Two-center approach to fully differential positron-impact ionization of hydrogen

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The two-center approach to positron-impact ionization of atomic hydrogen is shown to follow from the exact *post* form of the breakup amplitude [Kadyrov, Bray, Mukhamedzhanov, and Stelbovics, Phys. Rev. Lett. **101**, 230405 (2008)]. In such approaches distinct ionization amplitudes arise from each center for the same ionization process. The fully differential cross section for the positron-impact breakup of atomic hydrogen is calculated including direct ionization of the target and electron capture into the positronium continuum. We show that the coherent combination of the amplitudes leads to oscillations in the differential cross sections, whereas the incoherent combination does not. The latter has also the advantage of being consistent with the unitary close-coupling formalism.

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I. INTRODUCTION

Scattering in a three-body system is one of the central subjects of quantum mechanics. Positron scattering on the hydrogen atom is particularly important as the simplest example of a three-body problem with three distinguishable particles and a possibility of rearrangement (Ps formation). Though a kinematically complete picture of electron-impact ionization of atomic hydrogen is well understood, with calculations fully supporting experimental observations (see, e.g. [1], and references therein), this is not the case as far as its positron-hydrogen counterpart is concerned.

In this work we consider the fully differential positron-impact breakup of atomic hydrogen. Depending on the kinematical situation this process can be regarded as direct ionization (DI) or Ps formation in the continuum (PFC). PFC, an analog of a phenomenon known as electron capture into the continuum (ECC) in ion-atom collisions, was first calculated using the truncated (see below for explanation) Born [2] and 3C [3] approximations, where the total scattering wave function was approximated by the initial-channel one. In the truncated Born approximation (denoted hereafter as B0) the interaction of the incident positron with the target nucleus was also dropped and the final state wave function was taken as a product of the Ps continuum wave and a plane wave for the motion of the Ps relative to the proton. The 3C method used a three-body Coulomb-distorted wave [4,5] for the final state. Both approaches gave a singular structure in the fully differential cross section (FDCS). The divergence in the FDCS occurred when the scattered projectile and ejected electron have small relative momentum, corresponding to PFC.

The first experimental study of positron-impact ionization with fully determined kinematics has been carried out by Kövér and Laricchia [6]. They have measured the fully differential cross section for the single ionization of H_2 by 100-eV positrons. A small broad peak was found in the spectrum of the electron ejected in the forward direction at the so-called equal-energy-sharing point, when the scattered positron and ejected electron take away equal share of the total energy. Such a peak is indicative of PFC since the relative momentum of the outgoing electron and positron is small. Subsequently, Arcidiacono *et al*. [7] have performed a similar experiment with 50-eV positrons and revealed a very subtle picture. They have observed differences in the energies of the two light particles in the final state, with the electron spectrum being shifted to significantly lower energies and the scattered positron to higher energies than expected. The ejected electron energy was shifted down by about 2.5 eV relative to the equal-energy-sharing point which, for this incident energy, is at 18.2 eV. A similar picture has been observed when the H_2 target was replaced by He.

The aforementioned theoretical approaches have been applied to the positron-impact ionization of molecular hydrogen [8–10] to describe the experimental findings. A classical-trajectory Monte Carlo (CTMC) method has also been applied [10,11]. A common feature of all available approaches to the problem is that they lead to the FDCS that has a singular structure at the equal-energy-sharing point corresponding to PFC. The convolution of the raw results with the experimental energy and angular resolutions smears out the otherwise divergent cusp to a small shoulder, at the same time shifting it (the shoulder) to a lower energy. Such a shift obtained as a result of convolution is dependent on the experimental resolution. It should reduce when the experimental resolution is improved and, in principle, become too small to be observable when the resolution is sufficiently refined. As a result the shoulder should tend back to the singularity at its original position [11]. The question then is: Does the shift observed in the experiment by Arcidiacono *et al*. [7] actually represent any real physics? According to the approaches mentioned above, it does not. This is not the only controversy. Instrumental resolutions would indeed somewhat shift the spectrum of both electron and positron towards lower energies, therefore, they cannot be responsible for the shift of the positron spectrum in the opposite direction seen in the experiment [7]. This suggests that further investigations are required to understand the experimental findings. Ultimately, whether there is a permanent shift in the energy of the ejected electron and scattered positron, independent of the characteristics of the experimental apparatus, must be settled by a full (nonperturbative) low-energy quantum-mechanical approach.

