Ionization in positron-atom collisions

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Depending on the distribution of energy between the scattered positron and the ejected electron in the final channel, two competing processes are involved in positron-impact ionization of atoms, namely (a) direct head-on ionization of an electron and (b) positronium formation to the continuum. Using Faddeev's three-body scattering formalism for positron–hydrogen-atom collisions, we get an amplitude which takes account of both these processes. The doubly differential cross section thus obtained for the forward scattering angle shows a cusp when plotted against the emission energy. This cusp is due to the effect of positronium formation to the continuum and heretofore has not been predicted.

Two interesting competing processes are involved when an energetic positron ionizes an atom or a molecule. These are (a) direct ionization, whereby the emitted electron moves in the continuum relative to the residual ion, and (b) the electron capture (or positronium formation) to the continuum. In describing positron-impact ionization they cannot be separated from one another. That is to say, one does not really know for certain to which of the two centers—the residual ion or the scattered positron—the continuum electron is attached. When the ejected electron moves slowly away from the ion while the positron scatters away much faster, we may say that the electron is in an eigenstate of the residual ion and that direct ionization has taken place. If the velocity of the outgoing electron is small relative to the positron, with their center of mass moving much faster away from the ion, the final state is more an eigenstate of the electron-positron pair, and positronium formation to the continuum should be the dominant mechanism for ionization. As a result, the actual amplitude for positron-impact ionization should be a proper combination of these two physical possibilities. The ionization cross section is therefore not given by the algebraic sum of the individual cross sections. In this Brief Report, we consider the specific case of positron–hydrogen-atom collisions and use the three-body scattering formalism of Faddeev[1] to construct the final-state wave function for an ionizing collision. One essential feature of this approach is that all the interacting particles are treated equally without preference to any one particular pair. The total scattering amplitude for positron-impact ionization thus comes out naturally as an appropriate combination of the amplitude for direct ionization of an electron and the amplitude for positronium formation to the continuum, along with a component which describes the situation where all the interacting particles are asymptotically free. Our findings predict that when the available energy in the final channel is shared almost equally by the outgoing positron and the emitted electron, ionization occurs predominantly through the positronium formation to the continuum. In this case the triply differential cross section is highly enhanced in the forward direction and the doubly differential cross section at the forward angle shows a cusp at the energy point where the electron and the positron have exactly equal velocity.

Consider the incident positron, the atomic electron, and the proton as particles 1, 2, and 3, respectively. Relative to a fixed center in space, let their position vectors be denoted by $\mathbf{r}_j$ and their masses by m_j ($j=1,2,3$). Let us define the relative coordinate of the particles j and k by $\mathbf{R}_{jk}=\mathbf{r}_j-\mathbf{r}_k$ and the coordinate of their center of mass by $\mathbf{s}_{jk}=(m_j\mathbf{r}_j+m_k\mathbf{r}_k)/(m_j+m_k)$. The conjugate momenta $\mathbf{x}_{jk}$ and $\mathbf{q}_{jk}$ are given by $\mathbf{x}_{jk}=m_jm_k(\boldsymbol{v}_j-\boldsymbol{v}_k)/(m_j+m_k)$ and $\mathbf{q}_{jk}=m_j\boldsymbol{v}_j+m_k\boldsymbol{v}_k$, where $\boldsymbol{v}_j$ and $\boldsymbol{v}_k$ are the velocities of particles j and k, respectively. The residual interaction in the incident (positron + H atom) channel is $V_i=V_2+V_3$, where V_2 is the interaction between the particles 3 and 1, and V_3 is the interaction between the particles 1 and 2. We use atomic units throughout the work.

The transition matrix element for ionization may now be written as

$$T_{fi}=\langle\Psi_f^-|V_i|\psi_i\rangle=t_{23}+t_{31}+t_{12}-2t_0\ , \tag{1}$$

where the Faddeev wave function[1] Ψ_f^- for the final state is taken to be

$$\Psi_f^-=\Phi^{(23)}+\Phi^{(31)}+\Phi^{(12)}-2\Phi^{(0)} \tag{2}$$

(here we have retained only the first-order terms in the integral equation for the components of Ψ_f^- following Macek[2]), and the individual matrix elements are defined as

$$t_{jk}=\langle\Phi^{(jk)}|V_i|\psi_i\rangle,\quad t_0=\langle\Phi^{(0)}|V_i|\psi_i\rangle\ . \tag{3}$$

$\Phi^{(jk)}$ are the solutions of the two-particle subsystems interacting via potentials $V_{jk}(|\mathbf{r}_j-\mathbf{r}_k|)$, while the third particle propagates freely:[1,2]

$$\left[-\sum_{\alpha=1}^{3}\frac{1}{2m_\alpha}\nabla_\alpha^2+V_{jk}\right]\Phi^{(jk)}=E\Phi^{(jk)}\ , \tag{4}$$

E being the total energy available for the system. Asymptotically, $\Phi^{(jk)}$ goes to $\Phi^{(0)}$, where

$$\Phi^{(0)}=(2\pi)^{-9/2}\exp\left(i\sum_{\alpha=1}^{3}\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha\right)\ . \tag{5}$$

The wave function ψ_i for the incident channel is given by

$$\psi_i=(2\pi)^{-3}\exp(i\mathbf{k}_i\cdot\mathbf{r}_1+i\mathbf{q}_i\cdot\mathbf{s}_{23})\phi_0(\mathbf{R}_{23})\ , \tag{6}$$

where $\phi_0(\mathbf{R}_{23})$ represents the normal state of the hydrogen atom, and $\mathbf{k}_i$ and $\mathbf{q}_i$ are the initial values of the momentum.

