Optical potential study of positron–hydrogen-atom scattering at intermediate energies

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In this work, we will provide the full details of the coupled-channels-optical method as applied to study positron scattering from atomic hydrogen at intermediate energies. An optical potential method for the continuum has been implemented within the close-coupling framework that includes both the positron-hydrogen and positronium-proton channels. Elastic, excitation, ionization, positronium formation, and total cross sections are reported and compared to other available theoretical and experimental data.

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I. INTRODUCTION

Optical potential methods have been widely used in studying electron scattering by atoms at intermediate energies. Of the various optical potential methods that have been developed, the coupled-channels-optical method (CCOM) of McCarthy and Stelbovics [1] has been extensively used to study electron scattering from a number of atomic systems with much success. In this paper, we report an implementation of the CCOM to study positron scattering from atomic hydrogen at intermediate energies within the close-coupling formalism of Mitroy [2] that handles the positron-hydrogen and the positronium (Ps) proton channels explicitly in the close-coupling expansion. Earlier implementations have not taken into account this aspect except for the work that attempted to include virtual Ps formation via an optical potential [3]. The CCOM has provided a unique way of treating the continuum effects, and has recently provided some interesting results for electron-impact excitation of He to the third excited state [4] and n = 3 excitation of ground-state hydrogen [5].

Recently, we reported on the implementation of the CCOM [6] in the close-coupling (CC) formalism of Mitroy [2] and showed interesting results for the ionization and Ps formations at some intermediate energy region. Theoretical investigations of positron-hydrogen scattering in the intermediate-energy regime is formidable, as the theoretical methods must include many discrete states and the continuum in a practical manner. In this respect, the $L^2$ method has been attempted by Kernoghan et al. [7] and Mitroy [8]. They used a large $L^2$ basis of hydrogen states (30 and 28 states, respectively) together with the Ps(1s), Ps(2s), and Ps(2p) states to study positron scattering by atomic H at intermediate energies. These calculations have been done in coordinate space [7] and momentum space [8], but in principle should be equivalent. Nevertheless, there are differences between these two studies in the calculation of various cross sections, especially in the calculation of the ionization cross sections. These could be explained by the fact that the CC(28,3) calculation [8] has not allowed for the f states in the close-coupling expansion.

Our main motivation for the present work is to study the effects of using the CCOM for the positron-hydrogen scattering system. There is a lack of theoretical studies at these energies as compared for those at the low-energy region [9–14], and any new exciting results would provide the necessary impetus for further theoretical and experimental endeavors.

II. THEORETICAL DETAILS

The full theoretical details of the close-coupling formulation of the positron-hydrogen atom scattering system can be found in [2]. Here, we provide the main outline of the CC method and the details of the optical potential method. The Schrödinger equation for the positron-hydrogen atom system is

$$\left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} - E\right) \Psi(r_1,r_2) = 0, \quad (1)$$

where $r_1, r_2$ is the coordinate of the electron and the positron with respect to the proton, respectively, $r_{12} = |r_1 - r_2|$ and E are the total energy of the three-body system. Equation (1) can be written by using the relative ($\rho$) and center-of-mass coordinates ($R$) for any positronium channels. The relation between the coordinates can be written as

$$\rho = r_1 - r_2, \quad R = \frac{1}{2}(r_1 + r_2)$$

$$r_1 = R + \frac{1}{2} \rho, \quad r_2 = R - \frac{1}{2} \rho.$$

Thus Eq. (1) can be written as

$$\left(-\frac{1}{4} \nabla_R^2 - \nabla_\rho^2 + \frac{1}{|R - \frac{1}{2} \rho|} - \frac{1}{|R + \frac{1}{2} \rho|} - E\right) \Psi(\rho,R) = 0. \quad (2)$$

The Jacobian for the transformation between the two coordinate systems is

$$\int d^3r_1 \int d^3r_2 = \int d^3\rho \int d^3R. \quad (3)$$

The expansion of the wave function using the close-coupling approximation is
\[ \Psi(r_1, r_2) = \sum_a \psi_a(r_1) F_a(r_2) + \sum_\beta \phi_\beta(\rho) G_\beta(R), \]  