The close coupling methods are ideally suited to taking into account the two-center nature of the problem on an equal footing in a nonperturbative way [12–14]. The convergent close coupling (CCC) approach has been applied [14,15] to

calculations of integrated cross sections. Excellent agreement with the experiment has been obtained for the grand total, total Ps formation, and total breakup cross sections. However, an artifact of the two-center approach is that it treats DI and PFC as separate channels and the total breakup cross section has been calculated as a sum of the cross sections for the excitation of all positive-energy atomic and Ps pseudostates. This is what naturally follows from the formalism and corresponds to an incoherent combination of the contributions from DI and PFC. The next challenge is to extend the CCC approach to fully differential breakup processes. The question is then how to combine the amplitudes of DI and PFC, coherently or incoherently, to get the total fully differential cross section. To investigate this point we first derive the two-center approach from the surface-integral formulation of scattering theory [16,17]. This results in the requirement to obtain the corresponding ionization amplitudes from positive-energy states of both the atomic and positronium centers. The two sets come in momentum variables from different coordinate systems. The transformation into a single coordinate system is not straightforward, particularly due to the discretization, and is currently under investigation. However, we can utilize the Born approximation to answer the key question above. It allows an analytic treatment of the secondary energies involved in both centers, and is a limiting case for two-center close-coupling methods where the size of the expansion basis goes to infinity and the channels are decoupled.

The results presented here are a prerequisite for and pave the way to a full-scale nonperturbative two-center approach to a differential breakup problem in an arbitrary many-particle system which then can also address the aforementioned controversies in the positron-induced ionization.

The two-center formalism is given in Sec. II, where we describe how the breakup amplitude is extracted and give details of the calculations. The results of the calculations are presented in Sec. III. Finally, in Sec. IV we draw conclusions from this work. Atomic units are used throughout unless otherwise specified.

II. TWO-CENTER APPROACH TO BREAKUP IN POSITRON-HYDROGEN COLLISIONS

We consider the scattering of positron with momentum $\boldsymbol{k}_i$ incident on atomic hydrogen in the ground state. This may result in the elastic scattering, excitation of the target, or positronium formation. In addition, we assume that the energy of the projectile is sufficient to breakup the target leading to three unbound particles in the final state. Let $\boldsymbol{k}_1$ ($\boldsymbol{k}_2$) be the momentum of the scattered positron (ejected electron). In the surface-integral formulation of scattering theory the exact *post* form of the breakup amplitude is written as [16,17]

$$T = \langle \Phi_0^- | \overleftarrow{H} - E | \Psi_i^+ \rangle, \tag{1}$$

where Ψ_i^+ is the total three-body scattering wave function, Φ_0^- is the three-body Coulomb asymptotic state consisting of incoming waves representing the three unbound particles in the final state [5,18,19]. The three-particle Hamiltonian H is given as

$$H = H_0 + V_1 + V_2 + V_{12}, \tag{2}$$

where H_0 is the free Hamiltonian, V_1 (V_2) is the potential of interaction between the positron (electron) and the proton, V_{12} is the positron-electron interaction. The arrow on the Hamiltonian operator indicates that it acts on the bra state. The total energy is

$$E = k_i^2/2 + \epsilon_i^{\mathrm{H}} = k_1^2/2 + k_2^2/2, \tag{3}$$

where ϵ_i^{H} is the initial bound state energy of the target electron. The total wave function Ψ_i^+ satisfies the incoming plane wave and outgoing spherical wave boundary conditions [20].

We now introduce two projection operators

$$I_N^{\mathrm{H}} = \sum_{n=1}^{N} |\phi_n^{\mathrm{H}}\rangle\langle\phi_n^{\mathrm{H}}|, \tag{4}$$

$$I_M^{\mathrm{Ps}} = \sum_{m=1}^{M} |\phi_m^{\mathrm{Ps}}\rangle\langle\phi_m^{\mathrm{Ps}}|, \tag{5}$$

where ϕ_n^{H} (ϕ_m^{Ps}) are square-integrable pseudostates obtained by diagonalizing the H (Ps) Hamiltonian in a Laguerre basis. The main idea of the two-center close-coupling approach to e^+-H breakup consists in the following replacement in Eq. (1):

$$T \approx \lim_{N,M\to\infty} T_{N,M}, \tag{6}$$

where

$$T_{N,M} = \langle \Phi_0^- (I_N^{\mathrm{H}} + I_M^{\mathrm{Ps}}) | \overleftarrow{H} - E | (I_N^{\mathrm{H}} + I_M^{\mathrm{Ps}}) \Psi_i^+ \rangle. \tag{7}$$

Denoting the expansion of the total wave function as

$$|\Psi_{N,M}^+\rangle = |(I_N^{\mathrm{H}} + I_M^{\mathrm{Ps}})\Psi_i^+\rangle, \tag{8}$$

we write

$$\begin{aligned} T_{N,M} &= \langle \Phi_0^- (I_N^{\mathrm{H}} + I_M^{\mathrm{Ps}}) | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle \\ &= T_{N,M}^{\mathrm{H}} + T_{N,M}^{\mathrm{Ps}}, \end{aligned} \tag{9}$$

where

$$T_{N,M}^{\mathrm{H}} = \langle \Phi_0^- I_N^{\mathrm{H}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle, \tag{10}$$

$$T_{N,M}^{\mathrm{Ps}} = \langle \Phi_0^- I_N^{\mathrm{Ps}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle. \tag{11}$$

