Asymmetric Formation of Positronium Continuum States Following Positron-Impact Ionization of H_2

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The fully differential cross section for the positron- and electron-impact ionization of H_2 is calculated. For positron impact the results are contrasted against a recent experiment which evidently shows the influence of the electron capture to a low-lying positronium continuum state. From a detailed analysis it is deduced that the capture probability is dependent on the orientation of the electron-positron relative momentum vector with respect to the residual ion. Within the used model, this asymmetric positronium formation is traced back to the distortion of the positron motion by the two-center potential formed by the residual ion and the secondary electron. [S0031-9007(98)06857-4]

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A detailed understanding of correlated many-body scattering states is of fundamental importance for diverse fields of physics such as discharge and plasma physics, fusion physics, and physics of the upper atmosphere. Such continuum states are usually achieved as the final outcome of charged particle- and photon-impact ionization. Recent technological advances in multiple detection techniques have rendered possible an unprecedented insight into the properties of these states: the energy and momentum transfer to the many-body continuum can be probed independently by virtue of equivelocity heavy- and light-particle impact; for a fixed amount of energy and momentum transferred to the final state, the open reaction channels as well as the total potential surface can be varied using particle and antiparticle projectiles.

A unified description of all of these facets is a major challenge for current theoretical investigations.

The present study is motivated by a recent kinematically complete experiment [1] in which a H_2 molecule is ionized upon positron impact. The resulting final continuum states which consist of a positron and an electron moving in the field of H_2^+ [hereafter referred to as $(e^- e^+ H_2^+)$] have been simultaneously resolved in angle and energy.

Contrasting this final channel with that achieved in electron-impact ionization [two electrons in the double continuum of a residual ion, labeled hereafter by $(e^- e^- H_2^+)$], two distinctive differences can be noted.

(i) Evidently the total potential surface is markedly different in both cases [2] which results in completely different dynamics. This is particularly reflected by the decisively different threshold laws for total breakup (cf. [3–5] and references therein).

(ii) The indistinguishability of the two electrons introduces exchange effects in the case of $(e^- e^- H_2^+)$, i.e., the cross sections are statistical mixtures of triplet and singlet scattering cross sections. While this effect is absent in the case of $(e^- e^+ H_2^+)$, an additional channel opens, namely, that of positronium formation.

In the experiment of Kövér and Laricchia [1], capture of the ejected electron to low-lying positronium continuum states can be identified. This channel shows up as a rapid increase in the cross section when the electron approaches the positron in velocity space. The functional dependence of this enhancement is dictated by the electron-positron Coulomb density of states (CDS) (see below). Previous experimental and most of the theoretical work on positron-atom ionizing collisions concentrated on the analysis of the secondary electron spectra while the scattered positron is being undetected [6–15]. No unambiguous evidence as to the existence of the electron capture to the positron continuum has been found. On the other hand, the phenomenon of electron capture to the projectile's continuum (ECC) is well established in heavy ion-atom ionizing collisions both experimentally and theoretically [17–28]. From these studies it has been concluded that a theoretical description of the energy and angular distributions of the secondary electrons must account for the interaction of these electrons both with the residual ion and the projectile [29]. For light-particle impact, such as positron, the theoretical description is even more challenging, for in this case the projectile is deflected through very large angles [11,15]. In contrast, in the case of heavy-particle impact the projectile is scattered around the forward direction. Therefore, for the description of the $(e^- e^\pm H_2^+)$ final states, at least, a genuine three-body model is required. In this work we model the final state by a wave function originally derived for ion-atom collisions [16] and recently applied for electron and positron ionizing scattering [14] (atomic units, a.u., are used throughout; corrections due to finite electron mass as compared to that of the proton are neglected):

$$\begin{aligned}\Psi(\mathbf{r}_a,\mathbf{r}_b) \approx\ & (2\pi)^{-3} N_a N_b N_{ab} e^{i\mathbf{p}_a\cdot\mathbf{r}_a} e^{i\mathbf{p}_b\cdot\mathbf{r}_b} \\ & \times {}_1F_1[i\alpha_a, 1, -i(p_a r_a + \mathbf{p}_a\cdot\mathbf{r}_a)] \\ & \times {}_1F_1[i\alpha_b, 1, -i(p_b r_b + \mathbf{p}_b\cdot\mathbf{r}_b)] \\ & \times {}_1F_1[i\alpha_{ab}, 1, -i(p_{ab} r_{ab} + \mathbf{p}_{ab}\cdot\mathbf{r}_{ab})],\end{aligned} \tag{1}$$

where $\mathbf{r}_{a/b}$ are, respectively, the coordinates of the positron and the electron with respect to the residual ion,