(4)

where \( \psi_a \) is the hydrogenic state and \( \phi_\beta \) is the positronium state that satisfy the following conditions:

\[ \left\langle \psi_a(r_1) \left( -\frac{i}{\hbar} \nabla_1 - \frac{1}{r_1} - e_a \right) \psi_a(r_1) \right\rangle = 0, \]  

(5)

\[ \left\langle \phi_\beta(\rho) \left( -\frac{i}{\hbar} \nabla_\rho - \frac{1}{\rho} - e_\beta \right) \phi_\beta(\rho) \right\rangle = 0. \]  

(6)

By substituting Eqs. (5) and (6) into the Schrödinger equation (2) we obtain

\[ (E-H) \left( \sum_a \psi_a(r_1) F_a(r_2) + \sum_\beta \phi_\beta(\rho) G_\beta(R) \right) = 0, \]  

(7)

\[ (E-H) \left( \sum_a \psi_a(r_1) F_a(r_2) \right) + (E-H) \left( \sum_\beta \phi_\beta(\rho) G_\beta(R) \right) = 0, \]  

(8)

where the Hamiltonian \( H \) is defined as

\[ H = -\frac{i}{\hbar} \nabla_1^2 - \frac{i}{\hbar} \nabla_2^2 - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}. \]

By standard procedures, we obtain the following equations:

\[ (E + \frac{1}{\rho} \nabla_1^2 - e_a) F_a(r_2) = \sum_a \left( \psi_a \left( \frac{1}{r_2} - \frac{1}{r_{12}} \right) \psi_a \right) F_a(r_2) \]

\[ + \sum_\beta \left( \psi_a \left( (H-E) \right) \phi_\beta G_\beta \right), \]  

(9)

\[ (E + \frac{1}{\rho} \nabla_\rho^2 - e_\beta) G_\beta(R) = \sum_\beta \left( \phi_\beta \left( \frac{1}{r_2} - \frac{1}{r_1} \right) \phi_\beta \right) G_\beta(R) \]

\[ + \sum_a \left( \phi_\beta \left( (H-E) \right) \psi_a F_a \right). \]  

(10)

The momentum-space Lippmann-Schwinger equations for a positron with the momentum \( k \) incident on a hydrogen atom in state \( \psi_a \) are

\[ \langle k' \psi_{a'} | T | k \psi_a \rangle \]

\[ = \langle k' \psi_{a'} | V | k \psi_a \rangle \]

\[ + \sum_a \int d^3k'' \frac{\langle k' \psi_{a'} | V | k'' \psi_a \rangle \langle k'' \psi_a | T | k \psi_a \rangle}{(E^{++} - e_{a''} - \frac{1}{2}k''^2)} \]

\[ + \sum_\beta \int d^3k'' \frac{\langle k' \psi_{a'} | V | k'' \psi_\beta \rangle \langle k'' \psi_\beta | T | k \psi_a \rangle}{(E^{++} - e_{\beta''} - \frac{1}{2}k''^2)}. \]  

(11)

The optical potential \( V(Q) \) consists of a first-order static-exchange potential and a nonlocal complex polarization term. In principal, the effect of scattering into the neglected set \( Q \) of the reaction channel space is contained in the nonlocal polarization potential. The real and imaginary parts of the complex polarization potential describe virtual and real excitations of the \( Q \)-space channels, respectively. The set \( Q \) includes the target continuum channels and the remainder of the discrete channels that are not explicitly coupled in the coupled-channels calculation. The nonlocal potential is intractable, and thus we follow the localization procedure of McCarthy and Stelbovics [1].

In the present work, we are attempting to incorporate the local polarization potential into a coupled-channels calculation for \( e^+ - H \) scattering. Here we briefly discuss the approximations and numerical techniques that are used in evaluating the polarization potential for the continuum using the momentum representation. The polarization potentials for discrete excitations are omitted since these channels may be included in a practical coupled-channels calculation. The details of the approximations can be found elsewhere [1,15].

