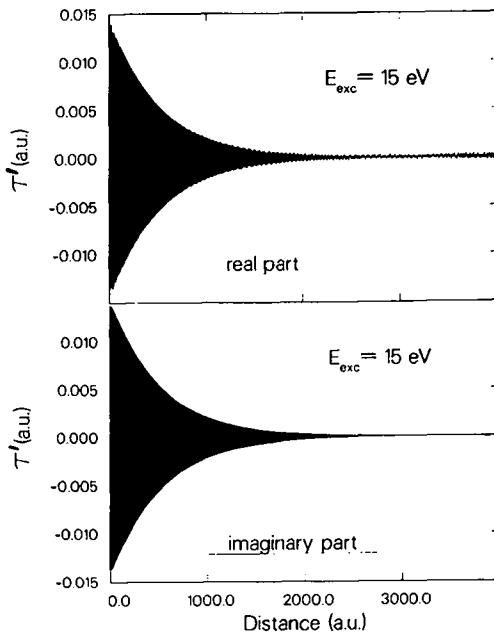


Fig1. Real and imaginary parts of the PCI function  $|r'\rangle$  as a function of radial distance, for the Xe  $N_5 - O_{2,3}O_{2,3}^1S$  transition. It is constructed using the Dirac-Fock method involving a superposition of 3000 central-field continuum wave functions  $|\tau\rangle$  and by taking the dipole interaction between the ground state and the 4d hole states into account.

$|\tau'|$  which describes how far the photoelectron escapes from the atom before it experiences the change in the potential due to the Auger decay. In this particular case ( $E_{exc} = 15eV, \Gamma_i = 0.11eV$ ) the average distance is about  $10^3$  a.u.

If  $Q = 0$  in Eq.(3)  $A(\kappa, \kappa') = \delta(\kappa - \kappa')$  in Eq. (5) and  $P_Q(\epsilon)$  reduces to the normalized Lorentzian profile. If  $Q = 1$  the Auger electron and photoelectron line shapes become distorted such that  $P_Q(\epsilon)$  peaks at  $\epsilon = \epsilon_A + \Delta$ , where  $\Delta$  is a positive PCI shift. The photoelectron line shape which is the mirror image of  $P_Q(\epsilon)$  peaks at  $\epsilon_p = E_{exc} - \Delta$ . The choice  $Q = 1$  accounts for the response of the photoelectron to the change of the ionic core potential produced by the Auger decay but neglects the screening of the ionic charge by the Auger electron. In this approximation, the Auger line shape has also been evaluated using Dirac-Fock central-field continuum and bound state wave functions and by incorporating the dipole interaction between the ground state and the final state.<sup>7</sup> Our rigorous quantum-mechanical as well as semiclassical calculations agree with results, based on Eq.(1) unless  $E_{exc}$  is very small.<sup>7</sup> In spite of this internal consistency the agreement with recent experiments<sup>10,11</sup> is poor at high excess energies.

In the time-dependent semiclassical approach the choice  $Q = 1$  in Eq.(3) corresponds to the assumption that the photoelectron is exposed instantaneously to a change of ionic core potential by one unit during the Auger decay. However, as realized by Ogurtsov<sup>12</sup>, it takes some time for the Auger electron to pass the previously emitted photoelectron. If  $E_{exc} \geq \epsilon_A$  it does not pass at all with the consequence that there should practically be no PCI distortion at these excess energies.<sup>2,10</sup> The semiclassical theory of this "no-passing" effect is in excellent agreement with recent experiments both regard to the shape<sup>2,10</sup> and shifts.<sup>2,10,11</sup>

In the time-independent picture the gradual time-dependent change of the screening of the core corresponds to an energy-dependent screening, i.e.  $Q = Q(\kappa)$ . It is a final-state effect due to the interaction of the two escaping electrons. Since the atomic structure of the core does not matter the functional dependence  $Q = Q(\kappa)$  may be determined by requiring that the product of two Coulomb wave functions corresponding to two undetermined effective charges has the same asymptotic phase as the exact angle-dependent solution for two continuum electrons in a Coulomb field.<sup>8</sup> Suppose that the charge of the core is  $Z + 1$ . Then it follows from taking the spherical average over the necessary condition for correctly describing the two continuum electrons in terms of the Coulomb wave functions that the fast electron sees the charge  $Z$  if the slow one is unscreened. On the other hand if the fast electron is assumed to be unscreened the slow one sees the charge  $Z + 1 - (\kappa_s/\kappa_f)$ , where  $\kappa_s$  and  $\kappa_f$  are the wave numbers of the slow and fast electron respectively. This result implies that the photoelectron is exposed to a change of the ionic charge during the Auger decay which is equal to

