Scattering of positronium from singly ionized helium and appearing resonances.

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Abstract

The coupled-channel model [Phys. Rev. A 59, 363 (1999)] that yields converged low-energy phase shifts, and exact binding and resonance features in Ps-H [Phys. Rev. A 59, 2058 (1999)] is applied to study Ps-He\(^+\) scattering. Similar to PsH, resonances appear in the \(S^-\), \(P^-\), \(D^-\), etc partial waves in the Ps-He\(^+\) system but in both the singlet and triplet scattering channels. The latter signifies possible Rydberg states of \(e^+\) around singlet and triplet helium. The S-wave singlet resonance at 2.79 eV agrees to that predicted earlier in \(e^+\)-He entrance channel (energy difference 16.64 eV) at 19.27 eV [Chem. Phys. Lett. 262, 460 (1996)].
Introduction: Ps-H is a fundamental few-body system containing the positronium atom and has got an active theoretical \[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14\] and recent experimental \[15\] interest. In this article, we present an investigation on ortho-Ps scattering from singly ionized helium atom. The system is apparently similar to the four-body Ps-H system, but provides the following additional interests. Firstly, within a similar four-body framework, we can study Ps scattering dynamics relating to an ionic target, where short-range exchange correlation is also present. So far, Ps-ion scattering studies have been confined mostly to bare ions \[16, 17\] (except a few studies \[18, 19\]) where there is no role for the Pauli exclusion principle to play in absence of indistinguishable fermions (electrons). Pauli exclusion principle introduces short-range exchange forces which become crucial for Ps scattering. Because, in absence of exchange, the potential in the elastic channel becomes exactly zero due to charge and mass symmetry of Ps \[20\]. Thus in order to have a comprehensive picture of the Ps-ion scattering dynamics, it is important to investigate Ps scattering from an ionic target that has indistinguishable fermions (electron or positron).

Secondly, we recall that, at low energies Coulomb interaction of positronium atom (Ps) with hydrogen like system, leads to interesting consequences like formation of resonances \[1, 2, 3, 4, 5, 6, 7, 8, 9\] and chemical binding \[5, 13, 14, 15\]. It has been interpreted in a Ps-H system that, the positron forms Rydberg states with the residual H\(^-\) ion \[2\]. The lowest order Rydberg state in the series lies below the Ps-H scattering threshold and leads to chemical binding. Higher order states lie above the scattering threshold and lead to resonances in the Ps-H continuum \[3\]. In Ps-H, the residual H\(^-\) can exist only in the singlet state and all these resonances and binding reported so far are in the singlet state. For Ps-He\(^+\) system, the positron shall find a residual helium atom which can have both singlet and triplet spin configurations, unlike the Ps-H case. So, in principle, in Ps-He\(^+\), resonances could appear in both the singlet and triplet scattering channels. Recently,
a metastable state for positronic helium \((e^+\text{He})\) is predicted \cite{21} with a binding energy of -2.2505916 Hatree and the state is found to be stable under dissociation into PsHe\(^+\) with a binding energy of -0.0005916 Hatree. The chemical stability of PsHe\(^+\) once again triggers the speculation of resonances like those obtained in the PsH system.

As in Ps-H \cite{8, 10}, we consider coupling of Ps-states to He\(^+\) ion and investigate target elastic processes. As He\(^+\) is a tightly bound system, we understand that target inelastic processes will not be significant owing to its small polarizability compared to that of the Ps. However, charge-transfer rearrangement like Ps+He\(^+\) → \(e^++\text{He}\) is a relevant process and is expected to have its impact over target-elastic and target-inelastic processes. However, we understand that such channels are relevant in a complete \textit{ab initio} calculation where explicit electron-electron correlation and continuum effects are essential to achieve convergence. Here, we are using regularized exchange-correlation potentials which are able to simulate the correlation and continuum effects \cite{8, 9, 11} (detailed in the theory section). So, we abstain from considering such channels explicitly. Since, their explicit inclusion in the present model may lead to overcompleteness of the Hilbert space.

