Doubly excited resonant states of positronium negative ion

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A nine-state close coupling approximation has been employed to investigate the e^-+Ps scattering up to the incident energy $n=4$ excitation threshold of the Ps atom. The *s*- and *p*-wave Feshbach resonances predicted by Ho [Phys. Lett. **102A**, 348 (1984) and Phys. Rev. A **60**, 2834 (1999)] have been noticed below all the thresholds up to $n=4$. The present study shows the success of close coupling model in predicting the resonances in the elastic channel.

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I. INTRODUCTION

An electron binds with a positronium atom (Ps) to form the positronium negative ion, where the two electrons are in a singlet spin state. This system and its charge conjugate counterpart consisting of two positrons and one electron were predicted to be bound by Wheeler [1]. A positronium negative ion has several doubly excited autodetaching states below the excitation thresholds of the Ps atom. This system has a fundamental importance since it provides a test for the charge conjugation in the leptonic systems, $e^+e^-e^-$ and $e^-e^+e^+$. This can be tested through an actual experiment for positron (or electron) impact on a Ps atom. Cross sections (for any process) for both systems are expected to be identical, if charge conjugation holds. This experimental study will also reveal the properties of matter and antimatter interactions.

Positronium negative ion Ps^- is the simplest member of the family of the three-body atomic systems interacting through the Coulomb forces. The present investigation can help in studying similar systems such as $\mu^+\mu^-\mu^-$ and $\bar{p}pp$, as the nonrelativistic Hamiltonian of these systems takes the same form, like that of Ps^-, if the energy and length scaled with the mass are used. The other three-body systems for which the odd particle is heavier than the other two identical particles and with Coulomb interaction can be similarly studied. These systems are, to name a few, $e^-\mu^+e^-$, $\mu^-p\mu^-$, $\mu^-d\mu^-$, and $\mu^-t\mu^-$ where μ, p, d, and t are muon, proton, deuteron, and triton, respectively. Resonance parameters of these systems can be obtained by the same technique as described previously.

There have been a large number of investigations on the resonances in e^-+Ps scattering associated with the $n=2$ threshold of the positronium atom in the recent past. Theoretical methods such as the complex-coordinate rotation method [2,3], the Kohn variational method [4], adiabatic treatment using the hyperspherical coordinates [5], and the hyperspherical close coupling method [6] have been used in these works. Burke *et al.* [18] have obtained the $^3P^e$ resonant state in the H^- continuum below the first excitation threshold of the H atom. It was expected that Ps^- should have a similar resonance in this spectrum. However, whether or not there is a $^3P^e$ resonant state of Ps^- below the $n=2$ threshold is a matter of controversy. Mills [7], who has used a variational method retaining two nonlinear and 70 linear parameters in a variational trial function, as well as Bhatia and Drachman [8], who have used a Raleigh-Ritz variational method with a generalized Hylleras wave function containing two nonlinear and 200 linear parameters, found no evidence for the existence of this state. Botero and Greene [9] have employed an adiabatic model using hyperspherical coordinates to predict the existence of resonances in Ps^-. They have also found no evidence for the existence of the $^3P^e$ resonant state for the system. However, Bhatia and Ho [10], using the complex-coordinate rotation method where two nonlinear and 1140 linear parameters have been employed, have given estimates for both the position and width for the $^3P^e$ state, like H^-. Therefore, it was necessary to carry out an *ab initio* calculation to obtain accurate results. Recently, Basu and Ghosh [11], using the close-coupling approximation (CCA) retaining the first six eigenstates of the bound Ps atom, have predicted the same. In a more recent study, Gilmore *et al.* [14] have employed a nine-state coupled pseudostate approximation and predicted the positions and widths of the resonances below the Ps $n=2$ threshold as well as the elastic cross sections in this energy region. They have also obtained the controversial $^3P^e$ state of Ps^-. Results of Gilmore *et al.* are quite reliable below the $n=2$ threshold. However, the models of Gilmore *et al.* can predict resonances only below the $n=2$ threshold, as they have included only the first three eigenstates ($1s$, $2s$, and $2p$) in their expansion scheme. The resonances associated with the higher Ps thresholds have been studied by Ivanov and Ho [12], using the complex-coordinate rotation method. Ghosh and Basu [13] have also studied the resonant states below $n=3$ threshold using a six-state eigen CCA and obtained results with a fair accuracy.

