Convergent close-coupling calculations of positron scattering on metastable helium

R. Utamuratov,* A. S. Kadyrov, D. V. Fursa, I. Bray, and A. T. Stelbovics
ARC Centre for Antimatter-Matter Studies, Department of Applied Physics, Curtin University, Perth 6152, Australia
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The convergent close-coupling method has been applied to positron scattering on a helium atom in the $2\,^3S$ metastable state. For this system the positronium (Ps) formation channel is open even at zero scattering energy making the inclusion of the Ps channels especially important. Spin algebra is presented for the general case of arbitrary spins. A proof is given of the often-used assumption about the relationship between the amplitudes for ortho-positronium and para-positronium formation. The cross sections for scattering from $2\,^3S$ are shown to be significantly larger than those obtained for the ground state.

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I. INTRODUCTION

There has been continuous interest in positron scattering from atoms and molecules over the past few decades. Being the simplest and most available antimatter particle, the positrons have been widely used as an alternative projectile for atomic scattering and in antimatter-matter interaction studies.

The theoretical studies of positron scattering on atoms and molecules are challenging because of the two-center nature of the problem. The effect of the second center associated with positronium (Ps) formation manifests itself from low to medium scattering energies, even below the Ps-formation threshold region. However, at energies below the Ps threshold it is still possible to get an accurate solution without including Ps-formation channels by using sufficiently high angular momentum states of a target as was shown in [1] in the case of positron scattering on the ground state of helium. But when the Ps-formation threshold is zero or negative then the importance of Ps channels significantly increases at low energies and in this situation single-center expansion calculations will be no longer accurate.

For many targets the Ps-formation channel is open starting from zero collision energy. Positron scattering on the $2\,^3S$ metastable state of helium is an example of such a system where the Ps threshold is negative (−2.06 eV). This system has not been yet studied either theoretically or experimentally at low energies. To the best of our knowledge, only a few theoretical calculations [2–4] have been reported at higher energies where the Ps-formation contribution is negligible. More recently Hanssen *et al.* [5] studied Ps formation in positron-metastable-He collisions at above 50-eV incident energies by including the Ps($1s$) state in their expansions.

Recently, we reported two-center convergent close-coupling (CCC) results of positron scattering on the ground state of helium [6,7] where good agreement between the theory and experimental data has been achieved. In this work we apply this formalism to positron scattering on metastable helium. As yet, no experimental studies have been conducted for positron-metastable helium scattering. The motivation for this study is mainly based on the following. First, we would like to check the applicability of the two-center CCC approach to a system with a negative Ps threshold. Second, the recent experimental achievements on electron scattering from metastable helium [8], in a group that also has a positron beam, may suggest that in the future there might be experimental data to test our calculations. Moreover, there are still unresolved differences between theory and experiment on electron scattering from metastable states of He [9,10]. Alternative studies using positrons instead of electrons may, therefore, shed more light on the reasons for such discrepancies.

II. FORMALISM

Consider scattering of positron on helium. In the nonrelativistic approach to the problem, the Hamiltonian for this system is written as

$$H = H_0 + \frac{2}{r_0} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} - \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_1|} - \frac{1}{|\boldsymbol{r}_0 - \boldsymbol{r}_2|}, \tag{1}$$

or, equivalently, in another set of the Jacobi coordinates,

$$H = H_0 + \frac{2}{\left|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho}\right|} - \frac{2}{\left|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho}\right|} - \frac{2}{r_2} + \frac{1}{\left|\boldsymbol{R} - \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}_2\right|} - \frac{1}{\rho} - \frac{1}{\left|\boldsymbol{R} + \frac{1}{2}\boldsymbol{\rho} - \boldsymbol{r}_2\right|}, \tag{2}$$

where

$$H_0 = -\tfrac{1}{2}\nabla_0^2 - \tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 \equiv -\nabla_\rho^2 - \tfrac{1}{4}\nabla_R^2 - \tfrac{1}{2}\nabla_2^2$$

is the free Hamiltonian of three particles and $\boldsymbol{r}_0$, $\boldsymbol{r}_1$, and $\boldsymbol{r}_2$ denote the positions of the positron, electrons 1 and 2, respectively, while $\boldsymbol{R} = (\boldsymbol{r}_0 + \boldsymbol{r}_1)/2$ is the position of the Ps center of mass (c.m.) relative to the helium nucleus and $\boldsymbol{\rho} = \boldsymbol{r}_0 - \boldsymbol{r}_1$ is the relative coordinate of the positron and electron 1. For scattering processes and collision energies of our interest we can simply neglect spin-orbit interactions. The Hamiltonian (1) conserves two-electron spin s, total spin S of three particles (two electron and positron), and its projection M. The two systems of coordinates $(\boldsymbol{r}_0,\boldsymbol{r}_1,\boldsymbol{r}_2)$ and $(\boldsymbol{R},\boldsymbol{\rho},\boldsymbol{r}_2)$ are shown in Fig. 1. We emphasize that since there are two electrons which can form Ps, there are two corresponding sets of Jacobi coordinates. When necessary we will refer to them explicitly as $(\boldsymbol{R}_1,\boldsymbol{\rho}_1,\boldsymbol{r}_2)$ and $(\boldsymbol{R}_2,\boldsymbol{\rho}_2,\boldsymbol{r}_1)$. Figure 1 shows one of