The action of the operator I_N^{H} leads to limiting the target subspace by replacing the full set of the H states (including non-L^2 continuum) with a set of L^2 states. This effectively screens the Coulomb interaction between the projectile and target constituents even in the continuum. Likewise, the action of operator I_N^{Ps} is to screen the Coulomb interaction between the proton and Ps in the Ps-formation channels. Consequently, we have

$$\begin{aligned} T_{N,M}^{\mathrm{H}} &= \langle \boldsymbol{k}_1 \psi_{\boldsymbol{k}_2}^{\mathrm{H}-} I_N^{\mathrm{H}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle \\ &= \sum_{n=1}^{N} \langle \psi_{\boldsymbol{k}_2}^{\mathrm{H}-} | \phi_n^{\mathrm{H}} \rangle \langle \boldsymbol{k}_1 \phi_n^{\mathrm{H}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle, \end{aligned} \tag{12}$$

$$\begin{aligned} T_{N,M}^{\mathrm{Ps}} &= \langle \boldsymbol{q} \psi_{\boldsymbol{p}}^{\mathrm{Ps}-} I_M^{\mathrm{Ps}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle \\ &= \sum_{m=1}^{M} \langle \psi_{\boldsymbol{p}}^{\mathrm{Ps}-} | \phi_m^{\mathrm{Ps}} \rangle \langle \boldsymbol{q} \phi_m^{\mathrm{Ps}} | \overleftarrow{H} - E | \Psi_{N,M}^+ \rangle, \end{aligned} \tag{13}$$

where $\psi^{\mathrm{H}-}_{\boldsymbol{k}_2}$ ($\psi^{\mathrm{Ps}-}_{\boldsymbol{p}}$) is the Coulomb wave representing the continuum state of H (Ps) with momentum $\boldsymbol{k}_2\,(\boldsymbol{p}), \boldsymbol{k}_1\,(\boldsymbol{q})$ is the momentum of the positron (Ps) in the final state relative to the proton. Here $\boldsymbol{p} = (\boldsymbol{k}_1 - \boldsymbol{k}_2)/2$ and $\boldsymbol{q} = \boldsymbol{k}_1 + \boldsymbol{k}_2$. Thus, $T^{\mathrm{H}}_{N,M}$ is simply the amplitude for direct ionization of H, while $T^{\mathrm{Ps}}_{N,M}$ is the amplitude for the Ps formation in the continuum and they are obtained upon the calculation of matrix elements for transitions between the generated pseudostates.

Two-center close-coupling approaches are based on using expansion (8) in the Schrödinger equation for Ψ^+_i. This leads to a set of coupled equations for the transition matrix elements. The formalism described above has been used in the two-center convergent close-coupling method developed in [14] and applied to calculations of the integrated cross sections. The total ionization cross section has been calculated as a sum of cross sections for the excitation of positive-energy pseudostates of both H and Ps. As mentioned before, this corresponds to an incoherent combination of the contributions from DI and PFC. The question then becomes: Is that a correct procedure within the two-center close-coupling formalism? We will answer this question by considering a limiting case when $N, M \to \infty$ and using the Born approximation to calculate the resulting amplitudes.

When $N, M \to \infty$ we have

$$\lim_{N,M\to\infty} T^{\mathrm{H}}_{N,M} \to \left\langle \boldsymbol{k}_1 \psi^{\mathrm{H}-}_{\boldsymbol{k}_2} \middle| V_1 + V_{12} \middle| \Psi^+_i \right\rangle, \tag{14}$$

$$\lim_{N,M\to\infty} T^{\mathrm{Ps}}_{N,M} \to \left\langle \boldsymbol{q} \psi^{\mathrm{Ps}-}_{\boldsymbol{p}} \middle| V_1 + V_2 \middle| \Psi^+_i \right\rangle. \tag{15}$$

