Two-center convergent close-coupling calculations for positron-lithium collisions

A. V. Lugovskoy,* A. S. Kadyrov, I. Bray, and A. T. Stelbovics
Department of Imaging and Applied Physics, Curtin University, Perth 6150, Australia
(Received 7 October 2010; published 14 December 2010)

We report on two-center convergent close-coupling calculations of positron-lithium collisions. The target is treated as one active electron interacting with an inert ion core. The positronium formation channels are taken into account explicitly utilizing both negative- and positive-energy Laguerre-based states. A large number of channels and high partial waves are used to ensure the convergence of the cross sections. We find the Ramsauer-Townsend minimum in total and elastic cross sections at an impact energy E of about 0.0016 eV. As found previously for H and He, the contributions to the breakup cross section from both the Li and the Ps centers become the same as the threshold is approached.

DOI: 10.1103/PhysRevA.82.062708 PACS number(s): 34.80.Uv, 36.10.Dr, 34.70.+e

I. INTRODUCTION

The physics of positron collisions with atomic targets is of practical and fundamental interest. Positron interactions with matter can be used to access a wealth of information on atomic and molecular structures and reaction mechanisms. Their understanding is crucial for the development and improvement of a number of high-tech applications such as positron-annihilation material analysis and cancer imaging. The two-center nature of the problem, atom and positronium, generates a particular challenge for theorists, while the generation of suitable positron beams is a substantial experimental challenge.

The last decade has seen significant advances in low-energy trap-based positron beams [1–3]. New high-resolution experiments have been conducted for a number of atomic and molecular targets, such as He [4], Ne and Ar [3], CO_2 [5], H_2 [6], and H_2O and HCOOH [7]. From the theoretical side there are several approaches to positron scattering, for example, the eikonal final state-continuum distorted-wave approximation [8,9], the exterior complex scaling method [10], the hybrid R-matrix approach [11], the momentum-space coupled-channel optical method [12], and the close-coupling method [13,14].

In this paper we study positron scattering from atomic lithium. For positron collisions with alkali-metal atoms, both elastic and rearrangement channels are open at all incident energies. Hence, the valid theoretical description has to treat appropriately the "competition" between the positive-charge centers, Li^+ and positron, for the valence electron. However, the first attempt to treat the problem was to use the one-center expansion of the total wave function over atomic orbitals [15–17]. This counterintuitive approach is consistent with the idea of basis completeness. But convergence of such expansions turned out to be very poor [18].

Another way to tackle the problem was to use the two-center expansion, where both atom and positronium states are taken into account on equal footing. This approach resulted in a better agreement with the experiment. For the positron-lithium case the two-center expansion was employed in Refs. [18–23].

In this paper we report two-center convergent close-coupling (CCC) calculations of positron scattering by atomic lithium. Previously, this method was implemented for positron collisions with hydrogen [24] and helium [25,26] targets. The use of complete bases on both centers resolved the issue of unphysical resonances [24] and resulted in excellent agreement between the theory and the experiment. Our purpose is to provide convergent results at energies where Ps formation is not negligible. At very low energies we identify a Ramsauer-Townsend minimum [19]. This structure has not previously been found for this collision system. The paper is organized as follows. In Sec. II we describe the theoretical approach together with the model potentials used. The results are presented in Sec. III, followed by concluding remarks.

II. THEORY

In this paper we follow the approach where a positron-lithium collision is treated as a three-body problem. The interacting particles are the incoming positron, the active (outer-shell) electron, and the Li^+ ion. The $1s$ electrons of the core do not participate directly in the collision event. They provide screening of the nucleus and take part in exchange with the active electron.

The scattering wave function Ψ satisfies the Shrödinger equation

$$(E - H)\Psi = 0, \tag{1}$$

where E is the total energy and

$$H = H_0 + V \tag{2}$$

is the Hamiltonian of this system, with H_0 and V being, respectively, the three-free-particle Hamiltonian and the sum of all two-body interactions. The Hamiltonian H_0 is used in two forms:

$$H_0 = -(1/4)\nabla^2_{\rho_\beta} - \nabla^2_{r_\beta}, \tag{3}$$

$$= -(1/2)\nabla^2_{\rho_\alpha} - (1/2)\nabla^2_{r_\alpha}, \tag{4}$$

corresponding to two different sets of Jacobi coordinates, $\{\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha\}$ and $\{\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta\}$; see Fig. 1. In this paper we follow the notations adopted in Ref. [27]. In our case, symbols α,e, and β indicate individual particles: positron, electron, and Li^+ ion, respectively. Also, they label the particle pairs so

*A.Lugovskoy@curtin.edu.au

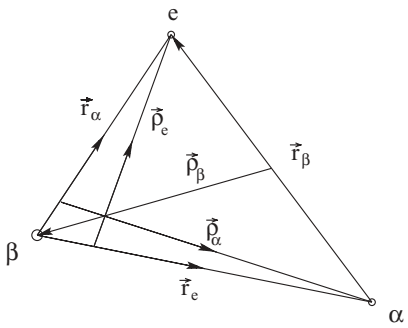

FIG. 1. Jacobi coordinates for positron (α), electron (e), and Li^+ ion (β).

that α indicates electron-Li^+,e indicates positron-Li^+, and β indicates electron-positron pair.

