# Momentum-space coupled-channel calculation for positron-helium scattering

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The momentum-space coupled-channel optical method has been applied to positron-helium scattering. The ionization continuum and the positronium formation channels are included via a complex equivalent-local optical potential. The positronium formation cross sections at the energy range from the threshold to 400 eV and the total scattering cross sections at the energies from 17 to 500 eV are reported and compared with available experimental measurements and theoretical calculations. The agreements between the present results and the corresponding measurements are satisfactory.

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# I. INTRODUCTION

Study of positron collision with atoms and molecules is a fundamental interesting topic. It can offer a new way to test our understanding of the basic interactions in many-body systems due to its unique features. The most important factor contributing to these features is the rearrangement process, namely, the positronium formation. This process is a twocenter problem, which presents a challenge to theoretical treatments. The positron impact ionization of atoms is another important process in the field of positron-atom collision. The breakup channel exhibits difficulties for manybody scattering theory coupled with the special problem of the long range of the Coulomb interaction. The overall scattering process includes all of the accessible channels and illustrates the significant features. The total scattering cross section provides a testing ground for both theory and experiment for positron scattering by atoms.

Helium atom, the simplest many-electron atom, is an ideal target for experimental and theoretical studies. The positronhelium scattering has the essential features that there is a significant ionization cross section and the positronium formation process plays a very important role. Ionization continuum and positronium formation channels are expected to contribute a large fraction of the total cross section for positron scattering. Study of positron collision with helium is a very sensitive test for theoretical methods. A number of experimental and theoretical activities on the studies of ionization, positronium formation, target excitation, and overall scattering processes in positron-helium scattering have been performed in the past two decades.

Measurements of the total cross sections of positronhelium scattering have been carried out by Stein *et al.* [1] at low impact energies and Kappila *et al.* [2] at medium and high energies. The single and direct ionization cross-section measurements have been performed by Fromme *et al.* [3], Mori and Sueoka [4], and Jacobsen *et al.* [5]. In recent years, detailed experimental studies of positron impact ionization have been complemented by Moxom *et al.* [6], Ashley *et al.* [7], and Murtagh *et al.* [8]. They have investigated various ionization processes: single, double, near-threshold triple, and total ionization. The experimental total positronium formation cross sections have been reported by Charlton *et al.* [9], Fornari *et al.* [10], Diana *et al.* [11], Fromme *et al.* [3], and Overton *et al.* [12]. Currently, Murtagh *et al.* [8] reported the total positronium formation cross sections for helium that were obtained by extracting from their measured total fragmentation cross sections.

On the theoretical side, McCarthy and Zhou [13] calculated the continuum contributions to positron scattering with helium via an equivalent local potential approximation. They gave the single and direct ionization cross sections from the threshold to 1 keV. Campeanu et al. [14] calculated the total ionization cross sections with a distorted wave approximation for positron impact energies 30-150 eV and Campbell et al. [15] calculated the ionization cross sections from the threshold to 150 eV with the pseudostate representation. Most recently, Wu et al. [16] presented the total fragmentation cross sections, i.e., the sum of positronium formation and single ionization cross sections, at energies from the first ionization threshold to 1 keV. The single-centered convergent close-coupling (CCC) method ([17]) has been applied in their calculation. In general, good agreements are found between theoretical calculations and experimental measurements.

Theoretical total cross sections for positronium formation have been calculated by Mandal *et al.* [18] using a distortedwave approximation at 24.5, 28, 40, 60, 100 eV, by Igarashi and Toshima [19] with the target continuum distorted-wave approach from 50 to 300 eV, by Schultz and Olson [20] with a classical trajectory Monte Carlo (CTMC) technique, by Sarkar *et al.* [21] in the high-energy second-order Born approximation from 100 to 2 keV, and by Hewitt *et al.* [22] using the one-electron model close-coupling approximation from 31.3 to 200 eV. Recently, a sophisticated close coupling calculation for the total cross sections of positronium formation has been performed by Campbell *et al.* [15] using a large number of basis states and pseudostates. The level of agreement of the positronium formation cross sections for helium with experimental measurements is less satisfactory.

