Coupled-channel optical calculation for positron–lithium scattering*

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Positron scattering with atomic lithium is investigated by using a coupled-channel optical method. The ionization continuum and positronium formation channels are taken into account via a complex equivalent-local optical potential. The positronium formation cross sections and the ionization cross sections, as well as the total scattering cross sections, are reported at energies above 3 eV and compared with available experimental and theoretical data.

Keywords: positron, lithium, positronium, ionization

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1. Introduction

The study of positron collisions with atomic targets is a topic of special practical and fundamental interest. It can offer a new way to obtain the information of atomic structures and test our knowledge of the basic interactions in many-body systems. The understanding of positron interactions with atoms is also necessary for the development of many high-tech applications. The most important feature of positron–atom scattering is the appearance of the rearrangement process, namely the positronium (Ps) formation channel, which is a two-center problem and presents a particular challenge to both theoretical treatment and experimental measurement.

In this paper, we focus on the study of positron–lithium scattering, which has attracted considerable attention in the past decades. Atomic lithium has a relatively simple structure and can be viewed to a certain degree as approximately one-electron atoms. An important feature of positron–lithium system is that the Ps formation process is always expected to play a very important role at low and intermediate energies since the Ps formation is energetically possible even at zero energy. The exact treatment of this rearrangement process is therefore necessary for theoretical investigations.

In the early calculations performed by Sarkar *et al.*[1] and Ward *et al.*[2] in the close-coupling framework, the Ps formation channels were neglected and the predicted cross sections were thus preliminary. In 1991, Basu and Ghosh[3] carried out the calculations for positron–lithium system with the Ps channels included. However, only the Li(2s, 2p) and Ps(1s) states were included in the calculation. After that, a number of studies for positron–lithium scattering were performed with the Ps channels incorporated. The Ps process was investigated by Hewitt *et al.*[4] using a close-coupling method with the basis consisting of Li(2s, 3s, 2p, 3p) and Ps(1s, 2s, 2p) states, by Gianturco and Melissa[5] employing a model potential approach, and by Bhattacharyya and Talukdar[6] with a screened hydrogenic model. Acacia *et al.*[7] reported the ionization cross sections using the distorted-wave approximation. Walters and coworkers performed a series of studies[8−10] in the close-coupling framework with different levels of approximation to investigate various scattering processes in positron–lithium collision. The Ps formation channels were taken into account and the effect of the ionization continuum was represented by a large number of pseudostates. Most recently, some new investigations of positron–lithium scattering were reported. The Ps formation process at very low energies was studied by Ward and coworkers[11−13] using the hypersperical hidden-crossing method (HHCM) and Le *et al.*[14] using the hypersperical close-coupling method (HSCM). Ratnavelu *et al.* reported various scattering cross sections for positron–lithium scattering[15,16] with a close-coupling optical model where the Ps states were

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included in the coupling and the contribution of ionization continuum was described via an optical potential. Last year, Lugovskoy *et al.*[17] presented a latest investigation for positron–lithium scattering using the two-center convergent close-coupling (CCC) method in which the ionization continuum and Ps formation channels were taken into account by utilizing both negative- and positive-energy Laguerre-based states, and the total scattering cross sections as well as the total Ps formation cross sections were reported.

On the experimental side, Surdutovich *et al.*[18] has reported the measurements for the lower limit of the total Ps formation cross sections for positron–lithium scattering. Unfortunately, there is no report of the experimental measurements for individual Ps formation cross sections, ionization cross sections and total scattering cross sections.

In this paper, we use the momentum-space coupled-channel optical (CCO) method[19] to investigate the positron–lithium collision at the energies above 3 eV. In this method, a complex equivalent-local potential is employed to describe the two-body Ps formation channels and the three-body ionization continuum. This method has been applied to the calculations of various scattering cross sections of positron collision with atomic hydrogen[19] and helium.[20] The level of the agreement between these results and the available theoretical calculated results, as well as the experimental measurements, is satisfactory.

2. Methods

The present CCO method consists of the solution of a discrete set of coupled Lippmann–Schwinger integral equations for $\boldsymbol{T}$-matrix elements

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

Here, the space of target states has been split into two parts. The P space consists of sufficient discrete states while the target ionization continuum and Ps formation channels are included in the Q space.