*R.Utamuratov@curtin.edu.au

them, where Ps is formed by electron 1; the second is obtained by exchanging electrons 1 and 2.

The total scattering wave function Ψ^{SM} for the system satisfies the Schrödinger equation,

$$(H - E)\Psi^{SM}(\boldsymbol{x}_0,\boldsymbol{x}_1,\boldsymbol{x}_2) = 0, \tag{3}$$

where E is a total energy and $\boldsymbol{x}_0,\boldsymbol{x}_1$, and $\boldsymbol{x}_2$ are all the coordinates of the particles including spin ones.

For positron scattering from atoms the system has two centers, one associated with the target atom and the other with Ps. In addition, positronium can be formed in both para (p-Ps) and ortho (o-Ps) states depending on spin projections of electron and positron which form Ps. The two-center convergent close-coupling approach to positron-He scattering is based on the expansion of the the total wave function Ψ^{SM} in terms of states of all asymptotic channels, that is,

$$\Psi^{SM} \approx (1 - P_{12}) \left\{ \sum_{\alpha}^{N_{\rm He}} \sum_{s_\alpha} F_{\alpha,s_\alpha}(\boldsymbol{r}_0)\psi_{\alpha,s_\alpha}(\boldsymbol{r}_1,\boldsymbol{r}_2)\chi_{s_\alpha SM}\big((0,(1,2)\big) + \sum_{\beta}^{N_{\rm Ps}} \sum_{s_\beta} [G_{\beta,s_\beta}(\boldsymbol{R}_1)\phi_i(\boldsymbol{r}_2)]\psi_\beta(\boldsymbol{\rho}_1)\chi_{s_\beta SM}\big((0,1),2\big) \right\}, \tag{4}$$

where the first term corresponds to expansion in terms of the helium wave functions ψ_{α,s_α} with expansion coefficients F_{α,s_α}. The second term corresponds to expansion in terms of the positronium states ψ_β with coefficients G_{β,s_β}. These coefficients, in turn, depend on spins s_α and s_β of He and Ps, respectively. However, since the total spin of the system is conserved during scattering and positron cannot change the target spin the coefficients F_{α,s_α} and G_{β,s_β} do not depend on S (this is in contrast to the electron scattering). The $N_{\rm He}$ and $N_{\rm Ps}$ are the numbers of the atomic and Ps states, respectively. Indices α and β denote the full set of quantum numbers (except spins) of the helium atom and Ps, respectively, and run over all the generated pseudostates. The singlet and triplet He states have $s_\alpha = 0$ and $s_\alpha = 1$, respectively. The second term allows for both electrons to form positronium and the sum over s_β takes into account positronium formation in para ($s_\beta = 0$) and ortho ($s_\beta = 1$) states. The residual ion of He^+ is described by ϕ_i. The antisymmetrization over two-electron permutations is included by the operator $(1 - P_{12})$, where P_{12} is a permutation operator which interchanges the electrons 1 and 2. The spin functions are defined as

$$\chi_{s_\alpha SM}\big((0,(1,2)\big) = \sum_{\mu_0,\mu_\alpha} C^{SM}_{\frac{1}{2}\mu_0\, s_\alpha\mu_\alpha}\chi_{\frac{1}{2}\mu_0}(0)\chi_{s_\alpha\mu_\alpha}(1,2), \tag{5}$$

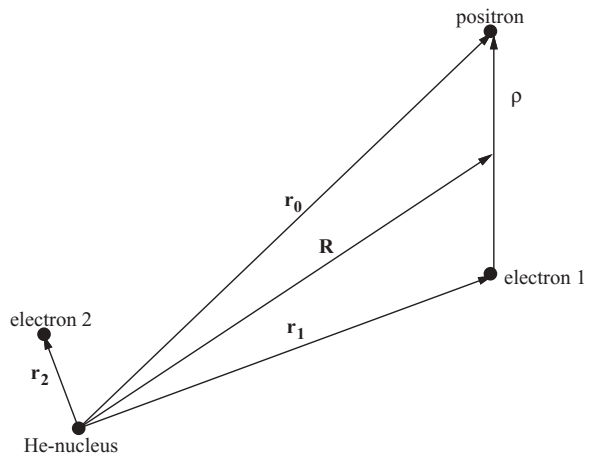

FIG. 1. Coordinate system for positron-helium scattering.