\textbf{Theory:} The theoretical formulation of the Ps-He\(^+\) scattering is very similar to that of the Ps-H system except the difference comes from the nuclear charge, in the interaction potential and target wave function. With an antisymmetrized total wave function \cite{7, 9, 11}, the momentum space Lippmann-Schwinger equation, for a particular electronic spin state \(S\), takes the following form \cite{11, 12}.

\[
f^{S}_{\nu',\mu',\nu\mu}(k_f, k_i) = B^{S}_{\nu',\mu',\nu\mu}(k_f, k_i) - \frac{1}{2\pi^2} \sum_{\nu''} \sum_{\mu''} \int dk'' \frac{B^{S}_{\nu''\nu',\mu''\mu'}(k_f, k'') f^{S}_{\nu''\mu'',\nu\mu}(k'', k_i)}{k''^2 - k''^2 + i0} \tag{1}
\]

where \(k_i, k_f\) are the initial and final momentum of the Ps atom with respect to the center of mass and \(k''^2 = \frac{2m}{\hbar^2} \{E - \epsilon_{\nu''} - \Upsilon_{\mu''}\}\); \(m\) is the reduced mass of Ps. \(E\) represents the total energy of the system; \(\epsilon_{\nu''}\) and \(\Upsilon_{\mu''}\) represent the binding energies of Ps and target.
respectively. We need to solve two sets of coupled equations corresponding to singlet and triplet scattering channels given by \( S = 0, 1 \). The corresponding spin-averaged input potentials are given by

\[
\mathcal{B}^{0,1}_{\nu'\mu'\nu\mu}(k_f, k_i) = B^D_{\nu'\mu'\nu\mu}(k_f, k_i) + (-1)^{0,1}B^E_{\nu'\mu'\nu\mu}(k_f, k_i)
\]

(2)

Where, \( B^D \) and \( B^E \) are the direct Born and Born-Oppenheimer (BO) exchange amplitudes, respectively. The expression for \( B^D \) can be simplified and be represented as [22]:

\[
B^D_{\nu'\mu'\nu\mu}(k_f, k_i) = -\frac{4}{q^2} < \phi_{\mu'}(r_1)|2 - e^{iq.r_1}|\phi_{\mu}(r_1) > \\
\times < \chi_{\nu'}(t_2)|e^{i\alpha_1/2} - e^{-i\alpha_1/2}|\chi_{\nu}(t_2) > ,
\]

(3)

where \( q = k_i - k_f \) and \( \phi_{\mu} \)'s and \( \chi_{\nu} \)'s are the eigenstates of \( \text{He}^+ \) and \( \text{Ps} \) atom, respectively. \( t_j = r_j - x; \) \( x \) and \( r_j \) are the coordinates of the positron and the electron of the \( \text{Ps} \) atom.

For \( B^E \), we use the following non-local form [10, 23], similar to that applied in \( \text{PsH} \) case:

\[
B^E_{\nu'\mu'\nu\mu}(k_f, k_i) = \frac{4}{Q^2} < \phi_{\mu'}(r)|e^{iq.r}|\phi_{\mu}(r) > \\
\times < \chi_{\nu'}(t)|e^{i\beta_1/2} |\chi_{\nu}(t) > ,
\]

(4)

where, \( Q^2 = (k_f^2 + k_i^2)/8 + C^2[(\alpha_{\mu'}^2 + \alpha_{\nu}^2)/2 + (\beta_{\nu'}^2 + \beta_{\nu}^2)/2] \). This form is arrived at by making use of the effective following type of transformations to the exact BO expression for excahnge:

\[
\int \chi_{\nu'}(x - r_2) \frac{1}{|r_1 - r_2|} d^3r_2 \approx \frac{1}{(C\beta_{\nu'})^2} \chi_{\nu'}(x - r_1)
\]

(5)

\[
\int \phi_{\mu}(r_2) \frac{1}{|r_1 - r_2|} d^3r_2 \approx \frac{1}{(C\alpha_{\mu})^2} \phi_{\mu}(r_1)
\]