The optical potential $V^{(Q)}$ can be expressed as the sum of the channel-coupling potential V and a nonlocal complex polarization potential $W^{(Q)}$ that accounts for the contribution of the states in the Q space, i.e., the ionization continuum and Ps formation channels in the present calculations. The polarization potential $W^{(Q)}$ is therefore has two parts, namely $W_{\mathrm{I}}^{(Q)}$ and $W_{\mathrm{Ps}}^{(Q)}$, that describe the ionization and Ps formation channels, respectively.

The matrix element of the polarization potential can be calculated as follows using the weak-coupling approximation:

$$\begin{aligned}&\langle \boldsymbol{k}'i|W^{(Q)}|j\boldsymbol{k}\rangle \\ &= \sum_{n\in Q}\langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle\frac{1}{E^{(+)}-E_n}\langle X_n^{(-)}|V|j\boldsymbol{k}\rangle, \end{aligned} \quad (2)$$

where $X_n^{(-)}$ represents the time reverse of the exact state vector for a reaction starting in channel n. The explicit form used for ionization is

$$|\Psi_n^{(-)}\rangle = |c\psi^-(\boldsymbol{q}_<), \boldsymbol{q}_>\rangle. \quad (3)$$

Here, $\boldsymbol{q}_>$ and $\boldsymbol{q}_<$ 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 $\langle \boldsymbol{r}|\psi^-(\boldsymbol{q}_<)\rangle$ is a Coulomb wave orthogonalized to the orbital from which the electron is removed. The $\langle \boldsymbol{r}|\boldsymbol{q}_>\rangle$ is a plane wave.

The model used for Ps formation is

$$\begin{aligned}&\langle \boldsymbol{k}'i|W_{\mathrm{Ps}}^{(Q)}|j\boldsymbol{k}\rangle \\ &= \sum_n\langle \boldsymbol{k}'i|V|X_n^{(-)}\rangle\frac{1}{E^{(+)}-\varepsilon_n-\boldsymbol{K}_{\mathrm{Ps}}^2}\langle X_n^{(-)}|V|j\boldsymbol{k}\rangle. \end{aligned} \quad (4)$$

The $X_n^{(-)}$ is orthogonalized to ψ_i from which the electron is captured

$$|X_n^{(-)}\rangle = (1-|\psi_i\rangle\langle\psi_i|)|\Psi_n^{(-)}\rangle, \quad (5)$$

$$\Psi_n^{(-)} = \Phi_\mu(\boldsymbol{k}_{\mathrm{Ps}}, \boldsymbol{R}, \boldsymbol{r}) = \varphi_\mu\, \mathrm{e}^{\,\mathrm{i}\boldsymbol{k}_{\mathrm{Ps}}\cdot\boldsymbol{R}}, \quad (6)$$

where $\boldsymbol{k}_{\mathrm{Ps}}$ is the momentum of the Ps center of mass and φ_μ is the wavefunctions of the Ps bound-states. The plane-wave $\mathrm{e}^{\,\mathrm{i}\boldsymbol{k}_{\mathrm{Ps}}\cdot\boldsymbol{R}}$ represents the motion of the Ps center of mass since only the short-range terms survive in the interactions between the Ps and the ionic core of the target. $\boldsymbol{r} = \boldsymbol{r}_{\mathrm{p}} - \boldsymbol{r}_{\mathrm{e}}$ and $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_{\mathrm{p}} + \boldsymbol{r}_{\mathrm{e}})$, where $\boldsymbol{r}_{\mathrm{p}}$ and $\boldsymbol{r}_{\mathrm{e}}$ are the coordinates of the positron and the electron.

A simple estimate of the cross section of ionization (direct ionization) is given by approximating the entrance channel $\boldsymbol{T}$ matrix element of Eq. (1) by its driving term, instead of solving the coupled-channel equations. This result is

$$\sigma_{\mathrm{I}} = \frac{2}{k}(2\pi)^3\mathrm{Im}\langle \boldsymbol{k}0|W_{\mathrm{I}}^{(Q)}|0\boldsymbol{k}\rangle. \quad (7)$$

The total cross section for the Ps formation is

$$\sigma_{\rm Ps} = \frac{2}{k}(2\pi)^3 {\rm Im}\langle \boldsymbol{k}0|W_{\rm Ps}^{(Q)}|0\boldsymbol{k}\rangle, \quad (8)$$

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

3. Results

In the present calculation, the target bound states of atomic lithium are represented by modified Roothan Hartree–Fock wavefunctions[21] in which the core polarization effect is taken into account by an semi-empirical potential. There are eight physical channels: 2, 3, 4s; 2, 3, 4p; 3, 4d included in P space. The optical potentials describing the target continuum are in the channel couplings 2s–2s, 2s–2p, 2s–3s, 2p–2p and the potentials for Ps formation in its $n = 1$ and $n = 2$ states are included in the channel coupling 2s–2s. The cross sections of positronium formation, direct ionization, and total scattering are reported at energies above 3 eV.

