Angular Distribution of Auger Electrons and Photons in Resonant Transfer and Excitation in Collisions of Ions with Light Targets

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It is shown that angular distributions of Auger electrons and x rays from deexcitation of doubly excited states produced in the resonant transfer and excitation of projectiles in collisions with light targets are, in general, not isotropic. The detailed theoretical results for the $2p^2\,{}^1D$ resonance in $F^{8+}+H_2$ are presented at a projectile energy of 20 MeV.

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Several experimental investigations of resonance transfer and excitation (RTE) in ion-atom collisions[1-13] have been reported. The doubly excited states produced in these collisions have been investigated by observations of x rays[1-5] (RTEX), of Auger electrons[6-11] (RTEA), and by coincidence measurements[12,13] of one x ray followed by a second x ray. All RTEX measurements, in which x rays are measured in coincidence with the charge state of the projectile, have been made at 90° with respect to the beam direction. The resolution in these experiments is not sufficient to distinguish the individual x-ray lines. This is in contrast to high-resolution RTEA experiments[6-10] where the Auger lines for a particular doubly excited state can be clearly identified. Some of these measurements are made in the beam direction,[6-9] 0° in the laboratory, and others[10,11] have been reported at 9.6° to 10.6° in the laboratory. The experiments, involving RTEX and RTEA, provide differential cross sections at a particular angle. Since no calculations of the expected angular distributions are available in the literature, the total experimental cross sections are typically deduced by taking the product 4π times the differential cross sections at one angle.

It is the purpose of this Letter to provide a theoretical framework which permits one to calculate the differential cross sections for a direct comparison with experiments. An example is given to elucidate these considerations on RTE in $F^{8+}+H_2$ collisions for the dominant $2p^2\,{}^1D$ state.

Consider an electron of energy ϵ and wave vector $\mathbf{k}_0$ incident on an ion of charge state q in the ground state $|\alpha_g\rangle$,

$$e^- + P^q(\alpha_g) \to P^q(\alpha_g) + e^- \times \text{elastic scattering} \quad (1)$$

$$\to P^{q-1*}(\alpha_d)$$

$$\to P^q(\alpha_j) + e^- \quad (2)$$

$$\to P^{q-1}(\alpha_f) + h\nu\,. \quad (3)$$

The processes (2) and (3) represent the formation of the doubly excited autoionizing state $|\alpha_d\rangle$ followed by the emission of an Auger electron leading to either the ground state ($j=g$) or other allowed final states $|\alpha_j\rangle$, or by the emission of a photon. Whenever the final state after x-ray emission $|\alpha_f\rangle$ is stable against autoionization, the process (3) is called the dielectronic recombination.[14] The electron differential cross section[15] for processes (1) and (2) for unpolarized electrons can be written as follows:

$$\frac{d\sigma}{d\Omega}(\alpha_g\epsilon\hat{\mathbf{k}}_0 \to \alpha_j\epsilon_j\hat{\mathbf{k}}_j) = \frac{1}{2\omega_g}\sum\left| f_{\rm el}(\epsilon,\theta)\delta_{\alpha g,\alpha j}\delta_{m_s,m_s'} + \sum_d \left(\frac{4\pi^3}{k^2}\right)^{1/2} \frac{\langle\alpha_j\epsilon_j\hat{\mathbf{k}}_j|V|\alpha_d\rangle\langle\alpha_d|V|\alpha_g\epsilon\hat{\mathbf{k}}_0\rangle}{\epsilon-(E_d-E_g)+i\Gamma(d)/2}\right|^2, \quad (4)$$

where the elastic-scattering amplitude[16] is designated by $f_{\rm el}(\epsilon,\theta)$. The summation (denoted by $\sum$) is over the magnetic quantum numbers of $|\alpha_g\rangle$, $|\alpha_j\rangle$, and the initial and final projection of electron spin m_s and m_s', respectively.

The incident-electron-beam direction, $\hat{\mathbf{k}}_0$ and $\hat{\mathbf{k}}_j$, represents the direction of the scattered electron. The statistical weight and the total energy of the ground state are denoted by ω_g and E_g, respectively. E_d and $\Gamma(d)$ are the energy and the total width of the doubly excited state $|\alpha_d\rangle$. The differential cross section for the emission of a photon in a particular direction with respect to the incident-beam direction is obtained by setting the elastic-scattering amplitude to zero and replacing the amplitude of Auger deexcitation in Eq. (4) by the appropriate radiative amplitude.