For potential V in Eq. (2) we use, in pairs, α,β, and e:

$$V = V_\alpha(r_\alpha) + V_e(r_e) + V_\beta(r_\beta), \tag{5}$$

where the electron-ion and positron-ion terms, V_α and V_e, are

$$V_\alpha(r) = V_{\rm st}(r) + V_{\rm ex}(r), \tag{6}$$

$$V_e(r) = -V_{\rm st}(r), \tag{7}$$

with $V_{\rm st}$ and $V_{\rm ex}$ being the static and exchange terms of the Hartree-Fock potential. The static term is calculated as

$$V_{\rm st}(r) = -\frac{Z}{r} + 2\sum_{\psi_j\in C}\int d^3r' \frac{|\psi_j(\boldsymbol{r}')|^2}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{8}$$

where Z is the charge of the nucleus and ψ_j are the states of the ion core C generated by performing the self-consistent-field Hartree-Fock (SCFHF) calculations [28]. The summation in Eq. (8) is done for all core states. The exchange between the active electron and core electrons is taken into account in the framework of the equivalent local-exchange approximation [29–31],

$$V_{\rm ex}(r,E_{\rm ex}) = \tfrac{1}{2}\{[E_{\rm ex} - V_{\rm st}(r)] - \sqrt{[E_{\rm ex} - V_{\rm st}(r)]^2 + \rho(r)}\}, \tag{9}$$

where

$$\rho(r) = \sum_{\psi_j\in C}\int {\rm d}\hat{\boldsymbol{r}}\,|\psi_j(\boldsymbol{r})|^2 \tag{10}$$

is the electron density distribution in the core and $E_{\rm ex}$ is an adjustment parameter. Finally, the electron-positron interaction V_β in Eq. (5) is the Coulomb potential.

Following the two-center CCC approach [27], wave function Ψ in Eq. (1) is sought as an expansion,

$$\Psi \approx \sum_\alpha^{N_\alpha} F_\alpha(\boldsymbol{\rho}_\alpha)\psi_\alpha^{N_\alpha}(\boldsymbol{r}_\alpha) + \sum_\beta^{N_\beta} F_\beta(\boldsymbol{\rho}_\beta)\psi_\beta^{N_\beta}(\boldsymbol{r}_\beta), \tag{11}$$

where $\psi_\alpha^{N_\alpha}$ and $\psi_\beta^{N_\beta}$ are atomic and positronium pseudostates, respectively, and F_α and F_β are their associated weight functions. Pseudostates $\psi_\alpha^{N_\alpha}$ and $\psi_\beta^{N_\beta}$ are generated by diagonalizing the one-particle Hamiltonians [32]

$$H_\alpha = -\tfrac{1}{2}\nabla_{\boldsymbol{r}} + V_\alpha(r) \tag{12}$$

and

$$H_\beta = -\tfrac{1}{4}\nabla_{\boldsymbol{r}} + V_\beta(r), \tag{13}$$

using the square-integrable orthogonal Laguerre basis,

$$\xi_{n,l}(r) = \left[\frac{\lambda_l(n-1)!}{(2l+1+n)!}\right]^{1/2}(\lambda_l r)^{l+1}\exp[-\lambda_l r]\,L_{n-1}^{2l+2}(-\lambda_l r), \tag{14}$$

where $L_{n-1}^{2l+2}(x)$ is the associated Laguerre polynomial and n ranges from 1 to the basis size N_l for $l = 0,1,\ldots,l_{\rm max}$. The complete sets of pseudostates contain both negative- and positive-energy states. Negative-energy states correspond to the bound states of the atomic target and positronium, while positive-energy states provide a discretization of their continuum spectra. The number of negative-energy states depends on the parameters λ_l and N_l, which are specific for every given orbital momentum number l.

TABLE I. Experimental and theoretical energies of several low-lying levels of lithium (in eV).

State	Expt.	SCHF	$N_l = 10$	$N_l = 50$
$2s$	−5.392	−5.342	−5.392	−5.392
$2p$	−3.544	−3.501	−3.614	−3.614
$3s$	−2.019	−2.009	−2.009	−2.019
$3p$	−1.558	−1.544	−1.540	−1.579
$3d$	−1.513	−1.512	−1.493	−1.514
$4s$	−1.051	−1.047	−0.589	−1.051
$4p$	−0.870	−0.865	−0.144	−0.879
$4d$	−0.851	−0.850	−0.316	−0.851

Table I reports the energies of a few low levels resulting from the Hamiltonian dioganalization with $N_l = 10 - l$ and $N_l = 50 - l$, with $E_{\rm ex} = -0.3831$ a.u.. These energy values are compared with the experimental data from Ref. [33] as well as the results of SCFHF calculations. The value of the local-exchange parameter $E_{\rm ex}$ was chosen so that the ground-level energy was equal to the experimental value. We see that the positions of the low-energy levels are well reproduced when a sufficiently large N_l is used. For $N_l = 50 - l$ the largest relative error is 1.9%. This is comparable with the 1.2% error for the energy obtained with the SCFHF method.