The interaction potentials $V_1 + V_{12}$ and $V_1 + V_2$ in e^+-H and Ps-p channels, respectively, represent the action of operator $H - E$ upon the corresponding final state wave functions on the energy shell. Thus, the breakup amplitude splits up into two components, the DI amplitude and the PFC one. Now we approximate Ψ^+_i by the wave function of the initial channel corresponding to the Born approximation. Thus the final DI and PFC amplitudes used in this work are written as

$$T^{\mathrm{DI}} = \left\langle \boldsymbol{k}_1 \psi^{\mathrm{H}-}_{\boldsymbol{k}_2} \middle| V_1 + V_{12} \middle| \phi^{\mathrm{H}}_i \boldsymbol{k}_i \right\rangle \tag{16}$$

$$= \left\langle \boldsymbol{k}_1 \psi^{\mathrm{H}-}_{\boldsymbol{k}_2} \middle| V_{12} \middle| \phi^{\mathrm{H}}_i \boldsymbol{k}_i \right\rangle, \tag{17}$$

$$T^{\mathrm{PFC}} = \left\langle \boldsymbol{q} \psi^{\mathrm{Ps}-}_{\boldsymbol{p}} \middle| V_1 + V_2 \middle| \phi^{\mathrm{H}}_i \boldsymbol{k}_i \right\rangle, \tag{18}$$

where ϕ^{H}_i is the wave function of the H ground state. Equation (17) follows as the term containing V_1 disappears due to the orthogonality of the H continuum and the ground-state wave functions. We emphasize that the corresponding term in T^{PFC} containing V_1 does not disappear since the Ps continuum is not orthogonal to the H ground state. The B0 method of Brauner and Briggs [2] did not include this term in their calculations. Therefore, the method is not the full first Born approximation. This is why we called their approach a truncated Born approximation.

A kinematically complete picture of the breakup process in a three-body system is described by a fully differential cross section. As shown above, in the two-center method it naturally follows that the breakup amplitude has two parts, one is from the direct ionization of hydrogen and the other is from positronium formation in continuum. We consider the case when the incident positron is scattered into a solid angle $d\Omega_1$ around the direction of $\Omega_1 = (\theta_1, \phi_1)$ with energy E_1, the electron of the target is ejected into a solid angle $d\Omega_2$ around the direction of $\Omega_2 = (\theta_2, \phi_2)$ with energy between E_2 and $E_2 + dE_2$, where $E_2 = k_2^2/2$ and $E_1 = E - E_2$. Then the coherently (COH) combined total FDCS is written as

$$\frac{d^5\sigma^{\mathrm{COH}}}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k_1 k_2}{k_i} |T^{\mathrm{DI}} + T^{\mathrm{PFC}}|^2. \tag{19}$$

For comparison we also calculate the FDCS for DI and PFC separately. They are written as

$$\frac{d^5\sigma^{\mathrm{DI}}}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k_1 k_2}{k_i} |T^{\mathrm{DI}}|^2, \tag{20}$$

$$\frac{d^5\sigma^{\mathrm{PFC}}}{d\Omega_1 d\Omega_2 dE_2} = (2\pi)^4 \frac{k_1 k_2}{k_i} |T^{\mathrm{PFC}}|^2. \tag{21}$$

Finally, we look at the incoherently (INC) combined total FDCS

$$\frac{d^5\sigma^{\mathrm{INC}}}{d\Omega_1 d\Omega_2 dE_2} = \frac{d^5\sigma^{\mathrm{DI}}}{d\Omega_1 d\Omega_2 dE_2} + \frac{d^5\sigma^{\mathrm{PFC}}}{d\Omega_1 d\Omega_2 dE_2}. \tag{22}$$

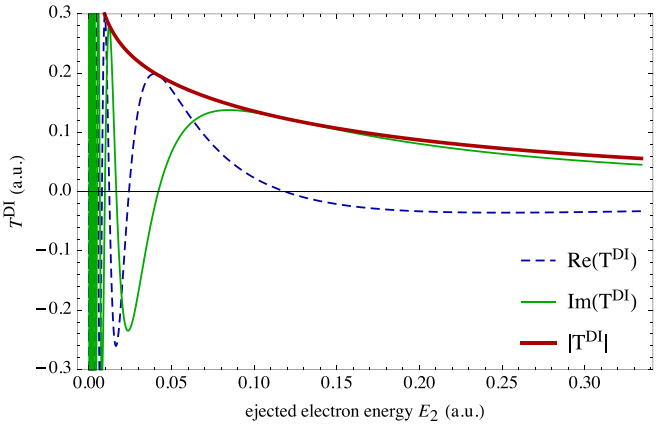

FIG. 1. (Color online) The amplitude for direct ionization of hydrogen by 50-eV positrons in the forward direction ($\theta_1 = \theta_2 = 0$).