$\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$, and $\mathbf{p}_{ab}$ is its conjugate momentum. The vector momenta of the emerging positron and electron are, respectively, labeled $\mathbf{p}_a$ and $\mathbf{p}_b$, and ${}_1F_1[a,b,c]$ is the confluent hypergeometric function. The normalization factors N_j are given by

$$N_j = \exp(-\pi\alpha_j/2)\Gamma(1 - i\alpha_j), \qquad j = a, b, ab\,, \tag{2}$$

with the Sommerfeld parameters being $\alpha_a = Z_p Z_t/p_a$, $\alpha_b = -Z_t/p_b$, and $\alpha_{ab} = -Z_p/(2p_{ab})$, where Z_p and Z_t are the projectile and the final-state ion charge, respectively. The cross section, differential in the energies E_a, E_b and the solid angles Ω_a, Ω_b of the escaping particles, is then given by

$$\sigma(\Omega_a, \Omega_b, E_b) = C|\langle\Psi(\mathbf{r}_a,\mathbf{r}_b)\,|V|\,\varphi_{\mathbf{p}_0}(\mathbf{r}_a)\Phi(\mathbf{r}_b)\rangle|^2, \tag{3}$$

where $C = (2\pi)^4 p_a p_b/p_0$ and $\varphi_{\mathbf{p}_0}$ is a plane wave describing the projectile incident with momentum $\mathbf{p}_0$. The H_2 target, as described by $\Phi(\mathbf{r}_b)$, is assumed to be composed of two noninteracting hydrogen atoms. Furthermore, the relaxation time of the final-state ion H_2^+ is supposed to be much longer than the interaction time so that a frozen-core approximation can be applied. In Eq. (3) the perturbation operator V is the scattering potential of the incoming particle from the active electron and the residual ion.

The first Born approximation (FBA) is obtained from this scheme in the limit $\alpha_a \equiv 0 \equiv \alpha_{ab}$. It is well known that the FBA yields cross sections that depend on the velocity of the impinging projectile and the square of its charge. Therefore, the FBA does not distinguish between particle and antiparticle impact at the same impact velocity.

In contrast, the full calculations (Fig. 1) reveal a drastic difference between reactions leading to $(e^- e^- H_2^+)$ or $(e^- e^+ H_2^+)$ continuum, in particular, in the region where the escaping particles emerge with equal velocities. This difference is readily understood from the CDS of the electron-electron and electron-positron subsystems that is described by $|N_{ab}|^2 = 2\pi\alpha_{ab}[\exp(2\pi\alpha_{ab}) - 1]^{-1}$. In the limit of $p_{ab} \to 0$, $|N_{ab}|^2$ attains the behavior

$$\lim_{p_{ab}\to 0} |N_{ab}|^2 \to -2\pi\alpha_{ab} \to \infty\,, \qquad \text{for } Z_p > 0\ (e^+ \text{ impact})\,, \tag{4}$$

$$\lim_{p_{ab}\to 0} |N_{ab}|^2 \to 2\pi\alpha_{ab}\exp(-2\pi\alpha_{ab}) \to 0\,, \qquad \text{for } Z_p < 0\ (e^- \text{ impact})\,. \tag{5}$$

From Eq. (4) it is clear that $\sigma(\Omega_a, \Omega_b, E_b)$ possesses a first order pole at $p_{ab} = 0$ in the case of e^+ impact that signifies the ECC channel. Because of the localized nature of this pole it is very important to account for the experimental resolution in order to compare with the experimental finding [30]. In fact, as shown in the inset (Fig. 1), the convolution with the experimental resolution, as given by Ref. [1], leaves only a small peak in the cross section at $p_{ab} = 0$. This is quite different from ion-atom collision where, due to the basically undeflected projectile, the ECC peak is much more pronounced even after convolution and with the scattered projectile being undetected (see, e.g., [27]).