Using the Feshbach formalism, the projection operators \( P \) and \( Q \) can be used to decompose the whole space of the target wave function into a subspace of wave function \( P \Psi \). The state in \( P \) space is a finite set that includes the ground state.

The projection operators are defined as

\[ P = \sum_{a \in P} | \psi_a \rangle \langle \psi_a |, \]  

(13)

\[ Q = 1 - P. \]  

(14)

In principle, expansion (13) should include the Ps states \( | \phi_\beta \rangle \langle \phi_\beta | \). Here we have neglected it and use the optical potential approach to allow only for the discrete states and the continuum of \( H \). Using the Schrödinger operator \( E^+ - \nu = \nu \), we can write the Schrödinger equation of the scattering system as

\[ \sum_{a'} \langle \psi_a | P(E^+ - \nu)(P + Q) | \psi_{a'} \rangle F_{a'} = 0, \]  

(15)
\[ \sum_{\alpha'} \langle \psi_{\alpha'} \rangle P(E^+ - K - \nu) (P + Q) \big| \psi_{\alpha'} \rangle F_{\alpha'} \]

\[= \sum_{\alpha'} \langle \psi_{\alpha'} \rangle P(E^+ - K - \nu) P \big| \psi_{\alpha'} \rangle F_{\alpha'} + \sum_{\alpha'} \langle \psi_{\alpha'} \rangle P(E^+ - K) Q \big| \psi_{\alpha'} \rangle F_{\alpha'} + \sum_{\alpha'} \langle \psi_{\alpha'} \rangle P \nu Q \big| \psi_{\alpha'} \rangle F_{\alpha'}. \] (16)

In this case, \( \nu = \nu_1 + \nu_2 + \nu_3 \) is the total potential, where \( \nu_1 \) and \( \nu_2 \) is the potential between the incident positron and the target electron with the core, respectively, while \( \nu_3 \) is the positron-electron potential considered. Using the various properties of the projection operators and other standard procedures, we obtain

\[ P(E^+ - K - \nu) P \psi = P(\nu_1 + \nu_3) Q \big[ (Q(E^+ - K - \nu) Q \big]^{-1} \times Q(\nu_1 + \nu_3) P \psi. \] (17)

\[ P(E^+ - K - \nu_2) P \psi = P(\nu_1 + \nu_3) P \psi + P(\nu_1 + \nu_3) Q \big[ (Q(E^+ - K - \nu_2) Q \big]^{-1} \times Q(\nu_1 + \nu_3) P \psi. \] (18)

From Eq. (18), we can define the optical potential \( V^{(\nu)} \) as

\[ V^{(\nu)} = (\nu_1 + \nu_3) + (\nu_1 + \nu_3) Q \big[ (Q(E^+ - K - \nu) Q \big]^{-1} \times Q(\nu_1 + \nu_3). \] (19)

By letting \( V = (\nu_1 + \nu_3) \), since the potential \( \nu_2 \) does not connect \( P \) and \( Q \) space, we simplify Eq. (19) as

\[ V^{(\nu)} = V + \nu Q \big[ (Q(E^+ - K - \nu) Q \big]^{-1} \times Q(\nu_1 + \nu_3). \] (20)

The second term of Eq. (19) is called the complex polarization term. So Eq. (20) can be simplified as

\[ V^{(\nu)} = V + W^{(\nu)}. \] (21)

The Green function can be written in detail, by making a spectral representation as discussed by Faddeev [16], and it is given as

\[ \frac{1}{Q(E^+ - K - \nu) Q} = \sum_{\nu} \frac{1}{E^{\nu+1} - E_{\nu}} \langle \Psi^{(-1)}_{\nu} \big| Q \rangle. \] (22)

The spectral index \( \nu \) is a discrete notation for the continuum. It defines the asymptotic partition of the three-body system into bound or ionized states and specifies the quantum numbers and momenta within each partition. We make the approximation that Green’s function is diagonal in \( Q \) space. The minimum requirement for this is that \( \nu_3 \) be diagonal in \( Q \) space, as it is, for example, if the state vectors of \( Q \) space are plane waves.