$$Q_d = 1 - \sqrt{E_{exc}/\epsilon_A} \quad (6)$$

if  $E_{exc} \leq \epsilon_A$  and is zero if  $E_{exc} > \epsilon_A$ .<sup>8</sup> Since Eq. (6) is independent of  $Q_i = Z$  one may put  $Q_i = 0$  as was done in Eq. (6). The identification of  $Q$  in Eq. (4) as the "dynamic" charge  $Q_d$  predicts in accordance with semiclassical models<sup>2,3</sup> and the experiments<sup>10,11</sup> that the PCI effect vanishes at  $E_{exc} \geq \epsilon_A$ . Detailed calculations show that the semiclassical line shapes<sup>2,3</sup> and hence also the measured ones<sup>11</sup> in the Xe  $N_5 - O_{2,3}O_{2,3}^1S$  case are represented very accurately by  $P_{Q_d}(\epsilon)$  provided  $E_{exc} \geq (\Gamma_i \epsilon_A)^{1/2}$ .<sup>8</sup> In fact our result is almost identical with a semiclassical model which assumes rectilinear trajectories<sup>3</sup> for the Auger electron and the photoelectron and which takes into account the energy gain of the Auger electron in a spherically average fashion.

If the averaging is not carried out the semiclassical line shape depends on the angle  $\Theta$  between the directions of the emission of the Auger electron and the photoelectron and is a special case of the Kuchiev-Sheinerman formula.<sup>3</sup> It is given by

$$P_{\Theta}(\epsilon) = (\Gamma_i/2\pi)[(\epsilon_A - \epsilon)^2 + \Gamma_i^2/4]^{-1} K(\epsilon) \quad (7)$$

where

$$K(\epsilon) = (\pi\xi/\sinh(\pi\xi)) \exp[2\xi \arctan 2(\epsilon_A - \epsilon)/\Gamma_i] \quad (8)$$

with  $\xi = \xi(\Theta) = -\kappa_p^{-1} + |\vec{\kappa}_p - \vec{\kappa}_A|^{-1}$ . Here  $\vec{\kappa}_p$  is the wave vector of the photoelectron and  $\vec{\kappa}_A$  that of the Auger electron. In the spherical averaged model  $\xi$  is replaced by  $\langle \xi \rangle = Q_d \kappa_p^{-1}$ , where  $Q_d$  is given by Eq. (6).

Figure 2 shows for the Xe  $N_5 - O_{2,3}O_{2,3}^1S$  case the dependence of the Auger electron line shape on  $\Theta$ .<sup>9</sup> The excess energy  $E_{exc}$  ranges from values below  $\epsilon_A = 30\text{eV}$  to values above it. In contrast to the profile measured in a non-coincidence experiment the distortion does not vanish at  $E_{exc} = \epsilon_A$  although it slowly disappears as  $E_{exc}$  becomes large. For low  $E_{exc}$   $\xi \simeq \langle \xi \rangle \simeq -\kappa_p^{-1}$ . Consequently  $P_\Theta(\epsilon)$  is nearly independent of  $\Theta$  and resembles  $P_Q(\epsilon)$ . For  $\Theta \geq 90^\circ$   $\Delta$  is always positive and  $P_\Theta(\epsilon)$  exhibits the same type of asymmetry as  $P_Q(\epsilon)$ . For  $\Theta < 90^\circ$  the shift and distortion can reverse themselves as shown in Fig. 2. When  $E_{exc} \simeq \epsilon_A$  and  $\Theta$  is small  $P_\Theta(\epsilon)$  depends strongly on  $\Theta$  and is very different from  $P_Q(\epsilon)$ . In this region, where  $\xi$  is nearly singular, final-state correlation effects may also become significant. Coincidence experiments would thus be of great interest.

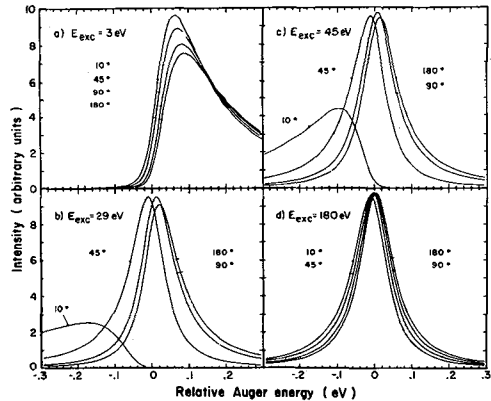


Fig.2. The line shape  $P_\Theta(\epsilon)$ , as a function of excess energy  $E_{exc}$  and angle  $\Theta$  between the wave vectors  $\vec{\kappa}_p$  and  $\vec{\kappa}_A$ , for the Xe  $N_5 - O_{2,3}O_{2,3}^1S$  transition.<sup>9</sup>

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