We test the present description of the two-body rearrangement channels by comparing the predicted total and individual Ps formation cross sections with available experimental and theoretical data within the impact energy region 3–60 eV in Figs. 1 and 2. For clarity and notational convenience in the discussion, we use CC(m, n) to describe the close coupling calculations with the basis of different size, where n is the number of Ps states and m is the number of bound states and pseudostates of the atomic target.

Figure 1 gives the present results for Ps(1s, 2s, 2p) formation cross sections compared with the theoretical results of CC(4,3) calculations of Hewitt *et al.*[4] and CC(29,3) calculation of McAlinden *et al.*[9] For Ps(1s) formation, all the theoretical results exhibit a similar trend in both shape and magnitude except that the results of McAlinden *et al.*[9] are a little higher than the other two calculations below 8 eV. The calculation of McAlinden *et al.*[9] also predict a structure at about 3.4 eV, which is amongst the Li($n = 3$) threshold but absent in other calculations. In Figs. 1(b) and 1(c), there are remarkable discrepancies existing in the theoretical predictions for Ps(2s) and Ps(2p) formation below 20 eV. The calculation of Hewitt *et al.*[4] produced the highest values and the results keep increasing with the decreasing energy which is much different with the energy dependence of other two calculations. The calculation of McAlinden *et al.*[9] lies significantly below other calculations for Ps(2s) formation at all energies and for Ps(2p) formation below 10 eV. Their calculation predicted a maximum near the threshold for both Ps(2s) and Ps(2p) formations. The present calculation also indicates a sharp increase for both Ps(2s) and Ps(2p) formation when the channel is open. For Ps(2s) formation, there is dip structure in the present results around 6 eV and the present Ps(2p) formation cross section decreases more rapidly after reaching the maximum at 5 eV.

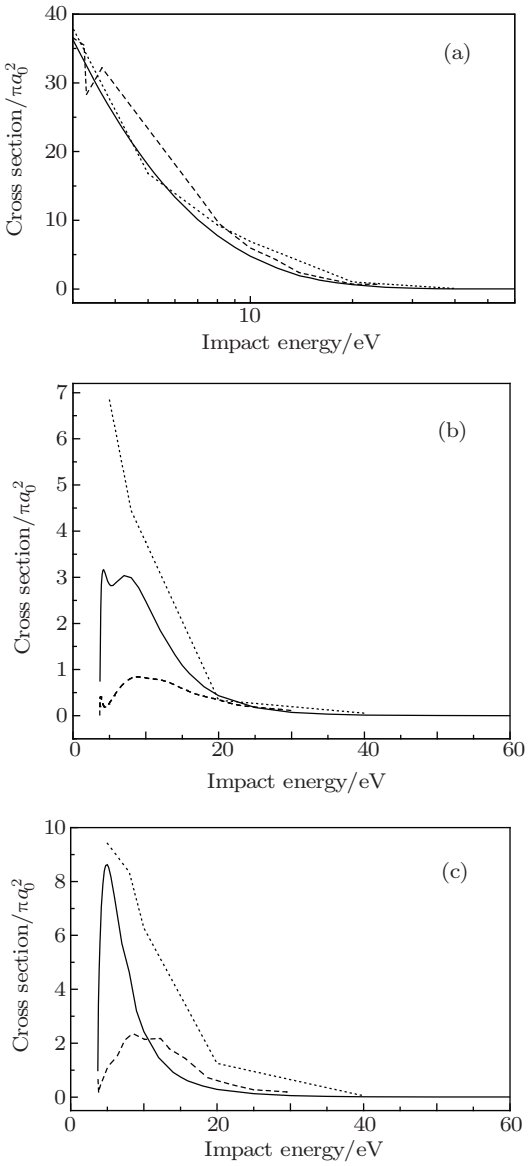


Fig. 1. Cross sections of (a) Ps(1s), (b) Ps(2s), and (c) Ps(2p) formation for positron–lithium scattering from 3 eV to 60 eV. Solid line, present results; dashed-line, CC(29,3) results from Ref. [9]; dotted line, CC(4,3) results from Ref. [4].