For the total scattering cross sections in the positronhelium system, theoretical calculations have been carried out by several different approaches: the distorted-wave second Born approximation method of Dewangen and Walters [23], the optical model of Byron and Joachain [24], and the

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eikonal-Born series method of Byron [25]. These calculations are all at impact energies above 100 eV, and positronium formation and ionization channels have been omitted. Recently, two basis-dependent methods (Campbell *et al.* [15] and Wu *et al.* [16]) have been developed, in which the target continuum and the rearrangement channels are explicitly included by employing pseudostates. The total scattering cross sections have been calculated by Campbell *et al.* [15] with two different pseudostate expansion models. In the first model, 27 states including the first three positronium states have been used in their coupled state expansion, and in the second model, six f pseudostates have been added to the previous 24 s-, p-, and d-state expansion. Wu et al. [16] applied the single-centered convergent close-coupling method to calculate the positron-helium scattering cross sections with two different models [CCC(FC) and CCC(MC)] at the energies from the ionization threshold to 1 keV. In the CCC(FC) model, target structure has been constructed based on the frozen-core approximation, and in the CCC(MC) model, the ground state of helium has been represented in the multiconfiguration expansion.

In this paper, we use the momentum-space coupledchannel optical (CCO) method [26] to study positron-helium collision at energies from the positronium formation threshold to 1 keV. In this method, a complex equivalent local potential is employed to describe the two-body positronium formation channels and the three-body ionization continuum. This method has been applied to calculate various scattering cross sections in positron-hydrogen, positron-alkali metals, and positron-magnesium systems [26–29]. The agreements between these results and available theoretical calculation results, as well as the experimental data, are satisfactory. In the present work, the present results of positronium formation cross sections and total scattering cross sections are reported.

### **II. THEORETICAL DETAILS**

The total scattering cross section is calculated by solving the momentum-space coupled-channel optical equation as follows:

$$\langle \mathbf{k}, \Phi_i | T | \Phi_0, \mathbf{k}_0 \rangle$$
  
=  $\langle \mathbf{k}, \Phi_i | V^{(Q)} | \Phi_0, \mathbf{k}_0 \rangle + \sum_{j \in P} \int d^3 \mathbf{k}' \langle \mathbf{k}, \Phi_i | V^{(Q)} | \Phi_j, \mathbf{k}' \rangle$   
 $\times \frac{1}{E^+ - \epsilon_j - \frac{1}{2} k'^2} \langle \mathbf{k}', \Phi_j | T | \Phi_0, \mathbf{k}_0 \rangle.$  (1)

Here the space of the target state has been split into two parts. The *P* space consists of all the discrete states  $\Phi_j$  including the ground state  $\Phi_0$ . The *Q* space includes target ionization continuum and positronium formation channels. Sufficient *P*-space states are included for convergence.

The optical potential  $V^{(Q)}$  is the channel-coupling potential V plus a complex polarization potential  $W^{(Q)}$  as follows:

$$W^{(Q)} = W_I^{(Q)} + W_{P_s}^{(Q)}, \tag{2}$$

where  $W_I^{(Q)}$  and  $W_{Ps}^{(Q)}$  stand for the parts of the polarization potential that describe the ionization continuum and the positronium formation process, respectively. The form used here for the matrix element of the polarization potential is given as

$$\langle \mathbf{k}' i | W^{(Q)} | j \mathbf{k} \rangle = \sum_{n \in Q} \langle \mathbf{k}' i | V | \Psi_n^{(-)} \rangle \frac{1}{E^{(+)} - E_n} \langle \Psi_n^{(-)} | V | j \mathbf{k} \rangle,$$
(3)

where  $\Psi_n^{(-)}$  represents the time reverse of the exact state vector for a reaction starting in channel *n*. The notation *n* is a discrete notation for the three-body ionization continuum or the two-body positronium formation channel. Spin dependence is implicit in the notation. For ionization, the model used is

$$|\Psi_n^{(-)}\rangle = |c\psi^{-}(\mathbf{q}_{<}), \mathbf{q}_{>}\rangle.$$
(4)

 $\mathbf{q}_{>}$  and  $\mathbf{q}_{<}$  are the greater and lesser, respectively, of the absolute momenta of the outgoing particles. The ionization continuum is described in the independent-particle model, where *c* is the remaining core and  $\langle \mathbf{r} | \psi^{-}(\mathbf{q}_{<}) \rangle$  is a Coulomb wave orthogonalized to the orbital from which the electron is removed.  $\langle \mathbf{r} | \mathbf{q}_{>} \rangle$  is a plane wave.