for the $e^+ + \text{He}$ channel, and

$$\chi_{s_\beta SM}\big((0,1),2\big) = \sum_{\mu_2,\mu_\beta} C^{SM}_{\frac{1}{2}\mu_2\, s_\beta\mu_\beta}\chi_{s_\beta\mu_\beta}(0,1)\chi_{\frac{1}{2}\mu_2}(2) \tag{6}$$

for the $\text{Ps} + \text{He}^+$ channel. Inner brackets indicate the bound particles.

As mentioned earlier positron scattering does not change the spin state of two electrons. Consequently, if the target is in the initial state with spin s then only the states with two-electron spin $s_\alpha = s$ can be excited. Therefore, by projecting (4) onto the initial spin state of the target $\chi_{sSM}\big((0,(1,2)\big)$ we can extract a particular part of the total wave function (4) for a given spin state of the target,

$$\Phi^{sS}(\boldsymbol{r}_0,\boldsymbol{r}_1,\boldsymbol{r}_2) = \langle \chi_{sSM}\big((0,(1,2)\big) \mid \Psi^{SM}\rangle. \tag{7}$$

In order to find the overlap on the right-hand side of Eq. (7) we perform spin algebra somewhat similar to the electron-helium scattering case presented in [11]. Using Eqs. (5) and (6) and the fact that spin functions χ_{sSM} form a complete set we get the following relations:

$$\begin{aligned}
&\chi_{s_\alpha SM}\big((0,(2,1)\big) \\
&\quad = \sum_{s'} \chi_{s'SM}\big((0,(1,2)\big)\langle\chi_{s'SM}\big((0,(1,2)\big)|\chi_{s_\alpha SM}\big((0,(2,1)\big)\rangle \\
&\quad = (-1)^{s_\alpha+1}\chi_{s_\alpha SM}\big((0,(1,2)\big), \qquad (8)\\
&\chi_{s_\beta SM}\big((0,(1,2)\big) \\
&\quad = \sum_{s'} \chi_{s'SM}\big((0,(1,2)\big)\langle\chi_{s'SM}\big((0,(1,2)\big)|\chi_{s_\beta SM}\big((0,(1,2)\big)\rangle \\
&\quad = \sum_{s'} c_{s_\beta s'S}\chi_{s'SM}\big((0,(1,2)\big), \qquad (9)
\end{aligned}$$

and using the previous two relations we also obtain

$$\chi_{s_\beta SM}\big((0,(1,2)\big) = \textstyle\sum_{s'}(-1)^{s'+1}c_{s_\beta s'S}\chi_{s'SM}\big((0,(1,2)\big), \tag{10}$$

where the overlap coefficients are given by the $6j$ symbol

$$c_{s_\beta s'S} = (-1)^{S-\frac{1}{2}}\sqrt{(2s_\beta+1)(2s'+1)}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s_\beta \\ S & \frac{1}{2} & s' \end{Bmatrix}. \tag{11}$$

Now we can rewrite the expansion (4), by explicitly writing the result of the $(1 - P_{12})$ operator and using the recoupling coefficients (11) we get:

$$\begin{aligned}\Psi^{SM} \approx & \sum_{\alpha}^{N_{\rm He}} \sum_{s_\alpha} F_{\alpha,s_\alpha}(\boldsymbol{r}_0)\big\{\psi_{\alpha,s_\alpha}(\boldsymbol{r}_1,\boldsymbol{r}_2) \\ & + (-1)^s \psi_{\alpha,s_\alpha}(\boldsymbol{r}_2,\boldsymbol{r}_1)\big\}\chi_{s_\alpha SM}(0,(1,2)) \\ & + \sum_{\beta}^{N_{\rm Ps}} \sum_{s_\beta s'} c_{s_\beta s' S}\big\{G_{\beta,s_\beta}(\boldsymbol{R}_1)\psi_\beta(\boldsymbol{\rho}_1)\phi_i(\boldsymbol{r}_2) \\ & + (-1)^{s'} G_{\beta,s_\beta}(\boldsymbol{R}_2)\psi_\beta(\boldsymbol{\rho}_2)\phi_i(\boldsymbol{r}_1)\big\}\chi_{s' SM}(0,(1,2)).\end{aligned} \tag{12}$$