III. RESULTS OF CALCULATIONS

In this paper we present results for 50- and 100-eV incident positron energies. The direct ionization amplitude T^{DI} and the part of the amplitude for Ps formation in continuum T^{PFC} containing V_2 are calculated in closed analytic forms, while the other part of T^{PFC} containing V_1 is calculated numerically. Figure 1 shows T^{DI} at 50-eV incident energy for the case when the positron is scattered, and the electron of the target is ejected, in the forward direction ($\theta_1 = \theta_2 = 0$), as a function of the ejected electron energy E_2 in the first quarter of the energy range. The amplitude infinitely oscillates and diverges as the energy goes to zero. Figure 2 shows T^{PFC} also as a function of E_2 at the same incident energy. This amplitude diverges at the equal-energy-sharing point (which is at 0.67 a.u.) with infinite oscillations. The infinite oscillations in both T^{DI} and T^{PFC} are due to the diverging Coulomb phases as k_2 and p

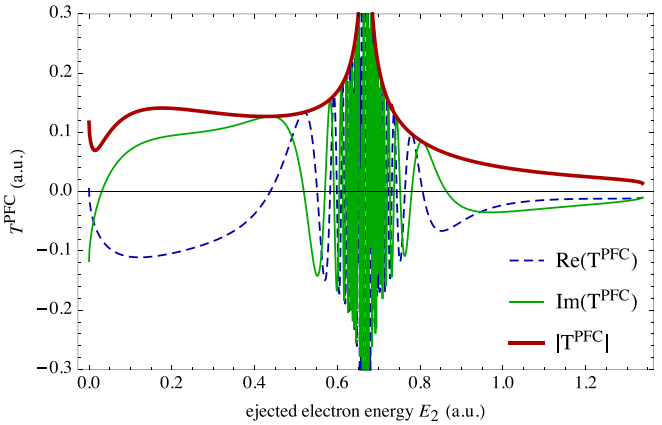

FIG. 2. (Color online) The amplitude for Ps formation in continuum in the forward direction ($\theta_1 = \theta_2 = 0$) in 50-eV positron collisions with hydrogen.

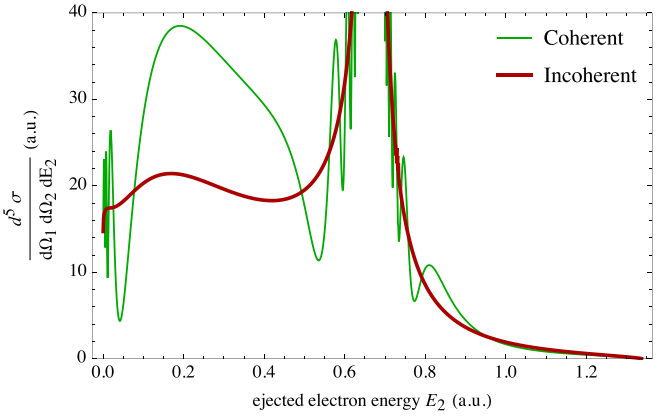

FIG. 4. (Color online) The FDCS from coherently and incoherently combined amplitudes for ionization of H by 50-eV positrons in the forward direction ($\theta_1 = \theta_2 = 0$).

vanish, respectively. Note that the magnitudes of both T^{DI} and T^{PFC} have no oscillations.

Using these amplitudes we have calculated the fully differential cross sections for positron impact breakup of the hydrogen atom. Figure 3 shows the raw unconvoluted FDCS in the forward direction for DI and PFC at 50-eV incident energy calculated from Eqs. (20) and (21) as functions of the ejected electron energy E_2. One can see that the FDCS for DI has a strong peak at small ejection energies and falls sharply before the equal-energy-sharing point is reached. We emphasize that the cross section is not singular at zero ejection energy, rather it has a definite finite value. As expected, the FDCS for PFC has a singularity at the equal-energy-sharing point. Also shown in this figure is the presently calculated FDCS for PFC corresponding to the B0 approximation of Brauner and Briggs [2] scaled down as indicated in the legend to enable comparison on the same scale. Figure 4 presents the raw results for the coherently and incoherently combined total FDCS in the same direction at the same energy. As one can see the DI and PFC amplitudes severely interfere with each other across the whole energy range, leading to a highly oscillatory result when they are combined coherently, while the result is smooth if they are combined incoherently. From physical grounds it is unlikely that the FDCS in the forward direction for the breakup of the hydrogen atom by positrons would have infinite oscillations for small ejected-electron energies, or near the equal-energy-sharing point. On the other hand, the incoherent combination yields smooth results, and is also consistent with the unitary nature of the close-coupling formalism. For example, we have found that the contribution to the breakup cross section from the two centers becomes the same as the threshold is approached [15]. There, the addition of cross sections from the positive-energy states implies an incoherent combination of amplitudes, and this also leads to satisfactory agreement with experiment for H [14] and He [21,22].