Substituting expansion (11) into (1) and following Ref. [27], one can derive the set of momentum-space coupled-channel equations for transition matrix elements,

$$T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) = V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) + \sum_{\gamma''}^{N_\alpha+N_\beta}\int \frac{d\boldsymbol{q}_{\gamma''}}{(2\pi)^3} \times \frac{V_{\gamma',\gamma}(\boldsymbol{q}'_\gamma,\boldsymbol{q}_{\gamma''})T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma''},\boldsymbol{q}_\gamma)}{\left[E + i0 - \epsilon_{\gamma''} - q_{\gamma''}^2/(2M_{\gamma''})\right]}, \tag{15}$$

where $\boldsymbol{q}_\gamma$ is the momentum of the free particle γ relative to the c.m. of the bound pair in channel γ ($\gamma = \alpha$ or β), ϵ_γ is the

corresponding pseudoenergy of the bound pair, and M_γ is its reduced mass. The effective potential $V_{\gamma',\gamma}$ is defined as

$$V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) = \langle \boldsymbol{q}_{\gamma'}|\langle\psi_{\gamma'}|U_{\gamma',\gamma}|\psi_\gamma\rangle|\boldsymbol{q}_\gamma\rangle, \tag{16}$$

where $|\boldsymbol{q}_\gamma\rangle$ is a plane wave representing the free particle γ and $U_{\gamma',\gamma}$ represents one of the following channel operators:

$$U_{\alpha,\alpha} = V - V_\alpha, \quad U_{\beta,\beta} = V - V_\beta, \quad U_{\alpha,\beta} = H_0 + V - E. \tag{17}$$

By performing partial-wave expansion in the total orbital angular momentum J, one can get from Eq. (15)

$$T^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma) = V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma) + \sum_{\gamma''}^{N_\alpha+N_\beta}\sum_{L''}\int \frac{dq_{\gamma''}\,q^2_{\gamma''}}{(2\pi)^3} \times \frac{V^{L'L''J}_{\gamma',\gamma}(q'_\gamma,q_{\gamma''})T^{L''LJ}_{\gamma',\gamma}(q_{\gamma''},q_\gamma)}{\left[E+i0-\epsilon_{\gamma''}-q^2_{\gamma''}/(2M_{\gamma''})\right]}, \tag{18}$$

where $V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)$ and $V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma)$ [and, similarly, $T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)$ and $T^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma)$] are related to each other by

$$V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma) = \sum_{L',M',L,M,J,K} Y_{L'M'}(\hat{\boldsymbol{q}}_{\gamma'})C^{JK}_{L'M'l'm'} \times V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma)C^{JK}_{LMlm}Y^*_{LM}(\hat{\boldsymbol{q}}_\gamma) \tag{19}$$

and

$$V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma) = \sum_{m',m,M',M}\int\int \mathrm{d}\hat{\boldsymbol{q}}_{\gamma'}\mathrm{d}\hat{\boldsymbol{q}}_{\gamma'}Y^*_{L'M'}(\hat{\boldsymbol{q}}_{\gamma'}) \times C^{JK}_{L'M'l'm'}V_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)C^{JK}_{LMlm}Y_{LM}(\hat{\boldsymbol{q}}_\gamma), \tag{20}$$

where Y_{LM} is a spherical harmonic and $C^{JK}_{L'M'l'm'}$ is a Clebsch-Gordan coefficient. The effective potentials $V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma)$ can be computed similarly to how it was done for the positron-hydrogen problem [27].

III. MATRIX ELEMENTS

Calculation of the effective potentials $V^{L'LJ}_{\gamma',\gamma}(q_{\gamma'},q_\gamma)$ is straightforward but tedious. In contrast to the hydrogen case, there is no analytical expressions for the potentials $V_e(r)$ and $V_\alpha(r)$. These potentials are available in numerical form only. This means that we cannot use intermediate analytical steps in calculation of the matrix elements, which increases the computation time significantly.

To calculate matrix elements for direct (atom-atom and positronium-positronium) transitions, one needs the spherical harmonic expansion of $V_{\alpha',\alpha}(\boldsymbol{q}_{\alpha'},\boldsymbol{q}_\gamma)$ and $V_{\beta',\beta}(\boldsymbol{q}_{\beta'},\boldsymbol{q}_\beta)$. In turn, this requires the spherical-wave expansion of $U_{\alpha,\alpha}$ and $U_{\beta,\beta}$. Using the approximation $r_e \approx \rho_\alpha$ (atomic c.m. assumed to be at the ion center), one gets