By projecting according to Eq. (7) we get the spatial part of the total wave function:

$$\begin{aligned}&\Phi^{sS}(\boldsymbol{r}_0,\boldsymbol{r}_1,\boldsymbol{r}_2) \\ &\quad \approx \sum_{\alpha}^{N_{\rm He}} \delta_{s_\alpha,s} F_{\alpha,s_\alpha}(\boldsymbol{r}_0)\big\{\psi_{\alpha,s_\alpha}(\boldsymbol{r}_1,\boldsymbol{r}_2) + (-1)^s \psi_{\alpha,s_\alpha}(\boldsymbol{r}_2,\boldsymbol{r}_1)\big\} \\ &\qquad + \sum_{s_\beta} c_{s_\beta s S} \sum_{\beta}^{N_{\rm Ps}} \big\{G_{\beta,s_\beta}(\boldsymbol{R}_1)\psi_\beta(\boldsymbol{\rho}_1)\phi_i(\boldsymbol{r}_2) \\ &\qquad + (-1)^s G_{\beta,s_\beta}(\boldsymbol{R}_2)\psi_\beta(\boldsymbol{\rho}_2)\phi_i(\boldsymbol{r}_1)\big\}.\end{aligned} \tag{13}$$

The Ps spin s_β can be 0 or 1; writing the sum over s_β explicitly we finally obtain

$$\begin{aligned}\Phi^{sS} \approx & \sum_{\alpha}^{N_{\rm He}} \delta_{s_\alpha,s} F_{\alpha,s_\alpha}(\boldsymbol{r}_0)\big\{\psi_{\alpha,s_\alpha}(\boldsymbol{r}_1,\boldsymbol{r}_2) + (-1)^s \psi_{\alpha,s_\alpha}(\boldsymbol{r}_2,\boldsymbol{r}_1)\big\} \\ & + \sum_{\beta}^{N_{\rm Ps}} \big\{\tilde{G}^{(s)}_\beta(\boldsymbol{R}_1)\psi_\beta(\boldsymbol{\rho}_1)\phi_\beta(\boldsymbol{r}_2) \\ & + (-1)^s \tilde{G}^{(s)}_\beta(\boldsymbol{R}_2)\psi_\beta(\boldsymbol{\rho}_2)\phi_\beta(\boldsymbol{r}_1)\big\},\end{aligned} \tag{14}$$

where we introduced

$$\tilde{G}^{(s)}_\beta(\boldsymbol{R}) = c_{0sS} G_{\beta,0}(\boldsymbol{R}) + c_{1sS} G_{\beta,1}(\boldsymbol{R}). \tag{15}$$

Let us consider now particular cases. For positron scattering from the ground state of helium, that is, when $s = 0$ and $S = \frac{1}{2}$, we get

$$c_{00\frac{1}{2}} = -1/2 \text{ and } c_{10\frac{1}{2}} = \frac{\sqrt{3}}{2}. \tag{16}$$

Therefore, according to Eq. (15) the corresponding expansion coefficient takes the form,

$$\tilde{G}^{(0)}_\beta(\boldsymbol{R}) = -\frac{1}{2} G_{\beta,0}(\boldsymbol{R}) + \frac{\sqrt{3}}{2} G_{\beta,1}(\boldsymbol{R}), \tag{17}$$

which agrees with the result derived in [7]. For positron scattering on the metastable states of helium with $s = 1$ there are two different couplings with the incoming positron's spin resulting in $S = \frac{1}{2}$ and $S = \frac{3}{2}$. When $S = \frac{1}{2}$ we have

$$c_{01\frac{1}{2}} = \frac{\sqrt{3}}{2} \text{ and } c_{11\frac{1}{2}} = \frac{1}{2}. \tag{18}$$

Therefore,

$$\tilde{G}^{(1)}_\beta(\boldsymbol{R}) = \frac{\sqrt{3}}{2} G_{\beta,0}(\boldsymbol{R}) + \frac{1}{2} G_{\beta,1}(\boldsymbol{R}). \tag{19}$$

If the spins couple to give $S = \frac{3}{2}$, then

$$c_{01\frac{3}{2}} = 0 \text{ and } c_{11\frac{3}{2}} = 1, \tag{20}$$

leading to

$$\tilde{G}^{(1)}_\beta(\boldsymbol{R}) = G_{\beta,1}(\boldsymbol{R}). \tag{21}$$

Finally, since Eqs. (19) and (21) represent the same amplitude we conclude that

$$G_{\beta,1} = \sqrt{3} G_{\beta,0}. \tag{22}$$

This relationship is often assumed and used in the literature, however, to our best knowledge, it has not been derived.

The procedures for constructing He and Ps states and for solving the scattering equations were given in Ref. [7]. The transition matrix elements are obtained in the same way as in [7] with account of different symmetry in the radial part of the total wave function (14).