This exotic system has also attracted experimental interest, as Mills [15] has produced it in the laboratory and measured its lifetime [16], whereas no experimental measure-

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ment has been carried out for e^-+Ps scattering yet. Ps beams have recently become available, and direct measurements of the total cross sections of the Ps scattering by simple atomic and molecular targets have been reported [17].

Burke and his collaborators [18] have used CCA in order to predict low-energy scattering parameters of e^-+H system. They have used a three-state CCA, six-state CCA, and six-state CCA with sixteen correlation terms in the expansion scheme. The CCA calculations included eigenwave functions of the H atom. They have predicted the doubly excited autodetaching states of the H^- system and also the $Q(1s-2s)$ and $Q(1s-2p)$ cross sections below the $n=3$ threshold of the hydrogen atom. Their predicted results are in very good agreement with those of experiment.

Both Ps^- and H^- belong to the same family in the sense that they both are three-particle bound systems. To be specific, all the particles in Ps^- are identical in mass tumbling about their center of mass, while H^- consists of two light particles undergoing correlated motion in the central force field of an "infinitely massive" proton. The binding energies of the ground states and the lowest $^1S^e$ states of Ps^- and those of H^- have a simple ratio (approximately a factor of $\frac{1}{2}$). This can be expected to hold good over the whole spectrum for both the negative ions. Below the first excitation threshold of Ps atom all the resonances as obtained have been confirmed by Ho [2,3], Bhatia and Ho [10], Ivanov and Ho [11], Basu and Ghosh [11], and Gilmore *et al.* [14]. Therefore, our wisdom suggests that resonances due to autodetaching states of Ps^- below the higher excitation thresholds of the Ps atom will also be obtained. Ivanov and Ho [12], using the complex coordinate rotation method, have obtained the resonant states below the higher excitation thresholds. The width and position of the first $^1S^e$ resonant state, below the $n=2$ threshold, predicted by Basu and Ghosh [11] differ significantly from those of Ho and Gilmore *et al.* The widths as well as positions of the other resonances differ to some extent. These suggest that our theoretical predictions are not convergent with added eigenstates in the expansion scheme. Therefore, further studies using a more elaborate basis set is warranted in predicting the resonances below the higher excited thresholds.

In the present work we decide to carry out a detailed study of the e^-+Ps scattering in the low-energy region using the close-coupling method retaining the first nine eigenstates ($1s$ to $4d$) of atomic positronium in the expansion scheme. Because the resultant close-coupling functions have the correct asymptotic form up to the energy corresponding to the excitation of the $n=5$ states, we argue that the results reported here can be considered to be quite reliable up to the $n=5$ threshold of the positronium atom. Our main motivation is to predict Feshbach resonances below the $n=3$ and $n=4$ thresholds and also to refine our previous results [11] below the $n=2$ threshold with the addition of higher excited eigenstates in the expansion scheme. Moreover, we are interested to find the suitability of close-coupling approximation in predicting resonances in the elastic channel. We conclude this introduction with a brief outline of the contents of this paper.

In Sec. II, we give a brief outline of the theoretical model applied by us. In Sec. III, we quote the scattering parameters for the e^-+Ps system using a nine-state CCA. We predict the doubly excited Feshbach resonant states for Ps^- ion below the $n=3$ and $n=4$ thresholds. We compare our results with those of the most accurate calculations of Ivanov and Ho [12]. Finally, conclusions inferred from this investigation will be given.

II. THEORY

Here, we consider a system in which all three particles have the same mass. Let $(\vec{r}_1,\vec{r}_2)$ be the position vectors of the two electrons in an arbitrary coordinate system and $\vec{x}$ be the coordinate of the positron. Then, the Hamiltonian for the system can be expressed as

$$H=-\frac{1}{2}\nabla_{r_1}^2-\frac{1}{2}\nabla_{r_2}^2-\frac{1}{2}\nabla_x^2+\frac{1}{|\vec{r}_1-\vec{r}_2|}-\frac{1}{|\vec{x}-\vec{r}_1|}-\frac{1}{|\vec{x}-\vec{r}_2|}. \tag{1}$$

We make use of the Jacobi coordinates $\left[\vec{\rho}_i=\vec{x}-\vec{r}_i,\vec{R}_i=\frac{1}{2}(\vec{x}+\vec{r}_i)\right]$ where the origin of the coordinate system lies with the ith electron, which is bound. Eliminating the center-of-mass motion, the Hamiltonian may be written as

$$H=-\frac{1}{2\mu(\mathrm{Ps})}\nabla_{\rho_i}^2-\frac{1}{2\mu(\mathrm{Ps}^-)}\nabla_R^2-\frac{1}{\rho_\mathrm{i}}-\frac{1}{\left|\vec{R}+\frac{1}{2}\vec{\rho}_\mathrm{i}\right|}+\frac{1}{\left|\vec{R}-\frac{1}{2}\vec{\rho}_\mathrm{i}\right|}. \tag{2}$$

Here, $\mu(\mathrm{Ps})=\frac{1}{2}$ and $\mu(\mathrm{Ps}^-)=\frac{2}{3}$ a.u. and $i=1$ or 2.