The forward direction is not special. Similar oscillations appear in the FDCS for other angles as well, if the underlying amplitudes are combined coherently. A typical example is shown in Figs. 5 and 6 at 50-eV incident energy for the case where the positron is scattered at 5°, and the electron

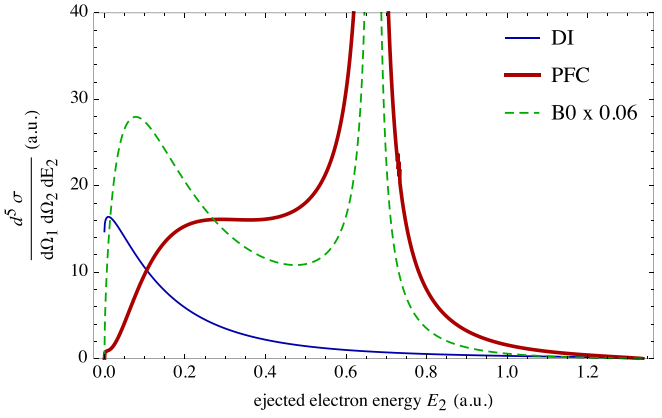

FIG. 3. (Color online) The FDCS for DI and PFC in e^+-H collisions at 50 eV in the forward direction ($\theta_1 = \theta_2 = 0$). Also shown is the present FDCS for PFC corresponding to the B0 approximation of Brauner and Briggs [2] scaled as shown.

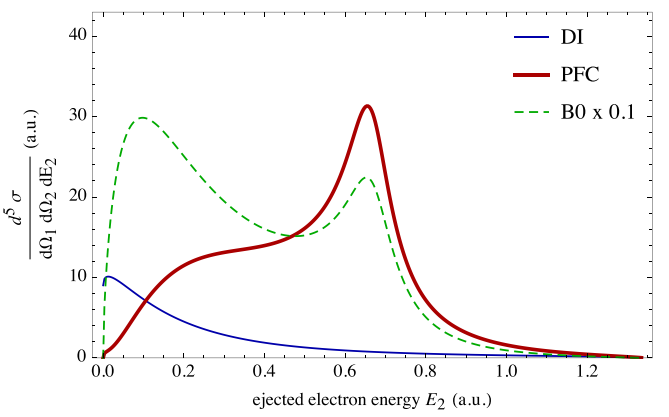

FIG. 5. (Color online) The FDCS for DI and PFC in e^+-H collisions at 50 eV for $\theta_1 = 5°, \phi_1 = 0, \theta_2 = 0$. Also shown is the present FDCS for PFC corresponding to the B0 approximation of Brauner and Briggs [2] scaled as shown.

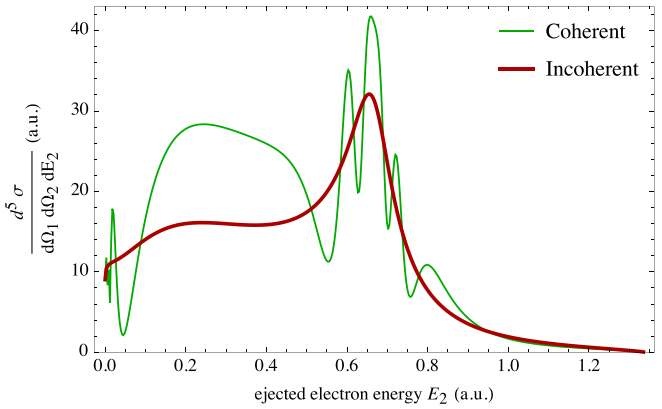

FIG. 6. (Color online) The FDCS from coherently and incoherently combined amplitudes for ionisation of H by 50-eV positrons for $\theta_1 = 5^\circ, \phi_1 = 0, \theta_2 = 0$.

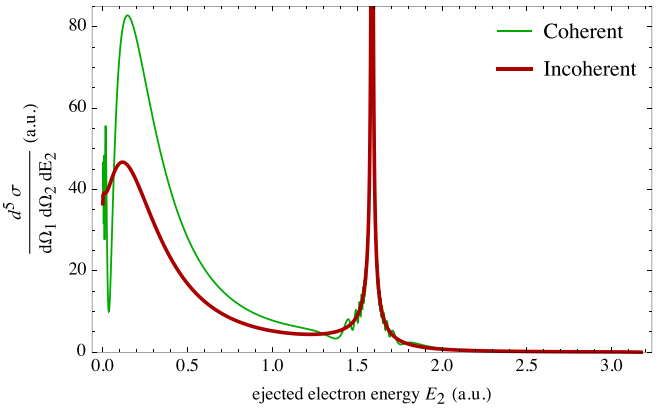

FIG. 8. (Color online) The FDCS coherently and incoherently combined amplitudes for ionization of H by 100-eV positrons in the forward direction ($\theta_1 = \theta_2 = 0$).

of the target is ejected in the forward direction ($\theta_1 = 5^\circ, \phi_1 = 0, \theta_2 = 0$). As the angle between the scattered positron and ejected electron increases the number of oscillations reduce further, however, the interference between DI and PFC remains significant.