$$U_{\alpha,\alpha} = V - V_\alpha = V_e(r_e) + V_\beta(r_\beta) \approx \sum_{\lambda=0}^{\infty}\frac{4\pi}{2\lambda+1}U^\lambda_{\alpha,\alpha}(\rho_\alpha,r_\alpha)[\boldsymbol{Y}_\lambda(\hat{\rho}_\alpha)\cdot\boldsymbol{Y}_\lambda(\hat{r}_\alpha)], \tag{21}$$

where

$$U^\lambda_{\alpha,\alpha}(\rho_\alpha,r_\alpha) = V_e(\rho_\alpha)\delta_{\lambda,0} - \frac{\min[r_\alpha,\rho_\alpha]^\lambda}{\max[r_\alpha,\rho_\alpha]^{\lambda+1}} \tag{22}$$

and

$$[\boldsymbol{Y}_\lambda(\hat{\rho}_\alpha)\cdot\boldsymbol{Y}_\lambda(\hat{r}_\alpha)] = \sum_{\mu=-\lambda}^{\lambda}[Y^*_{\lambda,\mu}(\hat{\rho}_\alpha)Y_{\lambda,\mu}(\hat{r}_\alpha)]. \tag{23}$$

Taking into account that $\boldsymbol{r}_e = -\boldsymbol{\rho}_\beta - \boldsymbol{r}_\beta/2$ and $\boldsymbol{r}_\alpha = -\boldsymbol{\rho}_\beta + \boldsymbol{r}_\beta/2$, we derive

$$U_{\beta,\beta} = V - V_\beta = V_e(r_e) + V_\alpha(r_\alpha) = \sum_\lambda \frac{4\pi}{2\lambda+1}U^{(\lambda)}_{\beta,\beta}(\rho_\beta,r_\beta)[\boldsymbol{Y}_\lambda(\hat{\boldsymbol{\rho}}_\beta)\cdot\boldsymbol{Y}_\lambda(\hat{\boldsymbol{r}}_\beta)], \tag{24}$$

where

$$\begin{aligned} U^{(\lambda)}_{\beta,\beta}(\rho_\beta,r_\beta) &= \frac{2\lambda+1}{2}\int_{-1}^{1}dz\,P_\lambda(z)\left[V_e\left(\boldsymbol{\rho}_\beta+\frac{\boldsymbol{r}_\beta}{2}\right)+V_\alpha\left(\boldsymbol{\rho}_\beta-\frac{\boldsymbol{r}_\beta}{2}\right)\right] \\ &= \frac{2\lambda+1}{2}\int_{-1}^{1}dz\,P_\lambda(z)\left\{V_\alpha\left(\sqrt{r^2_<+r^2_>-2zr_<r_>}\right)\right. \\ &\quad \left.+(-1)^\lambda V_e\left(\sqrt{r^2_<+r^2_>-2zr_<r_>}\right)\right\} \end{aligned} \tag{25}$$

and where $P_\lambda(z)$ is the Legendre polynomial of degree $l, r_< = \min(\rho, r/2)$ and $r_> = \max(\rho, r/2)$.

The matrix elements $V_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$ for rearrangement transitions are presented as a sum of two terms, $V^{(1)}_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$ and $V^{(2)}_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$, calculated separately. The first term is

$$\begin{aligned} V^{(1)}_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) &= \int\int d\boldsymbol{\rho}_\beta d\boldsymbol{r}_\beta e^{-iq_\beta\cdot\rho_\beta}\psi^*_\beta(\boldsymbol{r}_\beta) \times[(H_0-E)+V_\beta(r_\beta)+V_\alpha(r_\alpha)]\psi_\alpha(\boldsymbol{r}_\alpha)e^{iq_\alpha\cdot\rho_\alpha} \\ &= (2\pi)^3[\mathcal{E}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)\tilde{\psi}^*_\beta(\boldsymbol{p}_\beta)\tilde{\psi}_\alpha(\boldsymbol{p}_\alpha) \\ &\quad +\tilde{\psi}^*_\beta(\boldsymbol{p}_\beta)\tilde{g}_\alpha(\boldsymbol{p}_\alpha)+\tilde{g}^*_\beta(\boldsymbol{p}_\beta)\tilde{\psi}_\alpha(\boldsymbol{p}_\alpha)], \end{aligned} \tag{26}$$

where $\boldsymbol{p}_\alpha = \boldsymbol{q}_\beta - \boldsymbol{q}_\alpha, \boldsymbol{p}_\beta = \boldsymbol{q}_\beta/2 - \boldsymbol{q}_\alpha$, and $\mathcal{E}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) = p^2_\alpha/2 + q^2_\alpha/2 - E$. Functions with a tilde, $\tilde{\psi}_i(\boldsymbol{p})$ and $\tilde{g}_i(\boldsymbol{p})$, are the Fourier images of $\psi_i(\boldsymbol{r})$ and $V_i(r)\psi_i(\boldsymbol{r})$, respectively.