III. RESULTS

Based on our previous results for positron scattering from hydrogen [12] and helium [13], we know that smooth and pseudoresonance-free cross sections can be obtained if both centers are treated on equal footing, for example, by taking the same number ($N_l = N_0 - l, l \leqslant l_{\rm max}$) of Laguerre-basis states for both centers.

We present here calculations with the following basis sizes from both the atomic and the Ps centers:

(*a*) $N_0 = 15, l_{\rm max} = 0$,
(*b*) $N_0 = 15, l_{\rm max} = 1$,
(*c*) $N_0 = 15, l_{\rm max} = 2$,
(*d*) $N_0 = 15, l_{\rm max} = 3$,
(*e*) $N_0 = 17, l_{\rm max} = 1$.

With other targets, close-coupling calculations with pseudostates on a target center and only a few eigenstates on Ps may produce unphysical resonance features in the cross sections. To check whether this occurs with a metastable helium target as well we also performed calculations with the basis *c* for He and only the three lowest eigenstates (1*s*, 2*s*, and 2*p*) of Ps, results of which we denote as CC(41,3).

Results of the first four bases (*a*–*d*) will illustrate the convergence over increasing $l_{\rm max}$. The convergence over

TABLE I. Ionization energies of lowest triplet states of He in eV.

State	FC model	Experiment
$2\,^3S$	4.742	4.767
$2\,^3P$	3.573	3.622
$3\,^3S$	1.864	1.868
$3\,^3P$	1.566	1.580
$3\,^3D$	1.512	1.513
$4\,^3S$	0.944	0.993
$4\,^3P$	0.792	0.879
$4\,^3D$	0.791	0.851

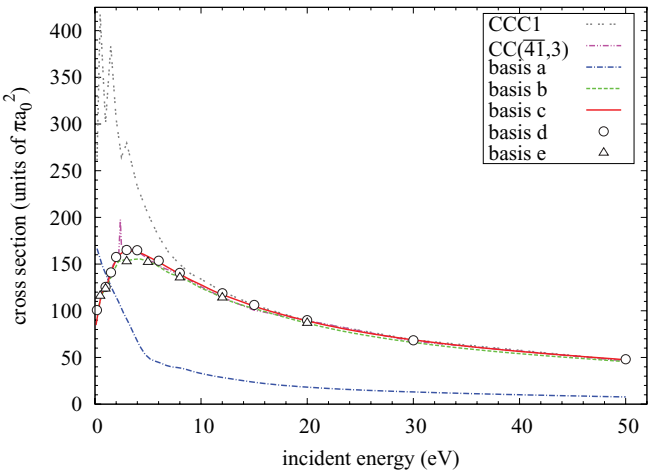

FIG. 2. (Color online) e^+-He($2\,^3S$) total cross sections. The calculations are described in the text.

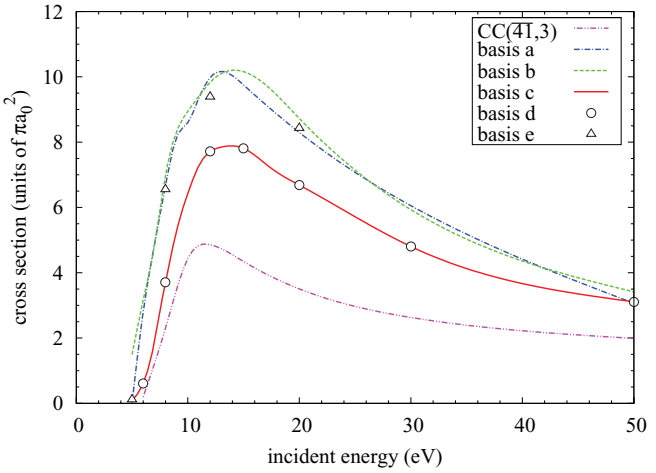

FIG. 4. (Color online) e^+-He($2\,^3S$) total breakup cross sections. The calculations are described in the text.

increasing N_0 can be seen by comparing the results of bases e and b.

For simplicity, all bases are generated with the Laguerre fall-off parameter set to $\lambda = 2$ for He, and $\lambda = 0.5$ for Ps. We used a frozen-core (FC) configuration interaction model to construct the triplet-state He wave functions. The lowest excited states are described sufficiently well within this model. Table I shows the lowest ionization energies of metastable He used in our calculations and compared to experimental values [14].

As seen from Table I, the lowest triplet states of He are sufficiently well described, and thus represent true eigenstates. Higher lying states diverge from true eigenstates and are referred to as pseudostates. By increasing the basis size, N_l, the number of true eigenstates can be increased to a given accuracy. The Ps states generated with the previously mentioned bases give a nearly exact ground and the lowest excited states of Ps.