Using the representation of \( Q \) and the spectral expansion of Green’s function, the momentum space representation of the polarization can be written as

\[ W_{\alpha \alpha'}(k, k') = \langle k \alpha | W^{(\nu)} | \alpha' k' \rangle \]

\[= \int dq \sum_{m, l, l'} \langle k \alpha | V | l \rangle \times \langle l | \Psi^{(-)}_{m} \rangle (E^{(+)} - E_{\alpha})^{-1} \times \langle \Psi^{(-)}_{m} | l' \rangle \langle l' | V | \alpha' k' \rangle, \] (23)

where \( \Psi^{(-)}_{m} \) is the three-body wave function for ingoing spherical-wave boundary conditions. By using the weak-coupling approximation \[1\], in which Green’s function of Eq. (23) is diagonal in \( Q \) space and denotes the overlap \( \langle l | \Psi^{(-)}_{m} \rangle \) by distorted wave \( \chi^{(-)}_l \), the polarization potential becomes

\[ W_{\alpha \alpha'}(k, k') = \int dq \sum_{l \in \Omega} \langle k \alpha | V | \chi^{(-)}_l \rangle \frac{1}{E - \frac{i}{2} \frac{1}{q^2}} \times \langle \chi^{(-)}_l \big| V \big| \alpha' k' \rangle. \] (24)

For the target continuum, the summation \( \Sigma_{l} \) is replaced by \( \int dq' \), where \( q' \) is the momentum of the ionized electron. In calculating the polarization potential for the continuum \( W_c \), we use the extreme screening approximation \[15,17\] in which the full Coulomb wave \( \psi^{(-)} \) is used for the slower positron or electron and a plane wave for the faster one. This is represented as

\[ |l\rangle = |\psi^{(-)}(q')\rangle, \quad |\chi^{(-)}_l \rangle = |q\rangle, \quad q \geq q', \]

\[ |l\rangle = |q'\rangle, \quad |\chi^{(-)}_l \rangle = |\psi^{(-)}(q)\rangle, \quad q < q'. \] (25)

Then the continuum potential can be written as

\[ W_c = \int dq \int dq' \langle k \alpha | v_3 | q \rangle \psi^{(-)}(q) \frac{1}{E^+ - \frac{i}{2} (q^2 + q'^2)} \times \langle \psi^{(-)}(q) | q \rangle | v_3 \rangle \alpha' k', \] (26)

where we have dropped the terms in \( v_1 \) as they correspond to heavy-particle knockout, which is a minor effect \[18\].

The approximation (25) is sometimes referred to as the Born-Oppenheimer (BO) approximation. This approximation is justified on the basis of the ability of the optical model to calculate ionization cross sections that are in reasonable agreement with experimental data. The total ionization cross section is related to the polarization potential for the continuum \[17\] by

\[ \sigma_1 = \frac{2}{k} (2 \pi)^3 Z(0), \] (27)

where \( k \) is the momentum of the incident positron and \( Z(0) \) is the imaginary part of the polarization potential \( W_c \) when \( |k_i| = |k_f| \) and \( i = f = 1 s \) for the \( e^+ - H \) case. Hence the continuum optical potential can be written as \( W_c = U + iZ \).
Schwinger equations for $e^+\text{-}H$ scattering has been well detailed in [1]. Minor modifications are needed to implement it for the $e^+\text{-}H$ case [2,21].

### III. Results and Discussions

The following calculations were performed. Here we use the CCO$(m,n)$ to denote the CCOM calculations that were performed.

(i) CC(3,3): This close-coupling calculation includes the hydrogen states $H(1s)$, $H(2s)$, $H(2p)$ together with the positronium states $Ps(1s)$, $Ps(2s)$, and $Ps(2p)$.