(6)

where \( \alpha_{\mu}, \beta_{\nu} \) etc are parameters of the Slater orbitals of \( \text{He}^+ \) and \( \text{Ps} \), respectively; with \( \alpha_{\mu}^2, \alpha_{\mu'}^2 \) representing the binding energies of \( \text{He}^+ \) in the initial and final states in Rydberg units, and \( \beta_{\nu}^2, \beta_{\nu'}^2 \) are the binding energies of the initial and final \( \text{Ps} \) states in atomic units (au), respectively. A dummy parameter \( C \), is introduced in the expression of \( Q^2 \), which can be
used to simulate the factor $C^2[(\alpha^2 + \alpha^2_m)/2 + (\beta^2 + \beta^2_{\nu})/2]$ close to the total ionization energy of the system in $au$ or facilitate any variation to this as has been effectively done for several electron impact cases [24]. It is of significant advantage that at asymptotic energies, both the value of the parameter $C$ and the regularized form above, do loose their significance and the exchange potential ($B^E$) and hence the solution of the coupled-equations coalesce, respectively, with those of the exact CC formalism. In the present work, however, we do not indulge to any fitting and rather paralyze the sensitivity of the parameter by re-introducing it in the following way: $Q_j^2 = (k_f^2 + k_i^2)/8 + (\beta^2_{\nu} + \beta^2_{\nu})/2 + C^2[(\alpha^2 + \alpha^2_m)/2]$ and by fixing $C^2 = 0.5$ so that the expression $(\beta^2_{\nu} + \beta^2_{\nu})/2 + 0.5[(\alpha^2 + \alpha^2_m)/2]$ yields the average binding energies (between initial and final channel) of the electron of Ps and He$^+$ in $au$, in which the calculation is performed.

**Numerical Procedures** : The three-dimensional LS equations, for a particular electronic-spin state ($S$) are decomposed to coupled one-dimensional partial wave equations, which are then solved by the method of matrix inversion [11, 17]. For the present ionic target, we register a slow convergence with respect to partial wave contributions, compared to the neutral atomic target. We had to employ as much as thirty partial waves at around 50-60eV incident energies, which is almost twice to that employed for Ps-H case. Also, the convergence is found to be slow with respect to the mesh points that discretizes the kernel of the coupled-equations. We take maximum 48 mesh points to discretize the kernel compared to a maximum 32 points taken for Ps-H. Present results are numerically convergent upto fourth significant digit.

**Results and Discussions** : We first discuss the results for the partial and total cross sections. In figure 1, we plot the angle integrated partial cross sections containing elastic and inelastic transitions of Ps. Elastic (thin solid curve), Ps(1s→2s) (dotted curve) and Ps(1s→2p) (short-dashed curve) transition cross sections are obtained by solving coupled equations using a 3-Ps-state expansion. Results for Ps(1s→$nlm$; 3 $\leq n \leq 6$),
discrete excitations (long-dashed curve) and ionization (dot-dashed curve) cross sections are obtained employing a first Born approximation including exchange. Total (target elastic) cross sections which are constructed from the results of Ps-elastic and all Ps-inelastic cross sections, are also plotted in this figure (thick solid curve). At low energies, the elastic and total cross sections have a sharp fall compared to those of the Ps-H system. Similar sharp fall in the cross section is also observed in the variational calculations for Ps-He$^+$ and Ps-p scatterings [19] and in the coupled-channel calculation for Ps-p scattering [17].

At low energies, Van Reeth and Humberston (VRH) [19], employing a two-channel Kohn variational method, observed a Ramsauer minimum for the elastic cross sections near 0.02 au of Ps energy and a gentle rise thereafter. We do not observe any such minimum in our elastic cross sections but otherwise observe a gross agreement with VRH. To understand the difference we recently perform a similar two-channel ab initio CC calculation employing exact exchange and considering the charge-transfer reaction Ps+He$^+ \rightarrow e^+ + $He. In our preliminary results [25] we also do not record any such Ramsauer minimum. Further insight seems warranted regarding the minimum.

At medium to high energies, we can expect the He$^+$ to behave more like a bare proton and we find our results to agree with those of Ps-p scattering cross sections. At 61.2 eV, the lowest energy considered by Ratnavelu et al [26], the elastic and Ps(1s$\rightarrow$2p) cross sections are given by 0.5068 $\pi a_0^2$ and 8.426 $\pi a_0^2$ while the present predictions for them are 0.5184 $\pi a_0^2$ and 8.198 $\pi a_0^2$ respectively. For Ps(1s$\rightarrow$2s) the agreement is not so close but fair; at 61.2 eV, the present prediction is 1.712 $\pi a_0^2$ compared to 1.166 of Ratnavelu et al [26]. While elastic and Ps(2p) cross sections agree so well, the difference in the Ps(2s) result is not clearly understood. Among all the partial cross sections, the ionization of Ps dominates the most and this, along with other Ps-inelastic processes, causes a maximum in the total cross section beyond the Ps excitation and ionization thresholds (5.1-6.8 eV).
This is a characteristic obtained in almost all Ps scattering calculations [8, 9, 10, 23, 27] and also observed in the measured data [28, 29, 30].