The total wave function for the system must be antisymmetric and the spatial part of the total wave function can be expressed as

$$\Psi(\vec{\rho}_i,\vec{R}_i)=(1\pm P_{12})\sum_n \omega_n(\vec{\rho}_i)F_n(\vec{R}_i). \tag{3}$$

Here, P_{12} is the electron exchange operator and ω_n is the wave function describing the bound state of the target Ps atom, while F_n denotes the moving electron. The total wave function Ψ will satisfy the following Schrödinger equation:

$$(H-E)\Psi=0. \tag{4}$$

The Schrödinger equation can be recast into two sets of coupled integral equations,

$$f^{\pm}_{n',n}(\vec{k}',\vec{k})=\{f^B_{n',n}(\vec{k}',\vec{k})\pm g^B_{n',n}(\vec{k}',\vec{k})\}-\frac{1}{2\pi^2}\sum_{n''}\int d\vec{k}''\times\frac{\{f^B_{n',n''}(\vec{k}',\vec{k}'')\pm g^B_{n',n''}(\vec{k}',\vec{k}'')\}f^{\pm}_{n'',n}(\vec{k}'',\vec{k})}{k^2_{n''}-k''^2+i\epsilon} \tag{5}$$

where f^+ stands for the space symmetric part, while, f^- stands for the space antisymmetric part. Here, f^B and g^B are the first Born and exchange scattering amplitudes, respectively (see Basu *et al.* [19]). After the partial wave analysis and performing some algebraic manipulations, the three-dimensional coupled inhomogeneous Eq. (5) reduces to one-dimensional coupled integral equation

TABLE I. s-wave phase shifts for $S=0$ and $S=1$ cases below the $n=2$ excitation threshold.

k in atomic units	$S=0$ Three-state CCA	$S=0$ Six-state CCA	$S=0$ Nine-state CCA	$S=0$ Ward *et al.* [4]	$S=1$ Three-state CCA	$S=1$ Six-state CCA	$S=1$ Nine-state CCA	$S=1$ Ward *et al.* [4]
0.05	2.416	2.441	2.452	2.547	−0.276	−0.272	−0.269	−0.250
0.10	1.862	1.888	1.894	2.049	−0.553	−0.548	−0.545	−0.5361
0.15	1.464	1.508	1.513	1.668	−0.810	−0.808	−0.806	−0.797
0.20	1.168	1.214	1.226	1.378	−1.043	−1.041	−1.037	−1.035
0.25	0.941	1.024	1.038	1.156	−1.258	−1.252	−1.249	−1.247
0.30	0.764	0.865	0.876	0.984	−1.439	−1.427	−1.422	−1.432
0.40	0.517	0.634	0.643	0.748	−1.746	−1.737	−1.733	−1.739
0.45	0.444	0.561	0.568	0.667	−1.873	−1.864	−1.860	−1.865

$$T^{J\pm}(\tau'\vec{k}';\tau\vec{k}) = B^{J\pm}(\tau'\vec{k}';\tau\vec{k}) - \frac{1}{2\pi^2}\sum_{\tau''} \times \int dk''k''^2 \frac{B^{J\pm}(\tau'\vec{k}';\tau''\vec{k}'')T^{J\pm}(\tau''\vec{k}'';\tau\vec{k})}{k_{\tau''}^2 - k''^2 + i\epsilon},$$

$$\text{where } \tau \equiv (n,l,L). \tag{6}$$

The uncoupled Eq. (6) has been solved by matrix inversion method [19].

We have studied the Ps^- system using the following basis sets:

(a) e^-+Ps$(1s,2s,2p)$,

(b) e^-+Ps$(1s,2s,2p,3s,3p,3d)$,

(c) e^-+Ps$(1s,2s,2p,3s,3p,3d,4s,4p,4d)$.

The basis sets (a) and (b) have been used in our earlier investigations [11,13]. However, in the present calculation model (c) has been employed.