(ii) CCO(3,3): In this calculation, the six states in (i) are used together with the continuum optical potentials in the 1s-1s, 1s-2s, 1s-2p, 2s-2s, 2s-2p, and 2p-2p couplings.

(iii) CC(6,3): This model is similar to CC(3,3) with the H basis states expanded to allow the $n=3[H(3s), H(3p), H(3d)]$ states.

(iv) CCO(6,3): The nine states are used with the continuum optical potentials in the 1s-1s, 1s-2s, 1s-2p, 2s-2s, 2s-2p, and 2p-2p couplings. Our calculations were done in the energy regime of 30–200 eV. Due to the time consuming nature, it was not possible to include the rearrangement kernel for all partial waves. The rearrangement matrix elements become extremely difficult to handle as $J$ increases [21]. In general, we allowed the Ps matrix elements for $J=\pm22$ and the Lippmann-Schwinger (LS) equations were solved. For $23\leq J\leq 50$, the LS equations were solved without the Ps matrix elements. For $J \geq 50$, we used the unitarized Born approximation [UBA(3,3)] model (which is naturally obtained from the Lippmann-Schwinger equations by discarding the off-shell part of the channel-free functions). In the CCO$(m,n)$ calculations, the continuum optical potentials were allowed for 0 $\leq J\leq 22$. The numerical techniques that were used to solve the LS integral equations are well documented [1,2,21]. In all the calculations reported here, we have used modifications suggested by Ratnavelu et al. [21] to perform the Gaussian integrations with a five-panel composite mesh. A quadrature mesh of 68 points was used for all the calculations.

#### A. Consistency of the CCO$(m,n)$ Calculations

The present work reports the implementation of the continuum optical potential in the close-coupling calculation of Mitroy [2] to study $e^+\text{-}H$ scattering. Furthermore, we have attempted to treat the optical potential only for the $e^+\text{-}H$ channels. In this section, we evaluate the consistency of our present calculations by studying partial-wave cross sections at 50 and 100 eV.

#### 1. 50 eV

In Figs. 2(a)–2(c), we depict the partial-wave cross sections for the elastic $H(1s\rightarrow1s)$, $H(1s\rightarrow2s)$, and $H(1s\rightarrow2p)$ transitions, respectively, at 50 eV. In the elastic case, we find that all models show convergence for $J\geq 2$. For $J = 0, 1, 2$, we find that the continuum potentials tend to decrease the cross sections quite significantly from the pure close-coupling calculations. Even for the low partial-waves, the convergence between CCO(6,3) and CCO(3,3) is good except at $J=0$ (where the difference is only minor).
In the H(1s→2s) transition, the convergence between all the models is observed for J > 4. The structure at J = 2 observed in the CC(6,3) and CC(3,3) models is enhanced very significantly with the use of optical potentials. The internal consistency of the CCO(m,n) calculations are excellent for all partial waves except probably at J = 0. The effect of the continuum has been to enhance the partial-wave cross sections for J = 1 and 2.

For the H(1s→2p) transition, we see a "two-band" qualitative shape. In the higher band, we find CC(6,3) and CC(3,3) showing their internal consistencies. In the lower band, we observe the CCO(6,3) and CCO(3,3) cross sections showing convergence. The qualitative shape is never distorted by using the optical potential approach (this point is vital for our later discussion). The continuum optical potentials tend to decrease the 1s-2p cross sections systematically. In studying all three transitions, we have seen that the qualitative shapes are not affected by the use of continuum optical potential calculations [CCO(6,3) and CCO(3,3)].

2. 100 eV

In Figs. 3(a)–3(c), we show the partial-wave cross sections for the elastic H(1s→1s), H(1s→2s), and H(1s→2p) transitions at 100 eV. As in the 50-eV case, similar trends are observed for the elastic case. In the H(1s→2s) case, the structure at J = 2 in the CC(6,3) and CC(3,3) mod-
els are confirmed with the CCO(6,3) and CCO(3,3) models. Unlike for the 50-eV case, the optical potential reduces the cross sections. The convergence also occurs only at larger $J>8$.