For Ps-He\(^+\), the major interest is about possible resonances, similar to Ps-H. This has become more relevant after Ryzhik and Mitroy [21] have found the theoretical evidence of a metastable Ps-He\(^+\) state with a small binding energy of -0.0005916 Hatree. So, with a possible molecule like feature, which has been predicted recently in PsH [31, 32], multiple resonances could prevail in the Ps-He\(^+\) system corresponding to various excited levels. As in the cases of Ps-H [9] and Ps-Li [33], we notice that there does not exist any resonant structure at the static exchange level and the resonances are manifested with the introduction of Ps-excited states in the coupling scheme. In figure 1, we plot the singlet and triplet scattering cross sections for a) \(S\)-wave, b) \(P\)–wave, and c) \(D\)-wave for the three-Ps-state model. As expected, multiple resonances are found in both the singlet and triplet scattering channels with each singlet state resonance is accompanied by a corresponding triplet state resonance. For Ps-H [2] and Ps-Li [33], it was assumed that the resonances are appearing due to Rydberg states of the positron around the singlet state \(H^-\) and \(Li^-\) ions, respectively and so resonances appeared there in the singlet channel only. However, in Ps-He\(^+\), the positron can have Rydberg states around both the singlet and triplet spin configurations of the helium atom and so resonances were expected in both the channels. The fact that each singlet state resonance is accompanied by a corresponding triplet state resonance and they appear in pairs is quite consistent with the energy spectrum of helium where each electronic singlet-state configuration has its triplet counterpart.

For S-wave, the singlet state resonances appear at 2.79 eV, 4.2 eV, and 4.85 eV, while the triplet state resonances appear at 3.28 eV, 4.51 eV and 4.94 eV (see fig-2a). The widths are approximately given by 0.07 eV, 0.04 eV and 0.02 eV for the singlet state resonances and 0.065 eV, 0.02 eV, and 0.0001 eV, for the triplet state resonances, respectively. We
note that, the triplet channel resonances appear beyond the corresponding singlet channel resonances, in the energy scale. In the spin-singlet channel, the short-range potential is attractive and it constructively combines with the long-range polarization potential, while for the triplet channel, the short-range potential is repulsive and it makes a destructive cancellation with the attractive polarization potential arising in the calculation through inclusion of $\text{Ps}(1s \rightarrow 2p)$ transition in the coupling. We understand that this could be the reason that the triplet channel resonances are placed beyond the singlet channel ones. The energy difference between corresponding singlet-triplet resonance pairs is found to diminish (0.49 eV, 0.31 eV, and 0.09 eV) gradually for higher order resonances. This is also consistent with the fact that the energy difference between singlet-triplet levels, diminish with higher excited states of helium. Similar features are also obtained for the $P-$ and $D-$wave resonances. In all the cases we find three pair of resonances below the first excitation threshold of Ps (at 5.1 eV).

From figure 2b, we see that the $P-$wave resonances appear at 3.55 eV, 4.64 eV, and 4.99 eV for the singlet state and at 3.65 eV, 4.71 eV, and 5.0 eV for the triplet state. The energy difference between singlet-triplet pairs are given by 0.10 eV, 0.07 eV, and 0.01 eV, respectively and are also diminishing with higher order resonances. For $D-$ wave resonances, the energy difference between a singlet-triplet pair diminishes further and the singlet and triplet resonances almost overlap with each other (see fig-2c). Their positions are given by 4.19 eV, 4.907 eV, and 5.096 eV for the singlet state and 4.2 eV, 4.909 eV, and 5.096 eV for the triplet state, respectively.