III. RESULTS AND DISCUSSIONS

We now start the presentation our results from the recent calculations. The s-wave phase shifts for the spin states $S=0$ and $S=1$, viz. singlet and triplet, respectively, are given in Table I. Table II represents the p-wave phase shifts for both the spin states. We have provided the results for basis sets (a), (b), and (c), viz. three-state CCA, six-state CCA, and nine-state CCA, respectively, using our method along with the variational results of Ward *et al.* [4], to find the relative importance of the addition of the eigenstate on the elastic phase shifts. For the singlet case, the rate of convergence of the phase shifts is slow for both the s- and p-wave results. However, the present results increase monotonically and tend toward the more accurate values of Ward *et al.* [4] with added eigenstates. In the triplet case, with the increase in energy ($k=0.2$ a.u. and above) the difference with the present results and those of Ward *et al.* is only in the third significant digit. We hasten to add that the triplet s- and p-wave phase shifts using nine-state CCA [model (c)] are marginally different from those of Ward *et al.* [4].

Feshbach resonances in the s- and p-wave scattering due to autodetaching states of the positronium negative ion below the $n=2$, $n=3$, and $n=4$ excitation thresholds of the positronium atom have been investigated in this present work. Resonances below $n=2$ and $n=3$ thresholds have been studied in earlier works [11,13]. In the present dissertation, we have again provided the results below the $n=2$ threshold in Table III using models (a), (b), and (c), as described earlier, to show the effect of added eigenstates on the positions and widths of the resonances. We have also provided the corresponding results using the complex coordinate rotation method (CCRM) [12] and also the nine-state pseudostate CCA predictions of Gilmore *et al.* [14] in the same table for

TABLE II. p-wave phase shifts for $S=0$ and $S=1$ cases below the $n=2$ excitation threshold.

k in atomic units	$S=0$ Three-state CCA	$S=0$ Six-state CCA	$S=0$ Nine-state CCA	$S=0$ Ward *et al.* [4]	$S=1$ Three-state CCA	$S=1$ Six-state CCA	$S=1$ Nine-state CCA	$S=1$ Ward *et al.* [4]
0.05	0.023	0.025	0.026	0.031	−0.009	−0.006	−0.004	−0.0004
0.10	0.157	0.164	0.170	0.192	−0.060	−0.051	−0.047	−0.0381
0.15	0.357	0.410	0.422	0.484	−0.153	−0.142	−0.138	−0.123
0.20	0.587	0.630	0.637	0.707	−0.267	−0.256	−0.252	−0.2347
0.25	0.665	0.709	0.712	0.784	−0.380	−0.371	−0.358	−0.353
0.30	0.673	0.704	0.710	0.778	−0.477	−0.432	−0.458	−0.4629
0.40	0.590	0.610	0.616	0.687	−0.655	−0.631	−0.610	−0.6343
0.45	0.554	0.560	0.568	0.641	−0.716	−0.684	−0.667	−0.687

TABLE III. Feshbach resonances below the $n=2$ excitation threshold. Positions of the resonances are given in electron volts and widths are given in mega-electron-volts in parentheses ( ).

Scattering case		Three-state CCA	Six-state CCA	Nine-state CCA	Gilmore *et al.* [14]	Ho [3], Bhatia and Ho [10], and Ivanov and Ho [12]
$^1S^e$	A	5.056 (8.0)	4.775 (6.0)	4.752 (2.6)	4.739 (1.2)	4.734 (1.2)
	B	*x*	5.070 (1.8)	5.069 (0.68)	5.081 (0.32)	5.069 (0.27)
$^3S^e$		*x*	5.090 (10.0)	5.082 (2.3)	5.083 (4.2×10^{-5})	5.074 (0.14)
$^1P^o$		5.086 (0.35)	5.098 (0.029)	5.098 (0.027)	5.094 (0.069)	5.084 (0.027)
$^3P^e$	A	*x*	4.934 (5.4)	4.887 (4.2)	4.812 (3.5)	4.808 (3.5)
	B	*x*	5.087 (0.32)	5.086 (0.29)	5.099 (0.48)	5.086 (0.44)

comparison. It is clear from Table III that with the addition of higher eigenstates in the calculation, the position of *s*-wave resonances has improved and our final results using the nine-state CCA model are in close proximity with those of CCRM [12] and Gilmore *et al.* [14]. This is also true for the widths of the resonances. The widths of the resonances below the $n=2$ threshold drastically reduce and approach the results of CCRM and those of Gilmore *et al.* [14]. The positions as well as the widths of the *p*-wave resonances using the nine-state model agree well with those of CCRM calculations [12] and Gilmore *et al.* [14] below the $n=2$ threshold of the Ps atom.