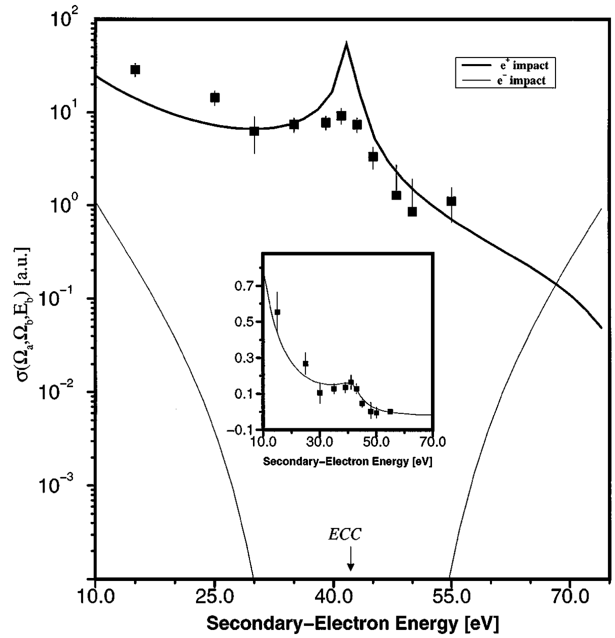

FIG. 1. The positron (thick curve) and electron (light curve) impact ionization cross sections of H_2 as a function of the secondary-electron energy. The solid squares are the experimental data of Ref. [1]. The incident energy is 100 eV. The absolute value of the experimental cross section is unknown. Both emerging particles are detected in the forward direction. The inset shows the positron calculations convoluted with the experimental resolution, as given by [1]. The position of the ECC peak is indicated.

For the following analysis it is important to note, however, that the general slope of σ around the ECC position is not much affected by the convolution, as can be observed in Fig. 1. Unfortunately, for the $(e^- e^- H_2^+)$ system there is no available experimental data in the present scattering geometry.

The obvious difference between e^- and e^+ impact, as seen in Fig. 1, is simply a reflection of the markedly different analytical behavior of (4) and (5). This effect also shows up in heavy-particle and antiparticle impact [31]. In our case, however, exchange introduces additional phenomena which can be unraveled by analyzing the quantity

$$\sigma^n(\Omega_a, \Omega_b, E_b) = \frac{\sigma(\Omega_a, \Omega_b, E_b)}{|N_{ab}|^2}\,. \tag{6}$$

For the case of Fig. 1 we depict in Fig. 2 the normalized cross section σ^n. As is more clear from Fig. 2, due to exchange in the case of e^- impact, σ^n (and σ) is symmetric with respect to the ECC position. Thus, for e^- impact exchange imposes a continuous σ^n at $p_{ab} = 0$.

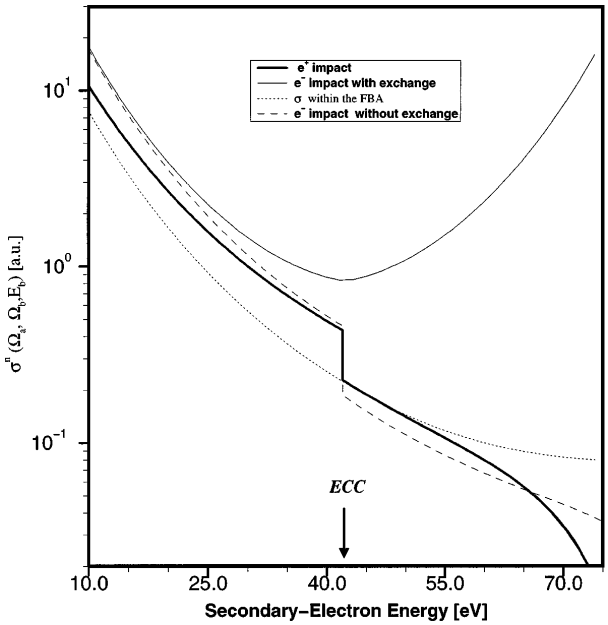

FIG. 2. The same as in Fig. 1, but the normalized cross section σ^n, as defined by (6), is considered. The cross sections σ^n for e^- impact with (light solid curve) and without (dashed curve) exchange are depicted along with σ^n for e^+ impact (solid thick curve). The cross section σ (3) (not σ^n) as predicted by the FBA is also shown (dotted curve, same results for e^- and e^+ impact).

Neglecting exchange reveals remarkable similarities between e^+ and e^- impact except for the region of very slow positrons in which case the repulsion between H_2^+ and the positron leads to a vanishing cross section [this is described by a positron-ion CDS, $|N_a|^2$, that behaves similar to Eq. (5) for slow e^+]. It is worthwhile to note that the slope of σ^n for e^+ and e^- (without exchange) is given by σ (not σ^n) as calculated within the FBA. In fact, even a plane-wave impulse approximation (PWIA) yields the same slope behavior of σ as within the FBA. The cross section σ^{PWIA} within the PWIA can be evaluated from the above model by setting $\alpha_a \equiv 0 \equiv \alpha_b, \alpha_{ab} \equiv 0$. The result is $\sigma^{\mathrm{PWIA}} = C/(2\pi^4 q^4)\,|\tilde{\Phi}(\mathbf{p}_{\mathrm{ion}})|^2$, where $\tilde{\Phi}(\mathbf{p}_{\mathrm{ion}})$ is the Fourier transform of Φ, $\mathbf{p}_{\mathrm{ion}}$ is the recoil momentum of the ion, and q is the momentum transfer. Thus the slopes of the σ as depicted in Fig. 1 are determined by the Compton profile of the initially bound state and the projectile-electron interaction potential in momentum space. Superimposed on that is then $|N_{ab}|^2$ and exchange requirements in the case of electron impact.