The second term, $V^{(2)}_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$, is

$$\begin{aligned} V^{(2)}_{\beta,\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) &= \iint d\boldsymbol{\rho}_\beta d\boldsymbol{r}_\beta e^{-iq_\beta\cdot\rho_\beta}\psi^*_\beta(\boldsymbol{r}_\beta)V_e(r_e)\psi_\alpha(\boldsymbol{r}_\alpha)e^{iq_\alpha\cdot\rho_\alpha} \\ &= (2\pi)^3\int\frac{d\boldsymbol{p}}{(2\pi)^{3/2}}\tilde{\psi}^*_\beta(\boldsymbol{p}'_\beta)\tilde{V}_e(\boldsymbol{p}-\boldsymbol{q}_\alpha)\tilde{\psi}_\alpha(\boldsymbol{p}'_\alpha), \end{aligned} \tag{27}$$

where $\boldsymbol{p}'_\beta = (\boldsymbol{q}_\beta/2) - \boldsymbol{p}, \boldsymbol{p}'_\alpha = \boldsymbol{q}_\beta - \boldsymbol{p}$ and $\tilde{V}_e(\boldsymbol{p})$ is the Fourier transform of $V_e(\boldsymbol{r})$. Equation (27) leads to the

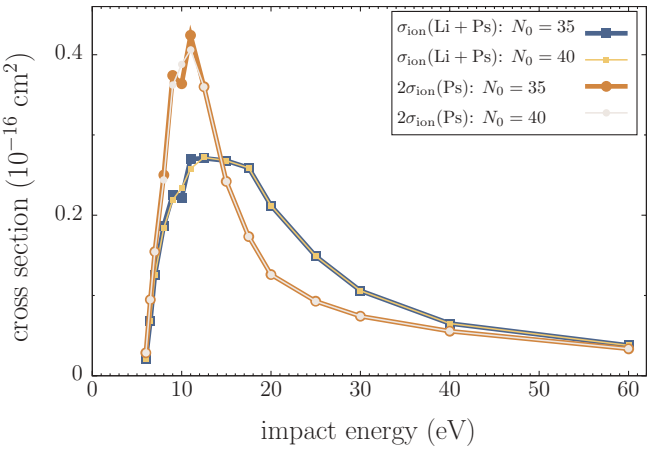

FIG. 2. (Color online) Breakup cross section $\sigma_{\rm ion}$(Li + Ps) and $2\sigma_{\rm ion}$(Ps) as functions of energy computed within the S-wave model; see text. Numbers of states used in calculations are indicated in the key.

following expression for its reduced matrix element:

$$\mathcal{V}^{L'L(2)}_{\beta\alpha}(q_\beta,q_\alpha) = \frac{1}{8\pi^3}\int_0^\infty dq\, q^2 Q'_L(q,q_\alpha) \sum_{m,m',M,M'} C^{L'l'J}_{M'm'K} C^{LlJ}_{MmK} \times \iint d\hat{\boldsymbol{q}}_\beta d\hat{\boldsymbol{q}} Y^*_{L'M'}(\hat{\boldsymbol{q}}_\beta) Y_{LM}(\hat{\boldsymbol{q}}) \tilde{\psi}^*_\beta(\boldsymbol{p}'_\beta)\tilde{\psi}^*_\alpha(\boldsymbol{p}'_\alpha), \quad (28)$$

where

$$Q^{(v)}_l(q,q_\alpha) = 2\pi \int_{-1}^{1} P_l(z) V_e(\boldsymbol{q} - \boldsymbol{q}_\alpha)\, dz, \quad (29)$$

with $z = \cos(\alpha)$ and α the angle between vector $\boldsymbol{q}$ and vector $\boldsymbol{q}_\alpha$.

Calculation of matrix elements, especially those for rearrangement transitions, is the most time consuming part of the CCC calculations. The system of close-coupled equations we need to solve is ill-conditioned due to the usage of the two center expansion, requiring the matrix elements.

IV. RESULTS

To obtain the transition matrix elements $T_{\gamma',\gamma}(\boldsymbol{q}_{\gamma'},\boldsymbol{q}_\gamma)$, the system of coupled momentum-space integral equations (17) is converted into equations for the K matrix and then solved numerically using real arithmetic [32]. Calculations are performed for a limited number of partial waves J. We found that the first 10 partial waves is enough for get reliable results for the positronium formation cross sections at all energies. Direct scattering channels require at least 10 more partial waves at the higher energies. Using the developed code we perform calculations with as many pseudostates from both centers as required for the convergence

We conduct calculations with different basis sets to be sure that our results are independent of the set parameters such as the exponential fall-off parameter λ_l and convergent when increasing the parameters contributing to the basis size,

$$N = \sum_{l=0}^{l^{\rm Li}_{\rm max}} N^{\rm Li}_l + \sum_{l=0}^{l^{\rm Ps}_{\rm max}} N^{\rm Ps}_l. \quad (30)$$

To make convergence issues simpler, we set $\lambda^{\rm Ps}_l = \lambda^{\rm Ps}$,$\lambda^{\rm Li}_l = \lambda^{\rm Li}$,$l^{\rm Ps}_{\rm max} = l^{\rm Li}_{\rm max} = l_{\rm max}$, and $N^{\rm Ps}_l = N^{\rm Li}_l = N_0 - l$. This way we reduce the number of parameters to just N_0, $l_{\rm max}$, $\lambda^{\rm Li}$, and $\lambda^{\rm Ps}$.