In Fig. 2, the present total Ps formation cross sections are displayed and compared with the experimental measurements of Surdutovich *et al.*[18] for the lower limit of the cross sections and the theoretical results of CC(4,3) calculations of Hewitt *et al.*,[4] CC(29,3)

calculation of McAlinden *et al.*,[9] CCO(5,6) calculation of Ratnavelu and Ng,[16] HSCC calculation of Le *et al.*,[14] and the two-center CCC calculation of Lugovskoy *et al.*[17] We can find that all the theoretical curves are in overall qualitative agreement with each other and they all lie above the experimental values below 7 eV. The present calculation above 7 eV confirms that the prediction of the lowest cross sections from McAlinden *et al.*[9] is more close to the experimental values. The present calculation shows a pronounced increase above 3.6 eV and reaches a maximum at 4 eV. This results from the sharp increase of the present calculated cross sections for Ps($n = 2$) formation which is started at 3.6 eV.

The difference of the theoretical calculations for Ps formation may be due to the treatment of the interactions of Ps formation process. In the calculation of Hewitt *et al.*,[4] the positron–ionic core interaction was taken to be the static potential between the positron and a variationally determined $Li^+(1s^2)$ wavefunction. McAlinden *et al.*[9] also employed the static potential to describe this interaction using a Hartree–Fock wavefunction for $Li^+(1s^2)$. Lugovskoy *et al.*[17] developed a new potential to describe the interactions. In the HSCC calculation of Le *et al.*,[14] the static core potential with a Hartree–Fock wavefunction and a dielectron correction were applied. In our model, we adopt the orthogonalization of the Ps states to the ground states of target atom to represent the interaction between the positron and the ionic core.

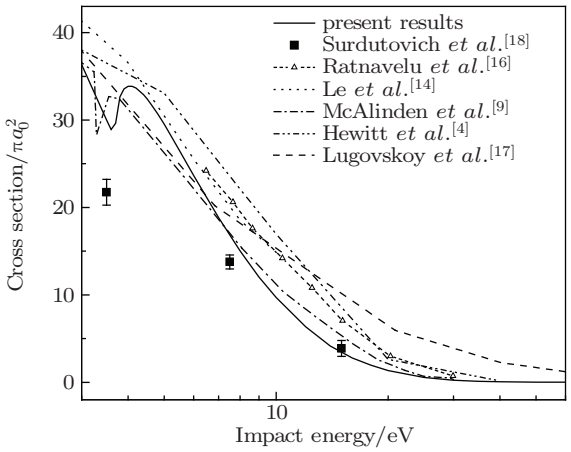


Fig. 2. Total Ps formation cross sections from 3 eV to 60 eV. Solid line, present results; blacksquare, experimental measurements from Ref. [18]; short-dashed line + △, CCO(5,6) results from Ref. [16]; dotted line, HSCC results from Ref. [14]; dash-dotted line, CC(29,3) results from Ref. [9]; dash-dot-dotted line, CC(4,3) results from Ref. [4]; dashed line, two-center CCC calculation from Ref. [17].

This model has been proved effective to produce accurate Ps formation cross sections in positron scattering with hydrogen and helium atoms.[19,20]

Figure 3 gives the present predicted ionization cross sections from the ionization threshold to 300 eV. The theoretical calculation results of McAlinden *et al.*,[9] Ratnavelu and Ng,[16] and Acacia *et al.*[7] are depicted for comparison. The theoretical predictions are similar in shape but obvious discrepancies can be found in the magnitude, especially at energies 10–30 eV. The different treatment of the break-up channels results in the differences. McAlinden *et al.*[9] employed a large number of positive-energy pseudostates to represent the ionization continuum and the ionization cross sections were calculated as the sum of excitations into these pseudostates. The calculation by Acacia *et al.*[7] was performed using the first Born approximation (FBA) within the framework of the distorted-wave theory. The present calculation and also Ratnavelu and Ng[16] applied an optical potential to describe the ionization continuum while the core polarization effect was not taken into account in the calculation of Ratnavelu and Ng.[16] We would appreciate further experimental and theoretical investigations to resolve the discrepancies.