Figure 2 shows the grand total cross sections calculated with different bases.

In addition to calculations with the two-center bases mentioned previously we also give convergent single-center results which were obtained with the basis of size $N_0 = 14$ and $l_{\max} = 8$. These are referred to as CCC1. As seen from Fig. 2 the single-center expansion approach though converged, can yield accurate results only at above 10 eV. At lower energies the approach cannot be relied upon. Results of CC(41,3) are almost indistinguishable from the fully convergent ones, except around 2 eV where there is a narrow pseudoresonance. Results of different bases a–e show that the convergence is achieved in both N_0 and $l_{\max}$. The most interesting feature with increasing $l_{\max}$ is the sudden change of the results from basis a, which is the s-wave model, to basis b with $l_{\max} = 1$. The reason for this is the big contribution of $2\,^3P$ excitation which is neglected in the s-wave calculations. As we can see, basis b, which only has s and p states, is quite sufficient to get the total scattering cross sections within 10% accuracy. The convergence is achieved with basis c, which has $14\,^3S$, $14\,^3P$, and $13\,^3D$ states. Adding F states (basis d), changes the results by no more than 1%.

Ps-formation cross sections are given in Fig. 3. The single-center model does not provide Ps-formation cross sections. Adding only three Ps states as in CC(41,3) exhibits pseudoresonance features, which indicate the necessity of treating both

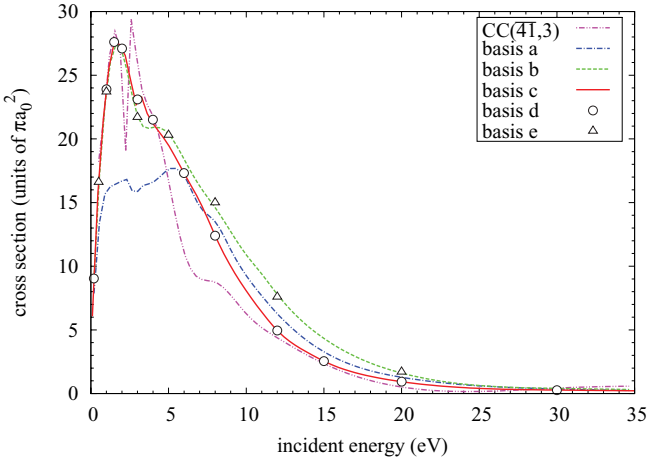

FIG. 3. (Color online) e^+-He($2\,^3S$) total Ps-formation cross sections. The calculations are described in the text.

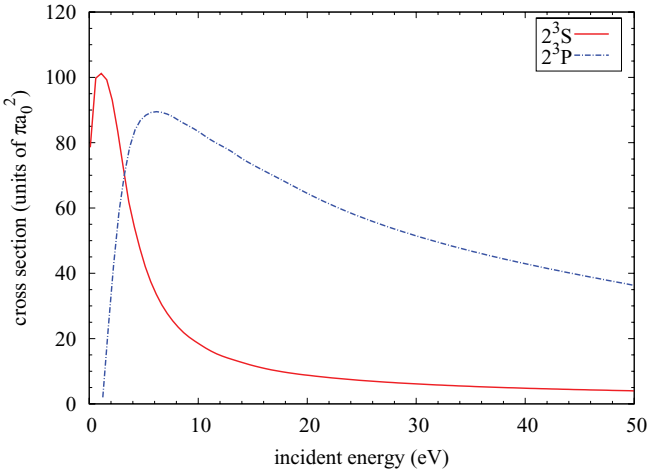

FIG. 5. (Color online) Elastic He($2\,^3S$) and He($2\,^3P$) excitation cross sections calculated using basis c ($l_{\max} = 2$); see text.

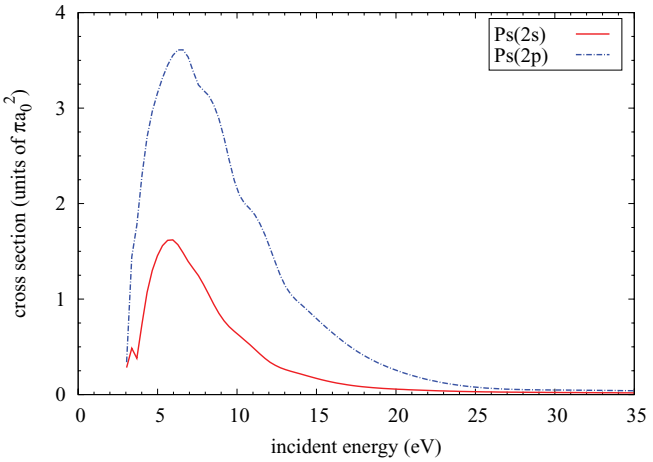

FIG. 6. (Color online) Ps(2*s*,2*p*) excitation cross sections calculated using basis *c* ($l_{max} = 2$); see text.