Given the commensurate treatment of both centers, we need to demonstrate that convergence is possible and that there is no double-counting of the ionization processes due to positive-energy states of both centers. We illustrate this in Fig. 2, within the S-wave model, where only 0 orbital angular momenta are retained. Presented are the total breakup cross section, $\sigma_{\rm ion}$(Li + Ps), as well as the positronium breakup cross section, $\sigma_{\rm ion}$(Ps), multiplied by two. The first one equals the sum of all

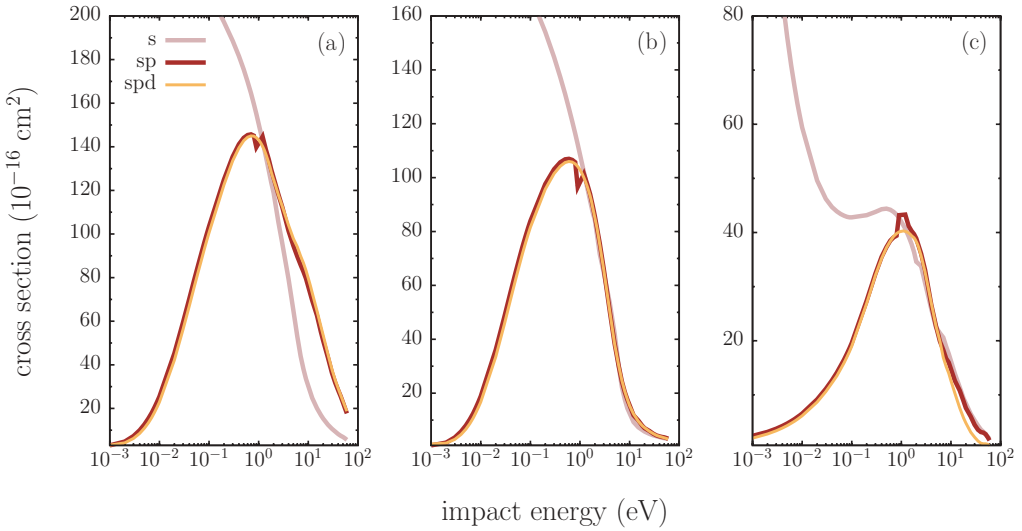

FIG. 3. (Color online) (a) Total, (b) elastic, and (c) positronium formation cross sections for positron-lithium collisions calculated using the two-center CCC method. The numbers of basis states were the same for both centers and were $N_0 = 20$ s states for the s basis, $N_0 = 10$ and $N_1 = 9$ for the sp basis, and $N_0 = 10$,$N_1 = 9$, and $N_2 = 8$ for the spd basis.

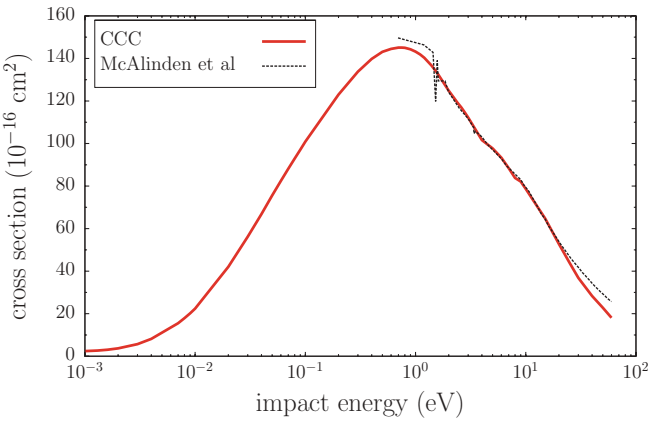

FIG. 4. (Color online) Total cross sections for positron-lithium scattering. CCC results [solid (red) lines] are compared with the data from Ref. [18] [dashed (black) line]. The *spd* basis as in Fig. 3 was used in calculations.

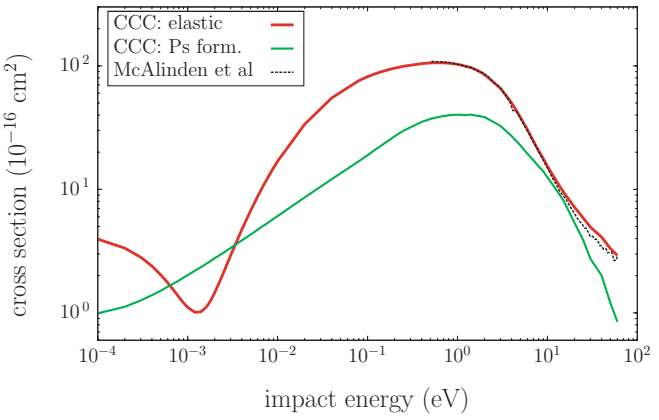

FIG. 5. (Color online) Same as Fig. 4 but for elastic cross sections. Also shown [dashed (black) line] is the positronium formation cross section. The CCC basis is the same as for Fig. 4.