The H($1s \rightarrow 2p$) transition also shows similar trends observed at 50 eV. The CCO(6,3) and CCO(3,3) models also tend to decrease the cross sections. By studying these two different energies to reflect the energy spectrum investigated, we find no abnormalities in the present CCO(6,3) and CCO(3,3) calculations. This provides a useful gauge of the correctness and consistency of the present CCO($m,n$) calculations.

B. Elastic and excited cross sections for the H($1s$) entrance channel

In Fig. 4(a), our present elastic cross sections are compared with the cross sections calculated by the CC(28,3) and the CC(30,3) models. We also depict the single-center convergent close-coupling (CCC) cross sections of Bray and Stelbovics [22].

The pure close-coupling models of CC(6,3) and CC(3,3) show the slow convergence in using just physical states of H at intermediate energies. The significant effects of the continuum optical potentials are very visible for all energies studied. The cross sections are reduced by as much as 20–30% at intermediate energies of $E<100$ eV. Below 40 eV, the CCO(6,3) and CCO(3,3) models predict larger cross sections than those of the CC(6,3) and CC(3,3). This sudden change in the systematic agreement at other energies might suggest that the validity of continuum optical potentials at low intermediate energies such as those at 30 eV is questionable. The approximations used to calculate the continuum optical potentials are of high-energy types and its validity at low intermediate energies of 30 eV may be compromised.

The $L^2$ calculations predict larger cross sections than the CCO models for the region studied except for those below 50 eV. Furthermore, below this energy label, the $L^2$ calculations show significant differences between themselves. We also observe the unphysical bump at 70 eV for the CC(28,3) model. This raises the question of convergence between these two models. What is the qualitative shape of elastic cross sections? To help us further, we also show the CCC elastic cross sections that have used 34 states (10s, 9p, 8d, and 7f) of H. It may be a coincidence that the CCC (which excludes the Ps effects) shows only minor differences to the $L^2$ models [7,8]. Bray and Stelbovics [22] conclude in their work that their CCC is probably only valid for $E>100$ eV, where Ps effects become negligible. Except for the general qualitative trends, there is need for further convergence studies to describe the elastic cross sections. For $E>150$ eV, the CCO calculations are within 5–10% of the CCC values. The CCC may be valid at the higher energies but it has been shown [21] that the Ps still has some influence for $E<20$ Ry. In Fig. 4(b), the present H($1s \rightarrow 2s$) excitation cross section with the CC(28,3) and CC(30,3) models is depicted. Due to the unavailability of the CCC numbers for the $e^+\text{-H}$ case, we also show the $e^-\text{-H}$ cross sections [23].

In general, all the qualitative features are reproduced by the models. The unphysical bump that was observed for CC(28,3) in the elastic case now appears in the CCO(6,3) and CCO(3,3) models. Repeated runs with different mesh sets have not altered the structure. Mitroy [8] attributes this structure to the improper handling of the continuum. We are quite sure the continuum has been handled properly in the present work (reflected in our ionization cross sections). There may be some other underlying explanation for these structures. The continuum potentials have a lesser effect for this transition. The effect at 30 eV brings CCO(6,3) and CCO(3,3) to quantitative and qualitative agreement with the $L^2$ models. The CCC for the $e^-\text{-H}$ case is shown to provide
a comparison for high energies. As expected, the small differences between the present models and the CCC for $E > 150 \text{eV}$ support the view that at high energies the target does not distinguish the $e^-$ or the $e^+$. The minor differences may be attributed to the neglect of the Ps channels in the CCC model.