We derived the expressions for the differential cross sections for the Auger electrons and the photons. The nonisotropic angular distribution in the rest frame of a doubly excited ion is a result of the fact that magnetic substates $|\alpha_d\rangle$ are, in general, not populated statistically. The formation of $|\alpha_d\rangle$ is a resonance process in which the incident electron is captured while exciting a bound electron. When the electron-beam direction ($\mathbf{k}_0$) is fixed as an axis of quantization, the expansion of $|\epsilon\hat{\mathbf{k}}_0\rangle$ contains spherical harmonics only with $m_l=0$ in the angular momentum representation. We note that the amplitude of formation, $\langle \alpha_d | V | \alpha_g \epsilon \hat{\mathbf{k}}_0 \rangle$, is identically zero when the magnetic quantum numbers (M_L, M_S) of $|\alpha_d\rangle$ are *not* the same as those of the initial state, consisting of the ground state $|\alpha_g\rangle$ and the free electron. Therefore, in general, the population of magnetic substates of $|\alpha_d\rangle$ are restricted by this selection rule as well as by the axial symmetry which demands that this should be independent of the sign of magnetic quantum number of $|\alpha_d\rangle$. The nonstatistical population of magnetic substates (and therefore leading to a nonisotropic distribution of the decay products) have been reported for nonresonant processes[17] such as inner-shell ionization by electron and proton impact. Similarly, the effects of autoionization resonances on the electron asymmetry parameter and alignment in photoionization is of current interest.[18]

Now we consider a hydrogenic ion of projectile charge Z_p, mass M, and energy E_p in collisions with light targets where other nonresonant processes[19,20] are expected to be not significant. The major contribution to RTE for such a case is the $2p^2\,{}^1D$ resonance, which can deexcite to only the ground state $1s\,{}^2S$ by Auger-electron emission with a rate A_a and to $1s2p\,{}^1P$ by x-ray emission with a rate A_r. The total width is $\Gamma_d \equiv \hbar(A_a+A_r)$. Appropriate formulas were derived using Eq. (4). The elastic-scattering amplitude can be well approximated by using the Coulomb amplitude[16] with an effective $Z = Z_p - 1$. Brandt[19] has reported on the general formulation of calculations of projectile ion-atom cross sections from ion-electron cross sections using the impulse approximation. Briefly in this model, the bound electrons of the target atom are treated as "*quasi*"-free electrons with a characteristic momentum distribution, when the projectile ion velocity is much larger than the electron velocity. Thus in the projectile rest frame the target electron has a continuous distribution of energies. It is also assumed that in this fast collision the momentum wave function $\Psi(\mathbf{p})$ of the target electron is undisturbed. Using the impulse approximation, and the general formulation of Brandt,[21] we obtain the doubly differential cross sections as follows:

$$\frac{d^2\sigma}{d\Omega\, d\epsilon} = \frac{d^2\sigma_{\rm el}}{d\Omega\, d\epsilon} + \frac{[C_R(\epsilon,\theta)+C_I(\epsilon,\theta)](\Gamma/2\pi)+A(\epsilon,\theta)(\epsilon-E_R)}{(\epsilon-E_R)^2+(\Gamma_d/2)^2}. \tag{5}$$

The resonant energy, E_R, is equal to $E_d - E_g$, and θ is the scattering angle in the projectile rest frame;

$$C_R(\epsilon,\theta) \equiv (D/4\pi)[1+\tfrac{10}{7}P_2(\theta)+\tfrac{18}{7}P_4(\theta)],$$

$$C_I(\epsilon,\theta) \equiv -\frac{(D/4\pi)Z\sin\Delta[(A_a+A_r)/A_a][P_2(\theta)/\sin^2(\theta/2)]}{(2\epsilon/\epsilon_0)^{1/2}},$$

$$A(\epsilon,\theta) \equiv -\frac{(D/4\pi^2)Z\cos\Delta[(A_a+A_r)/A_a][P_2(\theta)/\sin^2(\theta/2)]}{(2\epsilon/\epsilon_0)^{1/2}},$$

$$D(\epsilon,E_p) = (\pi^2\hbar^3/2m\epsilon)(\omega_d/\omega_g)[A_a^2/(A_a+A_r)](M/2E_p)^{1/2}J(Q).$$

The Compton profile[22] of the target is $J(Q)$, where

$$Q \equiv (M/2E_p)^{1/2}(\epsilon - E_p m/M),$$

with ω_d the statistical weight for the $2p^2\,{}^1D$ state. $P_l(\theta)$ is Legendre polynomial of order l and ϵ_0 is 27.21 eV;

$$\frac{d^2\sigma_{\rm el}}{d\Omega\, d\epsilon} = \left[\frac{Ze^2}{4\epsilon\sin^2(\theta/2)}\right]^2 \left[\frac{M}{2E_p}\right]^{1/2} J(Q),$$

which represents the binary-encounter electron contribution;

$$\Delta = 2\eta_2 - 2(mZe^2/\hbar^2 k)\ln[\sin(\theta/2)] - 2\eta_0,$$

where η_2 and η_0 are the Coulomb phase shifts for $l=2$ and $l=0$, respectively.