A much more delicate feature of the σ^n is the discontinuity at $p_{ab} \to 0$, i.e., the capture probability is dependent on whether $\mathbf{p}_a \to \mathbf{p}_b + \boldsymbol{\epsilon}$ or $\mathbf{p}_a \to \mathbf{p}_b - \boldsymbol{\epsilon}$, where $\epsilon \ll 1$. This behavior has also been encountered in ion-atom ionizing collisions (both experimentally and theoretically) [16,23,28,29,32–35] and has been dubbed *cusp asymmetry*. To my knowledge there is as yet no clear physical explanation of the origin of this asymmetry and, as will be shown below, this study sheds new light on this question but certainly does not resolve it.

Here we define the cusp asymmetry as

$$\Delta = \lim_{(E/2-E_b)\to 0^+} \sigma^n - \lim_{(E/2-E_b)\to 0^-} \sigma^n,$$

where E is the total excess energy. In the case of e^- impact the cusp asymmetry Δ is disguised by exchange (Fig. 2); its sign is the same as that observed in e^+ impact. This rules out an explanation of this asymmetry in terms of screening. Further calculations (not illustrated here for space limitations) showed the following: (a) The asymmetry diminishes at higher energies (>1 keV) and increases when the impact energy is lowered, and (b) the sign of the asymmetry is not dependent on the emission angles of the final-state products; i.e., if the ejected electron and the scattered projectile are detected both in the backward direction we end up with a behavior similar to that depicted in Fig. 2.

As mentioned above, the experimental data of Fig. 1 follow the slope of the calculated cross section and hence hint at the existence of Δ. Further ongoing experimental efforts should provide more insight into the exact value of Δ.

As realized in the early studies on ion-atom collision [32,33], a description of Δ requires a higher order treatment. This is obvious from Fig. 2. The FBA yields no asymmetry. In addition, if we neglect final-state

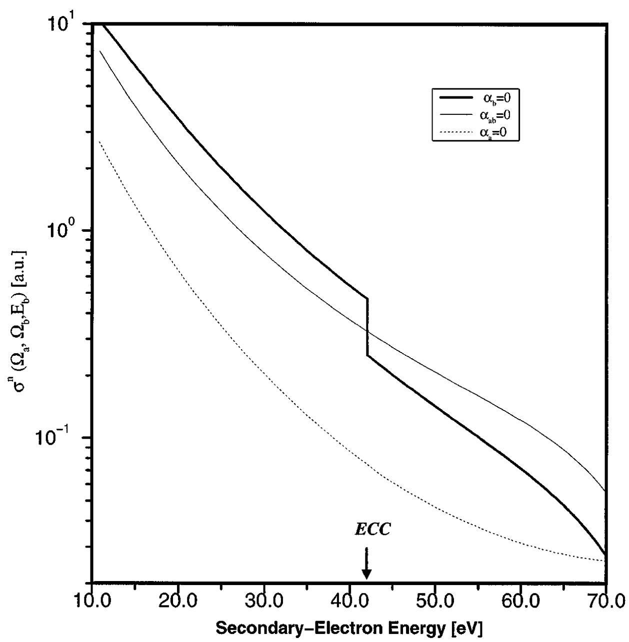

FIG. 3. The e^+-impact case for the same geometry as in Fig. 1 is studied. Neglect of the positron-residual ion final-state interaction [$\alpha_a \equiv 0$ in Eq. (1)] yields the dotted curve, whereas if we disregard the interaction between the emerging e^- and e^+ [$\alpha_{ab} \equiv 0$ in Eq. (1)] we end up with the solid light curve. The final-state interaction of the secondary electron with the ion has basically no influence on the cusp asymmetry [$\alpha_b \equiv 0$ in Eq. (1) leads to the thick solid curve].

interactions between the escaping particles (i.e., within an independent particle model) σ would be proportional to the FBA cross section [15] and we end up thus with vanishing Δ. Furthermore, as shown in Fig. 3, the final-state interaction of the ejected electron with the residual ion produces no contribution to Δ [i.e., Δ is invariant upon the substitution $\alpha_b \equiv 0$ in Eq. (1)]. In contrast, only the simultaneous final-state interaction of the positron with the emitted electron and the residual ion leads to an asymmetric ECC cusp. Neglecting one of these interactions results in a breakdown of Δ. In other words, within the present model, this asymmetric formation of positronium continuum states can be viewed as the result of the positron propagating in a two-center potential formed by the interaction with the continuum electron and the residual ion.

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