In Figure 4(c), the H($1s\cdot2p$) excitation cross sections are shown. We also depict the CCC cross sections for the $e^-\cdot H$ case. The effect of the continuum optical potential is quite significant and it systematically decreases the cross section over the whole range. Nevertheless, the qualitative shape of the CC(6,3) and CC(3,3) models is preserved by the CCO(6,3) and CCO(3,3) models. Our detailed consistency studies for 50 and 100 eV have shown that the qualitative shape has also been preserved for the partial cross sections studied in the $1s\cdot2p$ transition.

The differences between the present CCO works and the CC(28,3) and CC(30,3) works for $E < 70 \text{eV}$ are very dramatic. The "shoulder" in the cross section is only observed at lower energies for the $L^2$ calculation. The differences between the CC(28,3) and the CC(30,3) are minor at $E > 70 \text{eV}$ but show different qualitative and quantitative features for $E < 70 \text{eV}$, especially in the prediction of the "shoulder." The CC(28,3) model shows the feature at about 50 eV while in the CC(30,3) model it appears at about 40 eV. Below 40 eV, both these calculations show vast differences. Is this the reflection of the poor convergence of the $L^2$ methods? In fact, if the two models have not converged we would see the differences at higher energies rather that at low energies. Is there an underlying explanation for these differences? To provide an insight at the $1s\cdot2p$ mechanism, we are only able to show the CCC cross sections for the corresponding electron-hydrogen atom scattering (as the CCC values for the positron-H case are unavailable). These cross sections are about the same magnitude as the positron case. We also have a similar qualitative shape in the electron case with a broad shoulder appearing at about 35–50 eV. This suggests a similar physical mechanism underlies the $1s\cdot2p$ excitation of the H by positron or electron impact. The CCC cross sections show the same magnitude as the CCO models. The electron-H cross sections and the CCC positron-H cross sections show differences of about 2–5% at higher energies $E > 100 \text{eV}$.

### C. Positronium (Ps) formation cross sections

The present Ps formation cross sections in the Ps($1s$), Ps($2s$), and Ps($2p$) states are shown in Figs. 5(a)–5(c), respectively. The CC(28,3) cross section is also shown.

All the theoretical models predict the same qualitative shape for Ps($1s$) formation cross sections. In comparing the CC(6,3) and CC(3,3), we can visibly observe differences for $E < 40$. The inclusion of the $n=3$ states reduces the cross sections slightly at these energies. The continuum optical potentials also reduce the cross sections systematically for $E < 80 \text{eV}$. The differences between CCO(6,3) and CCO(3,3) with CC(28,3) are largest (about 10–15%) for $E > 40 \text{eV}$. The differences are smaller for higher energies and seem to converge for $E > 100 \text{eV}$. All the present calculations for the Ps($2s$) formation cross sections predict a similar qualitative shape with a sharp peak at about 40 eV. The magnitude of the peak is reduced with inclusion of the $n=3$ states. It is further reduced with the use of the continuum optical potentials. The differences between the CCO(6,3) and CCO(3,3) with the CC(28,3) are quite large for all the energies studied. The CCO(6,3), CCO(3,3), and CC(6,3) and CC(3,3) converge only for $E > 90 \text{eV}$. It is interesting to see that the differences with CC(28,3) are still significant for $E > 90 \text{eV}$. The Ps($2s$) cross sections of Kernoghan et al. [7] are also shown. We also observe a peak at about 30 eV. Is there a maximum in the Ps($2s$) cross sections? The present

![Image](image.png)

**FIG. 5.** Ps formation cross sections in (a) Ps ($1s$), (b) Ps ($2s$), (c) Ps ($2p$). The legend is the same as in Fig. 4 except CC(6,3) (---), CC(3,3) (-----), and CC(28,3) (----).
models and the CC(30,3) seem to show the structure that is absent in the CC(28,3) work.

The qualitative shape of the Ps(2p) formation cross sections is predicted by all the theoretical models. The differences shown by the various calculations resemble the similar situation as in the Ps(1s) formation. We also note that the Ps formation in the Ps(2p) state is about a factor of 10 smaller than the other transitions at \( E = 30 \text{ eV} \). The differences between the CC(28,3) and the CCO(6,3) are quite large (about 20–30\% for \( E < 50 \text{ eV} \). For large energies, all the models converge.