We may note that the transition amplitudes t_{23} and t_{12} in Eq. (1) correspond to the processes (a) and (b), respectively. The matrix element t_{31} corresponds to the case where the scattered positron moves in the continuum repulsive

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Coulomb field of the proton and is a natural outcome of the Faddeev equations. The term t_0 describes the situation where all the outgoing particles are asymptotically free and are represented by plane waves.

We have evaluated all the matrix elements into closed expressions. At most, a single-dimensional integration over 0 to 1 has to be performed numerically in t_{12} and t_{31} involving the potentials V_2 and V_3, respectively. In order to calculate the yield of electrons in the momentum range $d\mathbf{k}_2=k_2^2dk_2d\Omega_2$ for positrons scattered into the solid angle $d\Omega_1$, we use the formula[3]

$$\frac{d^2\sigma}{dk_2d\Omega_2}=\frac{4\pi^2k_2^2k_1}{k_i}\int|T_{fi}|^2d\Omega_1 \ . \tag{7}$$

The final integration for this doubly differential cross section is carried out numerically. We now discuss some of our main results.

Figure 1 displays the present triply differential cross section $d^3\sigma/dE_2d\Omega_2d\Omega_1$ for incident positron energies 100 and 250 eV at $\theta_1=4°$, $\phi_1=0°$, $\phi_2=180°$, and varying θ_2. We have chosen the ejected-electron velocity v_2 to be nearly

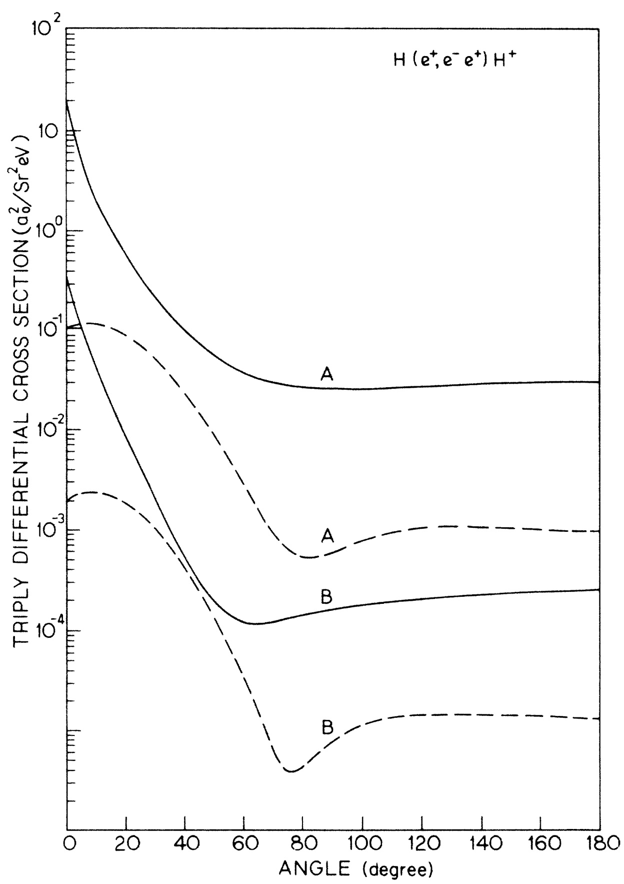

FIG. 1. Triply differential cross section as a function of the scattering angle θ_2 for $H(e^+,e^-e^+)H^-$ collisions. The solid lines (——) denote the present results and the broken lines (— — —) denote the direct-ionization Born results. Curves A are for incident positron energy $E_i=100$ eV, ejected-electron energy $E_2=44$ eV, and scattered positron energy $E_1=42.4$ eV. Curves B are for $E_i=250$ eV, $E_2=118$ eV, $E_1=118.4$ eV. The calculations are performed at $\theta_1=4°$, $\phi_1=0°$, $\phi_2=180°$, and varying θ_2 for both these energies.

equal to the velocity v_1 of the scattered positron for both these energies. The cross section thus calculated shows a sharp peak in the forward direction. The Born values of the direct-ionization cross section alone [obtained from $|t_{23}|^2$ of Eq. (3)] do not show any such behavior. It is apparent that the Coulomb normalization $N_{\mathbf{x}_{12}}$ of the wave function $\Phi^{(12)}$ in the matrix element t_{12} is responsible for such forward peaking, since

$$|N_{\mathbf{x}_{12}}|^2\sim 1/\mathbf{x}_{12} \ , \quad \text{when } \mathbf{k}_1\approx\mathbf{k}_2 \ .$$

From an analysis of the results of the individual matrix elements, it is found that all other components except t_{12} vary so slowly over the entire angular range that they seem almost to give a constant contribution towards the cross-section values, while t_{12} falls off rapidly from a forward peak. This indeed shows that the electron is actually dragged along with the positron in continuum states near the forward angle when $\mathbf{k}_1\approx\mathbf{k}_2$.