The model used for positronium formation is

$$|\Psi_n^{(-)}\rangle = \Phi_\mu(\mathbf{k}_{ps}, \mathbf{R}, \mathbf{r}) = \phi_\mu e^{i\mathbf{k}_{ps}\cdot\mathbf{R}},\tag{5}$$

where  $\phi_{\mu}$  is the bound state of the positronium and  $\mathbf{k}_{ps}$  is the momentum of the positronium center of mass. The plane wave  $\langle \mathbf{R} | \mathbf{k}_{ps} \rangle$  represents the motion of the positronium, since only short-range terms in the positronium-ion potential survive. The notation *n* is a discrete notation for the two-body positronium formation channel. **r** in Eq. (5) is the relative coordinate as follows:

$$\mathbf{r} = \mathbf{r}_p - \mathbf{r}_e,\tag{6}$$

where  $\mathbf{r}_p$  and  $\mathbf{r}_e$  are the coordinates of the positron and the electron respectively, and **R** is the coordinate of the positronium center of mass,

$$\mathbf{R} = \frac{1}{2} (\mathbf{r}_p + \mathbf{r}_e). \tag{7}$$

The optical potential matrix element for positronium formation is

$$\langle \mathbf{k}' i | W_{Ps}^{(Q)} | j \mathbf{k} \rangle = \sum_{n} \langle \mathbf{k}' i | V | \widetilde{\chi}_{n}^{(-)} \rangle \frac{1}{E^{(+)} - E_{n}} \langle \widetilde{\chi}_{n}^{(-)} | V | j \mathbf{k} \rangle, \quad (8)$$

$$|\tilde{\chi}_{n}^{(-)}\rangle = (1 - |\psi_{i}\rangle\langle\psi_{i}|)|\Psi_{n}^{(-)}\rangle, \qquad (9)$$

where  $|\Psi_n^{(-)}\rangle$  is orthogonalized to the ground state of helium  $|\psi_i\rangle$ , from which the electron is captured, and

$$(\varepsilon_i - H_T) |\psi_i\rangle = 0. \tag{10}$$

Here,  $H_T$  is the target Hamiltonian. The independent-particle model has been used for calculating the positronium forma-

tion optical potential matrix element.  $|\psi_i\rangle$  is represented by a Hartree-Fock wave function and expanded by STO's bases. The amplitude of the positronium formation potential has been calculated by using the numerical method of Cheshire [30].

An equivalent-local approximation has been made for the whole polarization potential for computational feasibility. The polarization potential matrix element is calculated with about ten points in the variable K, where

$$K = |\mathbf{k} - \mathbf{k}'|, \tag{11}$$

$$\frac{1}{2}k^2 = E - \epsilon_0, \qquad (12)$$

$$\frac{1}{4}K_{ps}^2 + \epsilon_{ps} = \frac{1}{2}k^2 + \epsilon_0.$$
(13)

This is achieved by an angular-momentum projection,

$$\langle \mathbf{k}' i | W^{(Q)} | j \mathbf{k} \rangle = \sum_{l''m''} C_{l'l'l''}^{m'm''m} U_{l'l''l}(K) Y_{l''m''}(\hat{\mathbf{K}}), \quad (14)$$

where

$$U_{l'l''}(K) = \sum_{m'm''} C_{l'l''l}^{m'm''m} \int d\hat{\mathbf{k}} \langle \mathbf{k}' i | W^{(Q)} | j \mathbf{k} \rangle i^{-l''} Y_{l''m''}(\hat{\mathbf{K}}).$$
(15)

A cubic spline interpolation is used for a general value of K. The equivalent-local potential is calculated by a multidimensional method using Cartesian momentum variables (McCarthy and Stelbovics [31]). The real part of the potential involves virtual excitation into Q space and the virtually formed positronium bound states. The imaginary part describes real excitation of continuum and the formation of positronium bound states. A simple estimate of the cross section of ionization (direct ionization) is given by approximating the entrance channel T-matrix element of Eq. (1) by its driving term, instead of solving the coupled-channel equations. This result is

$$\sigma_I = \frac{2}{k} (2\pi)^3 \operatorname{Im} \langle \mathbf{k} 0 | W_I^{(Q)} | 0 \mathbf{k} \rangle.$$
 (16)

The total cross section for the positronium formation is

$$\sigma_{ps} = \frac{2}{k} (2\pi)^3 \operatorname{Im} \langle \mathbf{k} 0 | W_{ps}^Q | 0 \mathbf{k} \rangle, \qquad (17)$$

where  $|0\rangle$  stands for the ground state of the target.