The differential cross section is obtained by taking an average of the second term in Eq. (5) over an energy interval which is larger than Γ_d;

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_{\rm el}}{d\Omega} + C_R(\epsilon=E_R,\theta) + C_I(\epsilon=E_R,\theta).$$

The second and third terms represent the contributions to the differential cross section, respectively, from the doubly excited state $2p^2\,{}^1D$ and the interference between the elastic and resonance channels.

To elucidate these points, now we consider $E_p = 20$ MeV in F^{8+} $(1s\,{}^2S) + H_2$ collisions where the doubly excited state $2p^2\,{}^1D$ is formed in RTE. In order to provide realistic plots, a profile of width 1.5 eV is folded in the cross sections. Figure 1(a) contains the doubly differential cross section at several angles $\theta = 180°$, $160°$, $140°$, $35°$, and $25°$ in the projectile frame of reference. The contributions arising from the resonance is illustrated in Fig. 1(b) by plotting $d^2\sigma/d\Omega\, d\epsilon - d^2\sigma_{\rm el}/d\Omega\, d\epsilon$. Several features are noteworthy. The Auger line profile is no longer Lorentzian, and this feature is more dramatically illustrated at $\theta = 35°$ and $25°$ in Fig. 1(b). The corresponding plots at these angles in Fig. 1(a) show a *dip* (rather than a peak) in the doubly differential cross sections. At the projectile energy considered here the scattering angle[23] in the laboratory frame is $\approx \frac{1}{2}(\pi - \theta)$.

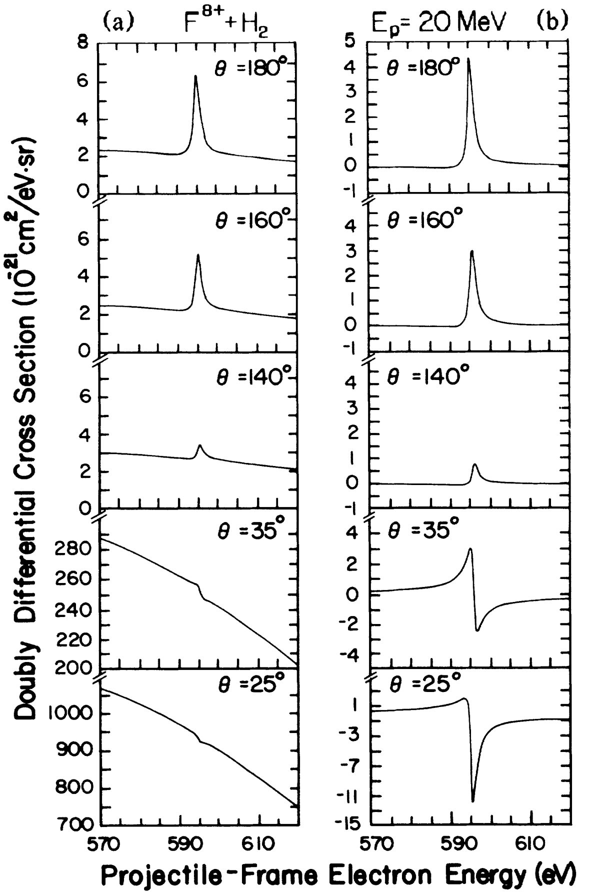

FIG. 1. (a) Doubly differential cross sections vs electron energy and different scattering angles θ_P in the projectile frame for $F^{8+}+H_2$ collisions at 20-MeV projectile energy. (b) The corresponding differences between the doubly differential cross sections and the contributions of the binary electrons $(d^2\sigma/d\Omega\, d\epsilon - d^2\sigma_{el}/d\Omega\, d\epsilon)$ are plotted vs electron energy and scattering angles in the projectile frame. The laboratory angles are given by $\approx (\pi-\theta)/2$ for this beam energy (Ref. 21). The strongest RTE state $2p^2\,{}^1D$ is only considered in this plot. Note that the contribution of this resonance appears as a dip (rather than a peak) and highly asymmetric profiles for $\theta \leq 35°$.