Similar results for the forwards direction, but at 100-eV incident energy are shown in Figs. 7 and 8. The oscillations in the coherently obtained TDCS at low ejected-electron energies still remain, however, those near the equal-energy-sharing point are significantly suppressed. As one can conclude from Fig. 7 this is due to the the fact that at 100 eV DI is significantly less likely to happen into this region than PFC.

Finally, we consider an example at a higher energy, where the total (integrated) *electron-impact* ionization cross section calculated using the Born approximation gives reasonably good agreement with the experiment. This is an energy region where the net contribution of exchange effects in electron-hydrogen collisions is negligible. Figures 9 and 10 depict the forward-direction FDCS at 500-eV incident positron energy. We show only a part of the energy range corresponding to small ejected-electron energies (less than the tenth of the whole energy region). From Fig. 9 we see that both DI and PFC cross sections decrease very rapidly with increasing E_2. It is well known that ionization by fast electrons leads predominantly to slow secondary electrons. The only difference in the positron-impact case is the presence of the δ-function-like spike at the equal-energy-sharing point. The coherent and incoherent FDCS (Fig. 10) also fall sharply as E_2 goes up. However, at extremely low ejected-electron energies we still see a strong interference between the DI and PFC amplitudes. This again might be indicating that there is an inconsistency between the two-center approach and coherent combination of amplitudes. This warrants further investigation. Figure 11 shows the behavior of the coherent and incoherent FDCS in the vicinity of the $E/2$ point, where the magnitude of oscillations in the coherent FDCS is defined by that of the DI amplitude. Likewise, the magnitude of oscillations at low E_2 (see Fig. 10) is determined by that of the PFC amplitude. Another interesting observation from these results is that even at energies as high as 500 eV one cannot ignore possible PFC when calculating the total breakup cross section. This means that at these energies the PFC effects in positron-hydrogen collisions are much

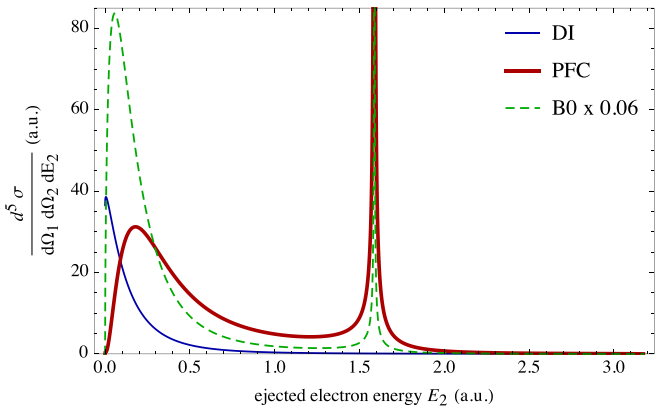

FIG. 7. (Color online) The FDCS for DI and PFC in e^+-H collisions at 100 eV in the forward direction ($\theta_1 = \theta_2 = 0$). Also shown is the present FDCS for PFC corresponding to the B0 approximation of Brauner and Briggs [2] scaled as shown.

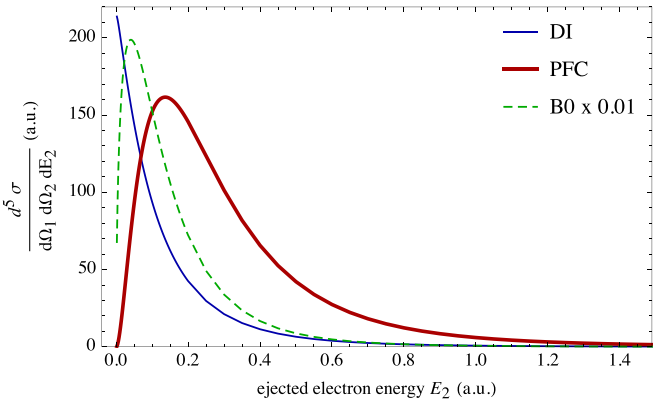

FIG. 9. (Color online) The FDCS for DI and PFC in e^+-H collisions at 500 eV in the forward direction ($\theta_1 = \theta_2 = 0$) at small ejected-electron energies. Also shown is the present FDCS for PFC corresponding to the B0 approximation of Brauner and Briggs [2] scaled as shown.