In Fig. 2 we show our results for the doubly differential cross section from Eq. (7) at the forward angle $\theta_2=0$ as a function of the electron energy for an incident energy 100 eV. The cross section produces a cusp when the relative velocity of the electron-positron pair $|v_1-v_2|\approx 0$. The position of the cusp peak is solely determined by the factor $|N_{\mathbf{x}_{12}}|^2$. While looking at the values of the cross section around this peak, one finds that its fall rate is much sharper at higher energies than its rise at lower energies. There is an obvious asymmetry around the cusp peak.

Furthermore, as the speed of the emitted electron gets slower and slower, the cross section as depicted in Fig. 2

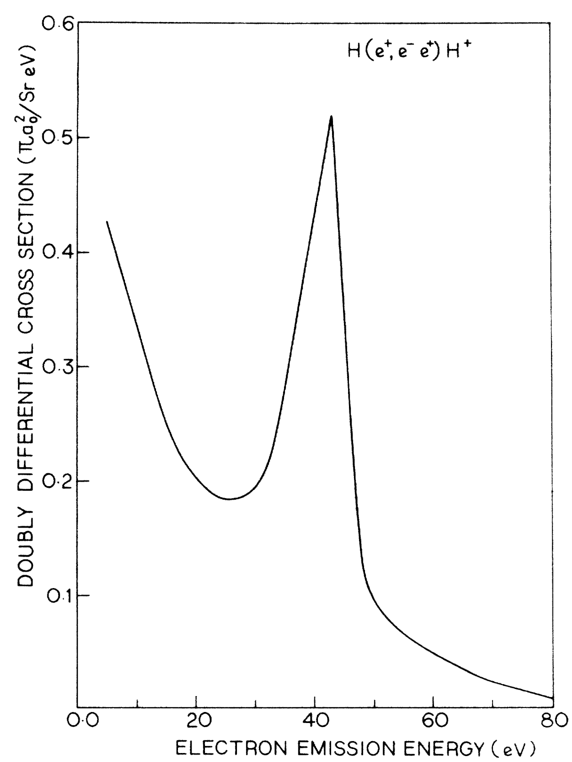

FIG. 2. Energy distribution of electrons ejected at the forward angle $\theta_2=0$ from atomic hydrogen by 100-eV positrons.

rises again rather rapidly and approaches a peak value at zero emission energy. Our results indicate that this maximum in the doubly differential cross section is mainly due to direct head-on collisions.

It may be mentioned that, in the case of electron scattering, ionization occurs only through direct head-on collisions.[4] In ion-atom collisions, on the other hand, the processes of (a) direct ionization and (b) electron capture to the continuum are simultaneously present.[2] When the ejected electron has nearly the same velocity as the scattered ion, the differential cross section shows a sharp peak in the forward direction. This is attributed to the electron being carried along with the projectile ion.[2,5–7] Similar features are also noticed for positron-atom collisions, as our present study shows. The ion-impact ionization, however, differs from the present case of incident positrons in several ways. The ion mass is many times higher than the incident positron mass. Merely exchanging the positron mass for the ion mass in the theory, as one might suspect, does not speak the whole truth of the physics in the two problems. We may recall that the internuclear interaction in ion-atom collisions can be ignored because of the argument that this interaction contributes to the determination of the phase of the amplitude only and not its magnitude. Now one cannot carry this argument over to the problem of positron collisons simply because the incident positron in a realistic situation cannot be described as following a classical straight-line trajectory with respect to the atomic nucleus, as is often done with justice in the case of ion-atom collisions. As we have noted earlier, the evaluation of the additional integrals involving the positron-nucleus interaction (V_2) is more difficult to carry out compared with the integrals involving the electron-nucleus interaction (V_3), which are obtained analytically. Also, while it is known that the second Born approximation does give the dominant contribution to the total charge-transfer cross section in ion-atom collisions, this is not true for the similar reaction of positronium formation in positron-atom collisions.[8] Thus, we feel that approximating the final-state wave function Ψ_f^- by the first term of the Neuman expansion of the Faddeev wave function is more justified for positrons than for incident heavy ions. In fact, the first-order Born-type expansion of the amplitude seems to be a satisfactory first step towards a qualitative understanding of the present problem of positron-impact ionization of atoms and molecules.

In conclusion, the present study shows the importance of positronium formation to the continuum in positron-impact ionization of atoms. Its effect on the doubly differential cross section is so pronounced that it can, we hope, be put to experimental test. Further theoretical work is under way to ascertain its role in the determination of the total ionization cross section.

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