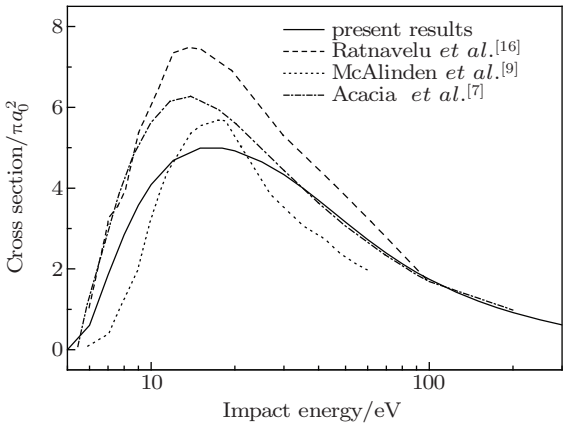


Fig. 3. The direct ionization cross sections from 5 eV to 300 eV. solid line, present results; dashed line, CCO(5,6) results from Ref. [16]; dotted line, CC(29,3) results from Ref. [9]; dash-dotted line, FBA results from Ref. [7].

The present total scattering cross sections at the energies 3–100 eV are shown in Fig. 4 and compared with CC(29,3) calculation of McAlinden *et al.*,[9] CC(2,1) calculation of Basu and Ghosh,[3] and the two-center CCC calculation of Lugovskoy *et al.*[17] In order to reveal the effect of ionization and Ps formation channels, the present results with two different models, namely CC for pure close-coupling and CCO

for the calculation with optical potential, are presented. Comparison shows that the inclusion of ionization and Ps formation channels reduces the cross sections below 10 eV and this effect is negligible at higher energies. Most of the theoretical calculations keep decreasing with the increasing incident energy and tend to converge above 10 eV where the ionization and Ps formation channels are proved to be unimportant. The exception is the CC(2,1) calculation of Basu and Ghosh,[3] which shows a significantly different energy dependence and exhibits larger cross sections above 6 eV. This may be attributed to the small size of the basis in their calculation. The present results lie obviously above the calculations of McAlinden *et al.*[9] and Lugovskoy *et al.*[17] below 10 eV. The difference is probably due to the different treatment of ionization and Ps formation channels. In the present model, the ionization and Ps formation channels are described via an equivalent-local complex potential while they are included in the CC(m,n) calculations by adding the Ps bound states and a number of pesudostates into the coupling.

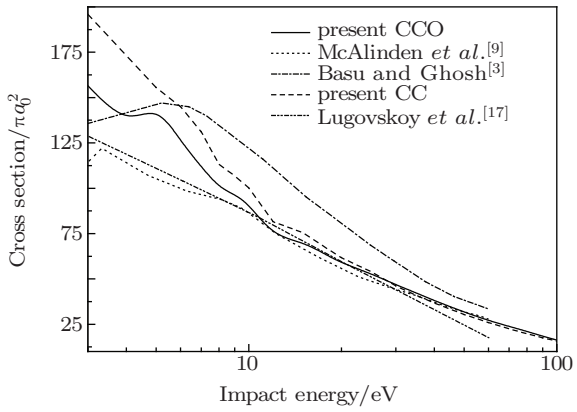


Fig. 4. Total scattering cross sections from 3 eV to 100 eV. Solid line, present CCO results; dash-dot-dotted line, two-center CCC calculation from Ref. [17]; dotted line, CC(29,3) results from Ref. [9]; dash-dotted line, CC(2,1) results from Ref. [3]; dashed line, present CC results.

4. Conclusion

Positron–lithium scattering was studied using the momentum-space coupled-channel optical (CCO) method in this paper. In the present calculations, a complex equivalent-local optical potential has been employed to describe the ionization and Ps formation channels. The total scattering cross sections and the cross sections of Ps formation and direct ionization are reported above 3 eV. The present results obtained are in reasonable agreement with available experimental and theoretical data. However, discrepancies still exist among the theoretical calculations, especially in the predictions for the individual Ps formation and the direct ionization cross sections. Further experimental and theoretical investigations are highly desirable in order to resolve the discrepancies.

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