cross sections over the positive-energy pseudostates of both centers,

$$\sigma_{\rm ion}({\rm Li}+{\rm Ps}) = \sum_{n:\epsilon_n^{\rm Li}>0} \sigma_n + \sum_{n:\epsilon_n^{\rm Ps}>0} \sigma_n \equiv \sigma_{\rm ion}({\rm Li}) + \sigma_{\rm ion}({\rm Ps}), \quad (31)$$

while the second, $\sigma_{\rm ion}$(Ps), is due to the contributions of just the positronium positive-energy pseudostates. We see excellent convergence for both $\sigma_{\rm ion}$(Li + Ps) and $\sigma_{\rm ion}$(Ps) when the number of states on each center goes from 35 to 40. The two values of N_0 yield indistinguishable results at all energies except in a small region around 10 eV. Thus, the two independent Li and Ps contributions to the breakup cross section are independently convergent. Furthermore, the fact that the curves converge on each other at threshold indicates that there $\sigma_{\rm ion}({\rm Ps}) \approx \sigma_{\rm ion}({\rm Li})$. Previously, such behavior was demonstrated for the cases of hydrogen [34] and helium [25]. We note that the system of equations becomes rapidly ill conditioned as N_0 is increased.

Having established convergence in a model problem, we now consider the full problem. Figure 3 shows the total, elastic, and positronium formation cross sections as functions of the impact energy. They where calculated using three different sets with $l_{\rm max} = 0$ (*s* basis), $l_{\rm max} = 1$ (*sp* basis), and $l_{\rm max} = 2$ (*spd* basis). Equal numbers of pseudostates were taken for both centers in our calculations. Figures 3(a)–3(c) reveal the significant difference in energy dependence between results calculated with the *s* versus the *sp* basis. Differences between the *sp*- and the *spd*-basis calculations are only marginal. These results suggest good convergence with N_0 and $l_{\rm max}$ for the presented transitions.

The grand total and elastic cross sections are presented in Figs. 4 and 5. They were calculated with the use of $N_l = 10 - l$ pseudostates for each center with $l_{\rm max} = 2$. Also shown, by dashed lines, are calculations from Ref. [18]. We see that the results are generally in good agreement. The only difference is the resonant-like structure in the total cross section near 1.6 eV. We found this structure and its position to be basis dependent. It disappears for sufficiently large bases on both centers. Also, for very low energies, CCC predicts a shallow Ramsauer-like minimum in both total and elastic cross sections near $E = 0.0016$ eV (see Fig. 5).

Figure 6 shows the positronium formation cross section. We compare our calculations [solid (red) and dashed (black) lines] with the experimental data from Ref. [35] and theoretical results from Refs. [18] and [23]. We also present results from a truncated basis that has only 3 eigenstates ($1s$, $2s$, and $2p$) for positronium and 29 states ($2s$-$9s$, $2p$-$9p$, $3d$-$9d$, and $4f$-$9f$) for lithium. The states were chosen so that their energies were in close correspondence to the energies of the mixed-basis states used in Ref. [18].

We see that all theoretical curves are in overall qualitative agreement with each other. Our truncated-basis calculations agree well with the results in Ref. [18], with both having a pseudoresonance, though at different energies. The differences can be attributed to the fact that we take into account the exchange part of the electron-electron interaction and, also, use slightly different lithium states. The exchange interaction was also taken into account in the hyperspherical close-coupling calculations [23]. Those authors obtained a resonance-free

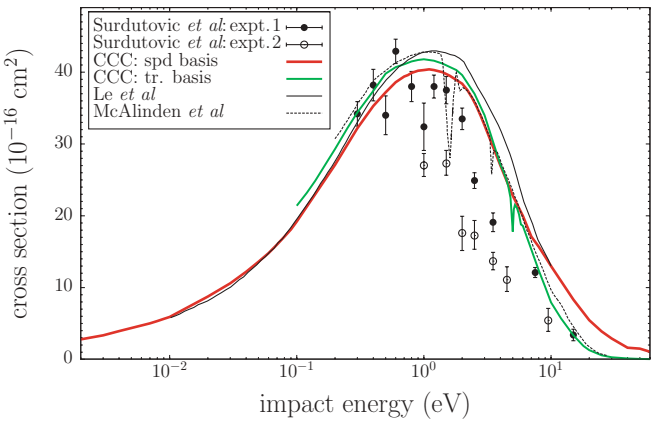

FIG. 6. (Color online) Total positronium formation cross section for e^+-Li along with experimental points [35] and theoretical calculations [18,23]. The CCC basis is the same as for Fig. 4. The truncated basis CCC calculation is an attempt to reproduce the states used in Ref. [18].

energy dependence for the positronium formation cross section. We see that the only slight disagreement of the CCC and their results is in the magnitude of the peak. The agreement with experiment is not at the level that we would hope for this relatively simple collision system.