### **III. RESULTS AND DISCUSSIONS**

In the present calculation, the *P* space consists of nine channels: 1, 2, 3, 4  ${}^{1}S$ ; 2, 3, 4  ${}^{1}P$ ; 3, 4  ${}^{1}D$ . The optical potentials describing the target continuum are in the channel couplings 1  ${}^{1}S-1$   ${}^{1}S$ , 1  ${}^{1}S-2$   ${}^{1}S$ , 1  ${}^{1}S-2$   ${}^{1}S$ , 1  ${}^{1}S-2$   ${}^{1}P$ , 2  ${}^{1}P$  -2  ${}^{1}P$ . The optical potentials for positronium formation in its n=1 and n=2 states are included in the channel coupling



FIG. 1. The present calculation of the positronium formation cross section is compared with available experimental data.

 $1 {}^{1}S - 1 {}^{1}S$ . Target bound states are represented by configuration-interaction (CI) wave functions. The basis used in the CI representation of these states consists of nine orbitals, namely, 1, 2, 3, 4s; 2, 3, 4p; 3, 4d, and the pseudo-orbitals  $\overline{s}$ ,  $\overline{p}$ ,  $\overline{d}$  [32].

We test the description of the two-body rearrangement channels by comparing the present total cross sections of positronium formation with available experimental measurements and theoretical calculations at the impact energy region from the positronium formation threshold to 300 eV in Figs. 1–3.

In Fig. 1, we display the comparison between the present total positronium formation cross section and available measurement data. From this figure, good agreement can be found between the present total positronium formation cross sections and most of the experimental data in both magnitude and shape in the whole energy region that we calculated, except for the discrepancies with the data of Fromme *et al.* [3] and Diana *et al.* [11] from 80 to 250 eV, where their results are higher than the present results and other measurement results.

In Fig. 2, the present total positronium formation cross sections for helium are compared with other theoretical calculation results: the distorted-wave approximation (DWA) calculations of Mandal *et al.* [18], the results of Schultz and Olson [20] using the classical-trajectory Monte Carlo (CTMC) technique, the close-coupling approximation calculations of Hewitt *et al.* [22] and Campbell *et al.* [15], and the



FIG. 2. The present positronium formation cross section is compared with the available theoretical calculations.



FIG. 3. The present positronium formation cross section is compared with the experimental data and the theoretical results at the low energy.

target continuum distorted-wave approximation calculations of Igarashi and Toshima [19]. Although all the calculations tend to merge above 100 eV, there are significant discrepancies under 100 eV. The results of Igarashi and Toshima [19] are a little lower than the present results. The results of Schultz and Olson [20] produced data well at high energies but overestimated the experimental data elsewhere. The close-coupling calculations of Hewitt et al. [22] agree well with the experimental data between 80 and 140 eV but are significantly smaller below 80 eV. Under 30 eV, the calculations of Campbell et al. [15], in which a large number of basis states and pseudostates are employed, have underestimated the experimental data. From Figs. 1 and 2, we can see that the present results are closer to the experimental data than other theoretical results. A noteworthy feature is that almost all the theoretical results get peak values at the energy, which is about 5-10 eV lower than the experimental measurements, except that the present results arrive at the maximum at 70 eV, which is very close to the experimental data.

We note that all the theoretical results mentioned above are at impact energies that are higher than 22 eV. The interaction of a low-energy positron with many-electron atoms is characterized by strong correlation effects. A low-energy positronium formation cross section provides a sensitive test for theoretical treatments. The present positronium formation cross sections in the energy region from the positronium formation threshold to 22 eV are displayed in Fig. 3, along with the experimental data and the variational calculations of Van Reeth and Humberston [33]. From this figure, a good agreement can be found between the present results and the experimental data of Murtagh *et al.* [8]. In the calculations of Van Reeth and Humberston [33], they used very flexible trial functions, including many short-range terms, to represent the distortion of the target and the positronium. Their results are very similar to the present results and to the experimental measurements in the shape and just about 10% lower in the magnitude.