In Fig. 6, we show the total Ps formation cross sections. The experimental measurements of Weber et al. [20] and the “best” measurement of Zhou et al. [24] are shown with the CC(28,3), CC(30,3), CCO(6,3), CCO(3,3), CC(6,3), and the CC(3,3) models. We have not shown the lower limit measurements of Zhou et al. [24] as they will clutter our graph. All our calculations only allow for the \( n = 2 \) Ps states; thus to calculate the total Ps formation cross sections, we have to use a scaling law of \( 1/n^3 \) for \( n \geq 3 \) [8]. The total Ps cross sections are calculated by

\[
\sigma_{\text{Ps,Total}} = \sigma_{\text{Ps}(1s)} + 1.6(\sigma_{\text{Ps}(2s)} + \sigma_{\text{Ps}(2p)}).
\]

The present CCO(6,3) and CCO(3,3) cross sections lie above the CC(28,3) calculation. The qualitative features of the total Ps formation cross sections are reproduced quite well by all the theories. The present data are within the experimental error bars of those of Weber et al. [20] but slightly above the latest measurement for \( E < 50 \text{ eV} \). The CC(30,3) data of Kernoghan et al. [7] are much lower than all other calculations but in good agreement with the “best” data of Zhou et al. [24] The effects of the continuum optical potential are clearly seen by comparing the CCO(3,3) and the CCO(6,3) with the CC(3,3) and CO(6,3), respectively.

**D. Ionization cross sections**

In Fig. 7, we show the ionization cross sections calculated with the CCO(3,3) and CCO(6,3) together with the CC(28,3) and CC(30,3) models. We also depict the ionization cross sections of Ratnavelu [15]. The present CCO(3,3) and CCO(6,3) confirm the qualitative and quantitative features of the continuum optical potential of Ratnavelu. This provides an indirect test that the continuum optical potential has been accurately incorporated in the present method. The present models also show excellent agreement with the UCL data from 30 eV onward. The lack of convergence of the \( L^2 \) calculations also suggests that further convergence studies must be done to explain the quantitative differences that exist between these two calculations at intermediate energies. Our calculations demonstrate that the CCO(3,3) and CCO(6,3) have converged over most of the energies. The inevitable question is now to reduce the experimental error bars so as to provide a much more discriminating test for theories.

**E. Total cross sections**

The total cross sections for the present models are shown together with the CC(28,3) and CC(30,3) in Fig. 8. The latest measurements of Zhou et al. [24] are also shown. The
CC(28,3) and CC(30,3) lie within the experimental error bars and do not show any disagreement with the experiments. The present models lie just below the lower bounds of the experimental data for $E<60$ eV. We observe that incorporating the $n = 3$ discrete states of H in the CCO(6,3) model enhances the cross sections from the CCO(3,3) model. It is also gratifying to see that the present CCO(6,3) cross sections are within 10–15% of the experiment and other theories for $E>60$ eV. The effect of the continuum optical potentials can be ascertained by comparing the CCO(6,3) and CCO(3,3) calculations with the corresponding CC(6,3) and CC(3,3) models.

IV. CONCLUSIONS

In summary, we have done an ab initio optical potential treatment of positron scattering from atomic hydrogen at intermediate energies. The continuum optical potential that has been implemented in our CCO(6,3) and CCO(3,3) models seems to be adequate to describe the ionization, total, and Ps formation cross sections. We have shown that the use of optical potentials in our CC calculation technique is comparable to some extent to the works of Mitroy [8] and Kernoghan et al. [7]. We believe that a definitive work may still be yet to be done in the large-basis $L^3$ method studies of the positron-hydrogen atom scattering system at intermediate energies. We also believe that a larger CCO should be attempted to study the convergence of the present method in the calculations of the various cross sections. Further theoretical studies as well as experimental measurements are also very desirable.

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