Now, we focus our attention to search for matching of these resonances to physical levels of the four-body Ps-He$^+$ system. It could be mentioned here that, in Ps-H, such correspondence has been found to exist [32]. The lowest order $S-$wave and $P-$wave singlet channel resonances are obtained at 2.79 eV and 3.55 eV. It is of interest to find that the lowest excited singlet $s-$state and $p-$state of He exist at 2.908 eV (58.292-
(54.4-6.8), and 3.47 eV (-57.73-(-54.4-6.8)). So, it is quite reasonable to believe that the above two resonances are the manifestations of the rearrangement levels $e^+\text{-He}(1s,2^1s$ and $e^+\text{-He}(1s2^1p)$ of the Ps-He$^+$ system.

Further, it is quite relevant to note that the above lowest $S$–wave singlet resonance at 2.79 eV corresponds quite well to the $S$–wave singlet channel resonance predicted in the $e^+-\text{He}$ entrance channel at 19.27 eV by Adhikari and Ghosh [18]. The correspondence becomes apparent when one takes into account the entrance channel energy difference of 16.64 eV between the two systems.

Manifestation of additional resonances seems to be quite relevant with the following new findings. Recently, Ryzhik and Mitroy [21] have concluded that PsHe$^+$ can exist in a metastable state with a small binding energy of -0.0005916 Hatree (resembling similarity to Ps-H). And secondly, Saito [31] and Biswas and Darewych [32] have recently found that the PsH system might have a molecule like feature, in addition to its proposed atom like feature [2] of a moving positron around a H$^-$ ion. So, the metastable PsHe$^+$ can lead to various excited levels before dissociation into Ps and He$^+$ or $e^+$ and He. These levels may well be reflected as Feshbach resonances in the scattering dynamics of Ps-He$^+$ and the additional resonances are thus worth further investigation.

**Conclusion:** In conclusion, we have studied positronium (Ps) scattering from singly ionized helium atom employing the model that yielded precise resonance positions and binding energies for PsH system. We find new resonances in both the singlet and triplet scattering channels. In the light of Ps-H and Ps-Li resonances, these are supposed to be due to the manifestation of positronic Rydberg states around the singlet and triplet states of the residual helium atom. We find strong correlation between few of the low lying resonances and some rearrangement levels of the four-body Ps-He$^+$ system. Although the S-wave resonance predicted earlier in the $e^+\text{He}$ entrance channel [18] is yet to be verified experimentally, we consider that the present work delivers a noteworthy information.
that a completely different type of investigation also reveal the same. In addition, the model predicts new resonances which seem to be of real interest because of the following two recently found physical features. Recently, Ryzhik and Mitroy [21] has reported a metastable state for the Ps-He$^+$ with a small binding energy of -0.0005916 Hatree. On the other hand, Saito [31] and Biswas and Darewych [32] have found that the four-body Ps-H system can have a molecule like manifestation, in addition to its proposed atom-like structure [2]. So, a possible molecule like feature for the metastable PsHe$^+$ system would certainly account for many of these additional resonances.

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Figure Captions:

Fig. 1: Angle integrated partial cross sections and target elastic total cross sections (in units of $\pi a_0^2$). Elastic (thin-solid curve), Ps($1s \rightarrow 2s$) (dotted curve), and Ps ($1s \rightarrow 2p$) (short-dashed curve) excitation cross sections using 3-Ps-state coupling. Ps($1s \rightarrow n = 3, 4, 5, 6$) discrete excitations (long-dashed curve) and Ps ionization (dot-dashed curve) cross sections using first Born approximation with regularized exchange. Total cross section is represented by the thick-solid curve.

Fig. 2: Variation of a) $S$–wave, b) $P$–wave, and c) $D$–wave singlet and triplet cross sections (in units of $\pi a_0^2$) for Ps-He$^+$ scattering for 3-Ps-state coupling.
Figure 2c

D-wave cross sections (in units of $\pi a_0^2$)

- Singlet
- Triplet

Incident Ps Energy (eV)
figure 1

Cross sections (in units of $\pi a_0^2$) vs Incident Ps Energy (eV).

- Elastic (CC)
- Ps(1s→2s) (CC)
- Ps(1s→2p) (CC)
- Ps(1s→n=3,6) (EB)
- Ps(1s→ion) (EB)
- Total
Figure 2b

Singlet
Triplet

P-wave cross sections (in units of \(\pi a_0^2\))

Incident Ps Energy (eV)
Figure 2a

Singlet
Triplet

S-wave cross sections (in units of $\pi a_0^2$)

Incident Ps Energy (eV)