The solid line in Fig. 2 is a plot of the differential cross section minus the contribution of binary encounter electrons $(d\sigma/d\Omega - d\sigma_{el}/d\Omega)$ versus angle in the projectile frame. Strongly peaked angular distribution at large-θ values (small laboratory angles) is evident. Contributions of the resonance, $C_R(\epsilon = E_R, \theta)$, to the differential cross section is shown by the dashed line. Recently, Benhenni *et al.*[24] have reported their preliminary results on the angular distribution of the Auger transition $1s2s2p^2\,{}^3D \rightarrow 1s^2 2s\,{}^2S$ in $O^{5+}+He$ collisions at 13-MeV projectile energy. The general features of the experimental results[24] are similar to the angular distribution in Fig. 2, which is for $F^{8+}+H_2$ collisions. This similarity is due, in part, to the fact that the angular distributions of the two resonances $C_R(\epsilon = E_R, \theta)$ is identical.

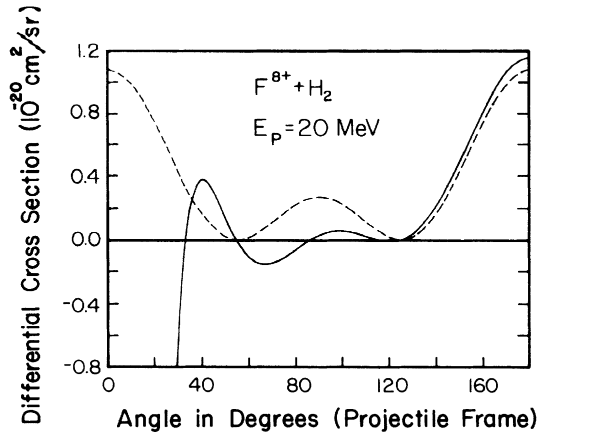

FIG. 2. Differential cross section vs angle in the projectile frame for $F^{8+}+H_2$ collisions at 20-MeV projectile energy. The solid line represents the differential cross section minus the contribution of binary encounter electrons (background $d\sigma/d\Omega - d\sigma_{el}/d\Omega$). For angles where the values are negative, there is a corresponding dip rather than peak in the doubly differential cross sections [Fig. 1(a)]. The dashed line represents only the contribution of the resonance, $C_R(\epsilon = E_R, \theta)$, as defined in the text.

Similarly for the $2p^2\,{}^1D\text{-}1s2p\,{}^1P$ x-ray transition,

$$\frac{d\sigma_x}{d\Omega} = \sigma_{\mathrm{RTEX}}(1s\,{}^2S \rightarrow 2p^2\,{}^1D\text{-}1s2p\,{}^1P)W_{d\text{-}f}(\theta),$$

where $W_{d\text{-}f}(\theta) = (1/4\pi)(1-\frac{1}{2}P_2)$ and σ_{RETX} is, in general, given by

$$\sigma_{\mathrm{RTEX}}(g \rightarrow d \rightarrow f) = (\pi^2\hbar^3/2mE_R)[(M/2E_p)^{1/2}J(Q)]F_2^*(d\text{-}f).$$

The satellite intensity factor is defined as follows:[25]

$$F_2^*(d\text{-}f) \equiv \frac{(\omega_d/\omega_g)A_a(d\text{-}g)A_r(d\text{-}f)}{\sum_a A_a + \sum_r A_r}.$$

Since for this case

$$(4\pi)(d\sigma/d\Omega)(\theta = 90°) = \tfrac{5}{4}\sigma_{\mathrm{RTEX}},$$

the assumption of isotropic angular distribution of x rays introduces an error of 25% in the deduced RTEX cross section from x-ray differential measurements at 90°. In general, the differential RTEX cross section, where many doubly excited states contribute but are not resolved in experiment, is given by

$$\frac{d\sigma_{(\mathrm{RTEX})}}{d\Omega} = \sum_{d,f}\sigma_{\mathrm{RTEX}}(g \rightarrow d \rightarrow f)W_{d\text{-}f}(\theta),$$

where $W_{d\text{-}f}(\theta)$ is characteristic x-ray angular distribution from the aligned doubly excited state $|\alpha_d\rangle$ to a final state $|\alpha_f\rangle$.

In conclusion, we have presented a theoretical framework which permits one to calculate the RTEA and

RTEX differential cross sections, and we have illustrated this procedure with a detailed example. We have shown that there is a significant anisotropy in the angular distributions of Auger electrons and x rays from collisionally aligned doubly excited states produced in resonant transfer and excitation of collisions of ions with light targets. These considerations suggest that the Auger electrons or x-ray differential cross-section measurement at a particular angle should be compared with the corresponding theoretical results in order to fully understand RTE in ion-atom collisions.

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$$\cos\theta_L = \frac{V_P + v_A\cos(\pi-\theta)}{[V_P^2+v_A^2+2V_P v_A\cos(\pi-\theta)]^{1/2}},$$

where V_P and v_A are the velocities of the projectile and the Auger electron, respectively.

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