centers with extended bases. Note that a similar pseudoresonance was obtained in positron scattering on the ground state [6]. Results of the *s* wave (basis *a*) underestimate around the peak and are not smooth around the Ps(2*s*) excitation threshold at 3.04 eV. Basis *b* seems sufficient to obtain reasonably convergent total Ps-formation cross sections. However, it still shows some instability around the Ps($n = 2$) excitation threshold and overestimates the convergent results at high energies. As in the case of the total cross section, basis *c* is sufficient to get convergent Ps-formation cross sections. The convergent total Ps-formation cross sections have a shallow and very narrow local minima at the Ps(n=2) excitation threshold. This minima appears as a result of a sharply decreasing Ps(1*s*) cross section and fast-rising Ps(2*s*) and Ps(2*p*) cross sections.

Figure 4 shows the total breakup cross section calculated as a sum of the cross sections for excitation of positive-energy pseudostates of He and electron capture into the Ps pseudocontinuum. As we go down to the ionization threshold region these two contributions approach each other confirming similar behavior observed in [15] for the positron-hydrogen scattering case. The CC(41,3) results are almost half the

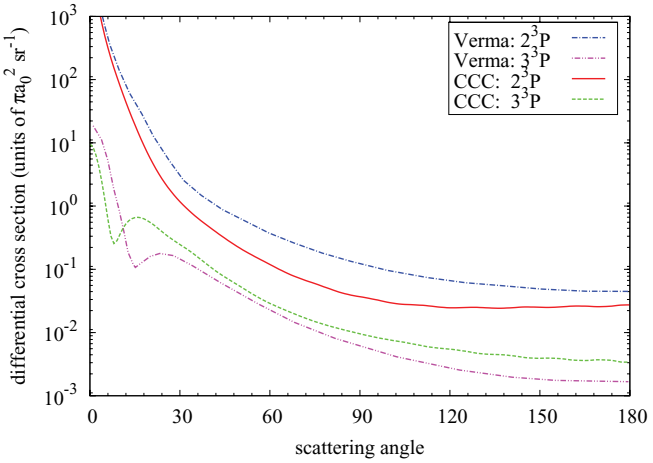

FIG. 7. (Color online) Angle differential cross section. The theoretical calculations are due to Verma and Srivastava [4] and present results are described in the text.

convergent results of the bases *c* and *d*. Interestingly, the bases *a* and *b* results are close to each other suggesting *p* states play little role in the total breakup process. Adding *d* states is significant, however, and has changed the results by around 20%. Adding even larger orbital momentum states (basis *e*) has not had a noticeable effect.

As can be seen from the results for the total, Ps-formation and breakup cross sections, basis *c* (including the *s*, *p*, and *d* states) is sufficient in *l* for convergent results. Therefore, in the cross sections that are presented further, we give only the results of basis *c*, unless otherwise stated.

The elastic He($2\,^3S$) and first excitation He($2\,^3P$) cross sections are given in Fig. 5. As seen from the figure, the elastic cross section reaches its maximum at 1 eV and then