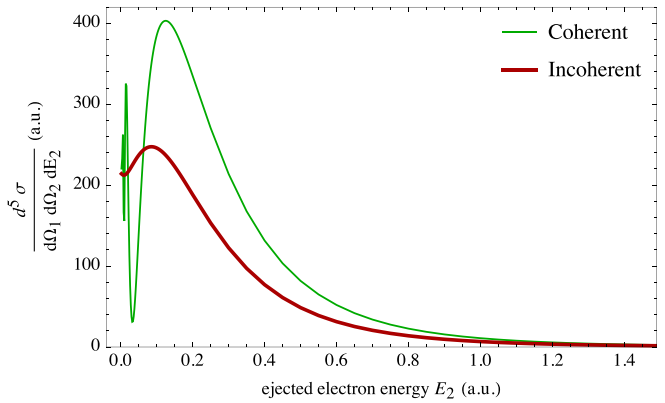

FIG. 10. (Color online) The FDCS coherently and incoherently combined amplitudes for ionization of H by 500-eV positrons in the forward direction ($\theta_1 = \theta_2 = 0$) at small ejected-electron energies.

larger than the electron-exchange ones in electron-hydrogen collisions. As far as differential calculations are concerned, our calculations show that the contribution from PFC cannot be ignored (in comparison to DI) even in the keV region.

IV. CONCLUSION

As discussed earlier, an explanation of the subtle features seen in the fully differential measurements of positron-induced single ionization of H_2 and He [7] requires the development of a sophisticated nonperturbative fully quantum-mechanical approach which could be applied at energies as low as 50 eV. The convergent close-coupling (CCC) method is ideally suited for taking into account the two-center nature of the problem on an equal footing in a nonperturbative way [14]. However, an artifact of this approach to the breakup problem is that it treats direct ionization and Ps formation in continuum as separate channels. Therefore, before the approach can be applied to fully differential studies a suitable way of taking into account of all channels contributing to breakup must be established. In this work we have investigated different ways of combining the contributions from DI and PFC to get the total fully differential cross section. To this end we have first demonstrated how the two-center approach follows from the surface-integral formulation of scattering theory [17]. Then we have performed calculations using the two-center Born approximation. This is a limiting case for two-center close-coupling methods where the size of the expansion basis goes virtually to infinity and the channels are decoupled. Using the two-center Born approximation we have analyzed the contributions to the breakup cross section from direct ionization of hydrogen and electron capture into the Ps continuum over a fine secondary electron energy mesh. A coherent combination of such amplitudes has been considered, and found to severely interfere with each other leading to strong oscillations in the resulting cross sections.

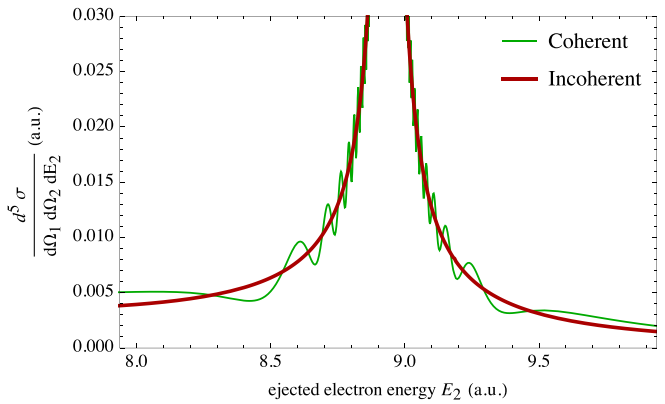

FIG. 11. (Color online) The FDCS coherently and incoherently combined amplitudes for ionization of H by 500-eV positrons in the forward direction ($\theta_1 = \theta_2 = 0$) in the vicinity of the equal-energy-sharing point.

Note that performing a similar investigation using the two-center close-coupling approach does not seem feasible at this stage. This is due to the fact that in this approach the amplitude for PFC emerges in a different set of variables than the DI amplitude. Therefore, before they can be combined, the PFC amplitude should be transformed into the variables of the direct channel. This multidimensional variable transformation is performed numerically and requires too many pseudostates to get the energy mesh fine enough to pick up the oscillations in the TDCS when the latter is calculated coherently. An advantage of the Born approach is that here the aforementioned variable transformation becomes straightforward.

Our convergent close-coupling calculations of the total cross section in positron-atom collisions using a single-center and different types of two-center bases show that the optical theorem, the fundamental principle of scattering theory, is satisfied regardless of the basis type used, provided the results are convergent [23]. In other words, the close-coupling formalism appears to preserve the unitarity when it is taken to convergence for any type of the basis used in expansion despite the two-center bases being overcomplete. This suggests that when channels are closely coupled oscillations in the coherent cross sections seen in the present work may somewhat decrease. However, the extent to which the difference between the coherent and incoherent cross sections would reduce, if it does at all, remains to be seen. Should this difference disappear completely, justifying exactly the same result we are getting for the grand total cross section [23] or is there some more intricate mechanism involved? As far as differential cross sections are concerned, implications of the overcomplete expansions customarily employed in multicenter problems have not been explored in the literature. We are working on this problem. The current work is just a step in this direction.

The results presented in this work pave the way to a nonperturbative two-center coupled-channel approach to a fully differential breakup problem in an arbitrary many-particle system which then can also address the aforementioned controversies in the positron-induced ionization of He and H_2. This work is currently in progress.

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