Another significant scattering process is the single direct ionization. A strict check for the description of the continuum is provided by comparing the present ionization cross sections with the experimental data and other theoretical calculations. This comparison has been made in the previous work of McCarthy and Zhou [13]. Here, we display the ion-



FIG. 4. The direct ionization cross section of McCarthy and Zhou [13] is compared with available experimental data.

ization cross sections compared with the latest experimental measurements and theoretical calculations in Figs. 4 and 5. The comparison with the experimental measurements is shown in Fig. 4. In general, a good agreement can be found with all of the experimental results in both shape and magnitude. The present ionization cross sections are close to the data of Mori and Sueoka [4] and Fromme *et al.* [3] from the ionization threshold to 200 eV, and a little higher than the data of Moxom *et al.* [6] and Ashley *et al.* [7] under 60 eV, which are renormalized to the electron impact ionization cross sections of Sorokin et al. [34] and Rejoub et al. [35]. The present ionization cross sections agree well with the data of Moxom et al. [6] from 200 to 1000 eV. The comparison with the available theoretical calculations is illustrated in Fig. 5. The present results are identical with the results of Basu *et al.* [36], particularly below 80 eV, and very close to the results of Campeanu *et al.* [14], which are obtained by a distorted-wave calculation. A disagreement exists between the present results and other theoretical results [15,20,37,38], including the pseudostates calculations of Campbell et al. [15], the results of Schultz and Olson [20] using the CTMC technique, the distorted-wave calculations of Moores [37] with close-coupled target states, and the coupled states calculations of Chen and Msezane [38].

The overall quality of the present description is tested by comparing the present total scattering cross sections with the experimental data [1,2,39] and other theoretical results including the results of Ashok Jain [40] and two different



FIG. 5. The direct ionization cross section of McCarthy and Zhou [13] is compared with the available theoretical results.



FIG. 6. The present calculation of the total cross section is compared with other experimental data and theoretical results.

close-coupling calculations (Campbell *et al.* [15] and Wu *et* al. [16]). The comparison is demonstrated in Fig. 6. The present results agree well with the measurement of Griffith et al. [39] and are a little lower than the data of Kauppila et al. [2] at 50–200 eV. In the close-coupling calculations of Wu et al. [16], two different models [CCC(FC) and CCC(MC)] are used. The CCC(FC) calculations and the 30-state calculations of Campbell et al. [15] overestimated the experimental measurements. The total cross sections of CCC(MC) calculations are systematically a little lower than the results of Kauppila *et al.* [2]. All of these calculations including ours are very similar to the experimental measurements on the behavior of energy dependence. However, significant disagreement exists in the position of the peak. The calculations of Campbell et al. [15] and Wu et al. [16] get their peak at about 60 eV, and the present results arrive at the peak around 40 eV, while the experimental measurements show the peak position at 50 eV. The disagreement between the present calculations and other theoretical calculations may be due to the

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different descriptions of the target continuum and positronium formation channels. In the calculations of Campbell *et al.* [15] and Wu *et al.* [16], where pseudostates are employed, the results are dependent on the size of pseudostates and the choice of their angular momenta. In the present calculation, a complex equivalent local potential has been employed to describe the two-body charge transfer process and the threebody continuum. In this optical potential model, only the single and direct ionization continuum has been included, while possible double ionization has been omitted. Although the single and direct ionization is the most important ionization process, the exclusion of double ionization, as well as the weak-coupling approximation and the equivalent-local approximation that are used in the present calculation, may lead to disagreement with the experimental data.

#### **IV. CONCLUSIONS**

The positron-helium scattering has been studied using the momentum-space coupled-channel optical (CCO) method. In the present calculations, a complex equivalent-local optical potential is developed to describe the positronium formation channel. The satisfactory agreement with the corresponding experiment measurements has demonstrated that the CCO method has some virtues as a tool to study positron scattering with atoms. Extensions of this method to positron scattering with many-electron atoms are straightforward.

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