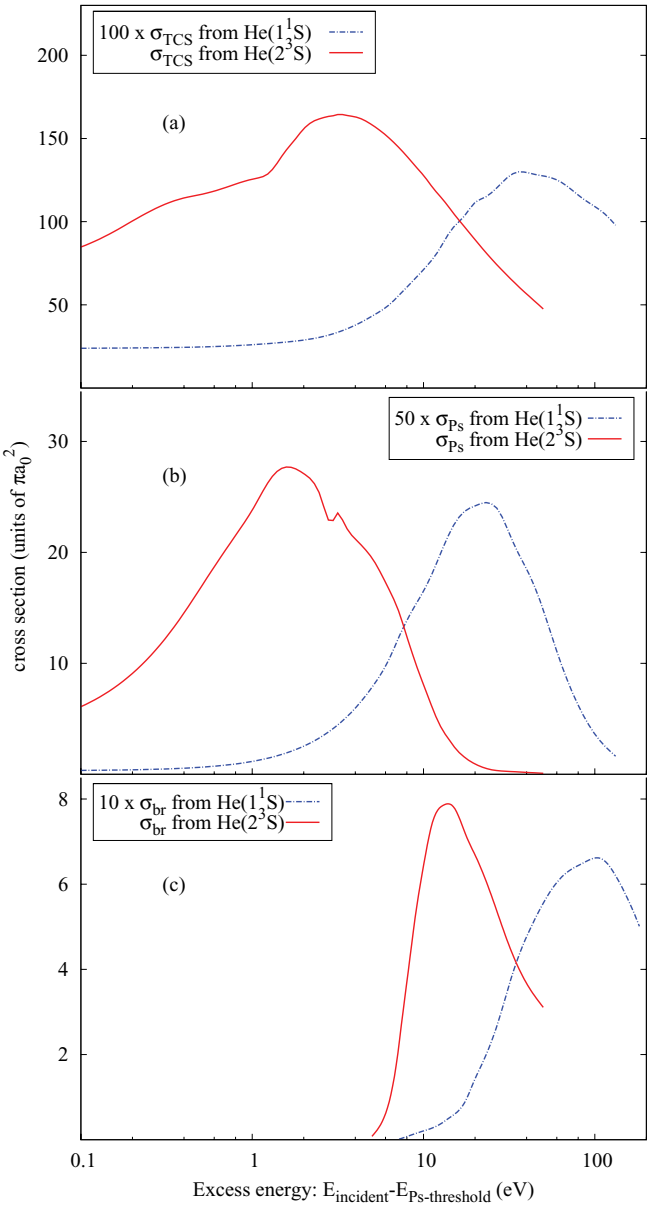

FIG. 8. (Color online) Comparison of (a) grand total, (b) total Ps-formation, and (c) total breakup cross sections for $e^+ + \mathrm{He}(1\,^3S)$ and $e^+ + \mathrm{He}(2\,^3S)$ scattering as a function of excess energy above the Ps threshold.

drops fast and stays stable starting from 20 eV. Excitation to $2\,^3P$ reaches its maximum around 6 eV and then slowly decreases. If we compare this figure with Fig. 2 we see that at higher energies the main contribution to total scattering comes from $2\,^3P$ excitation. Convergence in this channel requires inclusion of very high partial waves. We overcome this by implementing the Born subtraction method, using which we can get sufficiently accurate results by performing full close-coupling calculations only up to 20 partial waves. Recently, Murtagh *et al.* [16] have reported Ps formation in excited states in the positron scattering from the ground state of He, which are in good agreement with our calculations [7]. We present the corresponding results for He($2\,^3S$) in Fig. 6. We note that Ps($2p$) excitation is more than two times higher than for Ps($2s$) excitation. This is unlike the positron-He($1\,^1S$) case, where they have comparable magnitudes.

Lastly, we compare with the calculations of Verma and Srivastava [4] for angular differential cross sections (DCS) for $n\,^3S$ and $n\,^3P$ states, where $n = 2,3$, obtained by a distorted-wave approximation. Figure 7 shows DCS of $2\,^3S \rightarrow n\,^3P$ transitions at final positron energy of 20 eV (which corresponds to 21.2 and 23.2 eV scattering energy for $2\,^3P$ and $3\,^3P$, respectively). At this relatively high energy the contribution of Ps formation is negligible and the two-center results for atomic excitation become much the same as the single center ones. We can see qualitative agreement between our results and the calculations of Verma and Srivastava [4]. Our results for $2\,^3S \rightarrow 2\,^3P$ are a bit lower than the results of [4] above 20°. In the case of $2\,^3S \rightarrow 3\,^3P$ both methods predict a minimum at around 10°–15°.

Comparison of the integrated cross sections for positron scattering from He($2\,^3S$) and He($1\,^1S$) is given in Fig. 8. Relative magnitudes of cross sections vary substantially depending on the processes. The breakup cross section of He($2\,^3S$) is around 10 times higher than for He($1\,^1S$) at its peak, while for Ps formation this difference is around 50 times. The total scattering cross section of He($2\,^3S$) is almost 100 times larger than for He($1\,^1S$). The large relative ratio of cross section in the case of He($2\,^3S$) to He($1\,^1S$) shows the importance of the studies from excited states.

IV. CONCLUSION

Positron scattering from metastable He($2\,^3S$) has been theoretically studied at low energies. The results show that presence of excited states in the experimental target gas chamber may significantly enhance the cross sections demonstrating the importance of this process in understanding positron scattering from helium. Therefore, we hope that the present work will generate interest in the considered collision system from both experimentalists and other theorists.

Convergent results for total, Ps-formation and breakup cross sections have been obtained with high accuracy of convergence. Our studies also confirm the applicability of two-center convergent close-coupling method to systems with zero Ps-formation threshold. The main conclusions of previous two-center CCC studies apply to the $e^+ + \mathrm{He}(2\,^3S)$ system, too, namely the necessity of using a similar number of pseudostates from both centers to avoid unphysical resonances.

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