Resonance positions below the $n=3$ threshold have been presented in Table IV. We have used the six-state CCA and nine-state CCA for the investigation; results of Ho have also been quoted for comparison. The third resonance (C) in the singlet *s*-wave case has not been obtained using the six-state CCA but with a larger basis set, viz. nine-state CCA, it has been predicted. This feature has also been observed for the resonances below the $n=2$ threshold. The resonance positions for the $^1S^e$ case are quite close to the corresponding results of CCRM. The second resonance (B) in the singlet *p*-wave case, though obtained using the six-state CCA model is absent in our more refined calculation using the nine-state CCA model. Ho and Bhatia had also obtained this resonance [10], but this is absent in a more elaborate calculation by Ivanov and Ho [12]. The resonance for the $^3S^e$, $^3P^o$, and $^3P^e$ cases below the $n=3$ threshold have been investigated using the nine-state model. The resonance positions are in close agreement with those of Ivanov and Ho.

TABLE IV. Feshbach resonances below the $n=3$ excitation threshold. Positions of the resonances are given in electron volts and widths are given in mega-electron-volts in parentheses ( ).

Scattering case		Six-state CCA	Nine-state CCA	Ho [3], Bhatia and Ho [10], and Ivanov and Ho [12]
$^1S^e$	A	5.865	5.858	5.839
	B	6.023	6.007	5.988
	C	*x*	6.032	6.030
$^3S^e$		*x*	6.006	6.001
	A	5.944	5.946	5.939
$^1P^o$				
	B	6.028	*x*	*x*
	A	*x*	5.853	5.851
$^3P^o$				
	B	*x*	6.004	5.995
$^3P^e$		*x*	5.941	5.940

Table V represents the resonances below the $n=4$ threshold. All the resonances, as obtained by CCRM have been predicted by the present calculation using the nine-state CCA model. The positions of the resonances obtained by both methods differ slightly from each other. Moreover, from the trend of the results, we conclude that with the inclusion of a more elaborate basis set in the calculation these differences will be minimized. We would also like to add that we have not provided the widths for the resonances above the $n=2$ thresholds, however, our primary values of widths differ marginally from the CCRM predictions.

IV. CONCLUSION

The scattering of electrons (positrons) by a positronium atom has been reinvestigated using close coupling approximation. Three basis sets are employed to find the relative importance of eigenstates on the elastic scattering parameters. The accuracy of this model depends on the fact of how much the employed basis set covers of the total scattering space in the calculations.

TABLE V. Feshbach resonances below the $n=4$ excitation threshold. Positions of the resonances are given in electron volts and widths are given in mega-electron-volts in parentheses ( ).

Scattering case		Nine-state CCA	Ho [3] Bhatia and Ho [10], and Ivanov and Ho [12]
$^1S^e$	A	6.274	6.251
	B	6.331	6.324
	C	6.338	6.329
$^3P^0$	A	6.259	6.254
	B	6.331	6.326
	C	6.340	6.334

The *s*- and *p*-wave Feshbach resonances due to autodetaching doubly excited states of Ps^- are predicted below the $n=2$, $n=3$, and $n=4$ thresholds of the positronium atom. The present nine-state CCA results are in fair agreement with those of Ho [3], Bhatia and Ho [10], and Ivanov and Ho [12] and Gilmore *et al.* [14] below the $n=2$ threshold. The results of Gilmore *et al.* are reliable only below the $n=2$ threshold while our nine-state model predictions holds good up to the $n=5$ threshold of the Ps atom. Positions of the resonances below $n=3$ and $n=4$ thresholds obtained using the nine-state model are in good agreement with those of Ho [3], Bhtia and Ho [10], and Ivanov and Ho [12]. Our *s*- and *p*-wave elastic phase shift values are approaching the corresponding variational predictions of Ward *et al.* [4]. The addition of higher eigenstates, i.e., using model (c), in the expansion scheme modified our previous results, and they approach the more accurate results.

The present findings indicate that the entire spectrum of the positronium negative ion and hydrogen negative ion are analogous, scaled approximately by a factor of 2. Our conclusion from this work is that the CCA model is very successful in predicting the Feshbach resonances in the elastic channel.

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