V. CONCLUSION

The two-center CCC method has been developed to calculate positron scattering with lithium atoms, where the positronium formation channel is taken into account explicitly. Direct scattering and positronium formation cross sections have been calculated for a broad range of energies of practical interest. Convergence in the calculated cross sections was demonstrated by increasing the basis sizes and orbital angular momentum of the included states for each of the centers. The results obtained are in good agreement with available theoretical data. Our calculations reveal a shallow Ramsauer-like minimum in the total and elastic cross sections near 0.0016 eV. We would appreciate further experimental investigation to see if the present discrepancy with experiment can be resolved.

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council. We are grateful for access to the Australian National Computing Infrastructure Facility and its Western Australian node Ive.

[1] C. M. Surko, G. F. Gribakin, and S. J. Buckman, J. Phys. B **38**, R57 (2005).
[2] S. J. Gilbert, J. P. Sullivan, C. M. Surko, and S. J. Buckman, *APS Meeting Abstracts* (APS, College Park, MD, 2001), p. 5038.
[3] A. Jones, P. Caradonna, C. Makochekanwa, D. Slaughter, D. Mueller, J. P. Sullivan, and S. J. Buckman, J. Phys. Conf. Ser. **194**, 012033 (2009).
[4] P. Caradonna, A. Jones, C. Makochekanwa, D. S. Slaughter, J. P. Sullivan, S. J. Buckman, I. Bray, and D. V. Fursa, Phys. Rev. A **80**, 032710 (2009).
[5] A. Zecca, L. Chiari, A. Sarkar, M. A. P. Lima, M. H. F. Bettega, K. L. Nixon, and M. J. Brunger, Phys. Rev. A **78**, 042707 (2008).
[6] A. Zecca, L. Chiari, A. Sarkar, K. L. Nixon, and M. J. Brunger, Phys. Rev. A **80**, 032702 (2009).
[7] C. Makochekanwa *et al.*, New J. Phys. **11**, 103036 (2009).
[8] P. A. Macri, J. E. Miraglia, J. Hanssen, O. A. Fojón, and R. D. Rivarola, J. Phys. B **37**, L111 (2004).
[9] P. Macri and R. Barrachina, Nucl. Instrum. Methods Phys. Res. Sect. B **266**, 393 (2008).
[10] P. L. Bartlett, A. T. Stelbovics, T. N. Rescigno, and C. W. McCurdy, Phys. Rev. A **77**, 032710 (2008).
[11] K. Bartschat, Phys. Rev. A **71**, 032718 (2005).
[12] Y. Cheng and Y. Zhou, Phys. Rev. A **76**, 012704 (2007).
[13] J. Mitroy, Aust. J. Phys. **46**, 751 (1993).
[14] G. Ryzhikh and J. Mitroy, J. Phys. B **30**, 5545 (1997).
[15] S. J. Ward, M. Horbatsch, R. P. McEachran, and A. D. Stauffer, J. Phys. B **22**, 1845 (1989).
[16] K. P. Sarkar, M. Basu, and A. S. Ghosh, J. Phys. B **21**, 1649 (1988).
[17] P. Khan, S. Dutta, and A. S. Ghosh, J. Phys. B **20**, 2927 (1987).
[18] M. T. McAlinden, A. A. Kernoghan, and H. R. J. Walters, J. Phys. B **30**, 1543 (1997).
[19] S. Guha and A. S. Ghosh, Phys. Rev. A **23**, 743 (1981).
[20] M. Basu and A. S. Ghosh, J. Phys. B **19**, 1249 (1986).
[21] M. A. Abdel-Raouf, J. Phys. B **21**, 2331 (1988).
[22] R. N. Hewitt, C. J. Noble, and B. H. Bransden, J. Phys. B **25**, 2683 (1992).
[23] A.-T. Le, M. W. J. Bromley, and C. D. Lin, Phys. Rev. A **71**, 032713 (2005).
[24] A. S. Kadyrov and I. Bray, J. Phys. B **33**, L635 (2000).
[25] R. Utamuratov, A. S. Kadyrov, D. V. Fursa, and I. Bray, J. Phys. B **43**, 031001 (2010).
[26] R. Utamuratov, A. S. Kadyrov, D. V. Fursa, I. Bray, and A. T. Stelbovics, J. Phys. B **43**, 125203 (2010).
[27] A. S. Kadyrov and I. Bray, Phys. Rev. A **66**, 012710 (2002).
[28] I. Bray, Phys. Rev. A **49**, 1066 (1994).
[29] J. B. Furness and I. E. McCarthy, J. Phys. B **6**, 2280 (1973).
[30] B. J. Albright, K. Bartschat, and P. R. Flicek, J. Phys. B **26**, 337 (1993).
[31] J. Migdalek and W. E. Baylis, Phys. Rev. A **24**, 649 (1981).
[32] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[33] L. J. Radziemski, R. Engleman, and J. W. Brault, Phys. Rev. A **52**, 4462 (1995).
[34] A. S. Kadyrov, I. Bray, and A. T. Stelbovics, Phys. Rev. Lett. **98**, 263202 (2007).
[35] E. Surdutovich, J. M. Johnson, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. A **65**, 032713 (2002).