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High-lying resonances in Ps-H scattering below the Ps^-H^+ threshold

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In this work, we carry out an investigation of high-lying S-wave resonances in Ps-H scattering below the Ps^--H^+ threshold. The method of complex-coordinate rotation is used together with highly correlated wave functions containing all six interparticle coordinates. Using such Hylleraas-type bases up to 6412 terms, the energy positions for the $1S$–$8S$ states in the Rydberg series converging to the Ps^- threshold, as well as the four widths for the $2S$–$5S$ states, are calculated. The energies for the $5S$–$8S$ states of this Rydberg series are then used to fit into the quantum defect formula, from which the energy levels for higher members of the Rydberg series can be estimated.

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I. INTRODUCTION

Positronium hydride PsH is a four-body atomic system which consists of two electrons, one positron, and one proton. This system has attracted considerable theoretical activity and been observed in the laboratory [1]. PsH has a bound S state (see [2,3], and references therein), lying below the Ps+H dissociation threshold. There also exist other Rydberg states, a result of the Coulomb interaction between the positron and the negatively charged H^- ion [4]. Such Rydberg states lying in the continuum would appear as resonances in Ps-H scattering (see the energy levels in Fig. 1). Using the stabilization method and the complex-rotation method, Huston and Drachman first calculated an S-wave resonance lying below the e^+-H^- threshold [5]. A subsequent calculation using the complex-coordinate-rotation method refined its energy and width, confirming the importance of the configuration of the H^- ion [6]. In recent years, several investigations on the resonances in Ps-H scattering have been carried out [7–11], including our calculations for the S-, P-, D-, F-, and G-wave resonances [7,8]. Resonances below the doubly excited $2s^2\ {}^1S^e$ state of H^- in Ps-H scattering have also been calculated [12]. S-wave resonances with triplet-spin (relative to the two electrons) states in Ps-H scattering have been reported in the literature [13]. Very recently, using an effective potential approach, Di Rienzi and Drachman [14] carried out a calculation for higher-lying resonances in Ps-H scattering below the Ps^--H^+ threshold and reported resonance energies for the Rydberg series with S, P, and D symmetries. Motivated by these activities in this energy region [14,15] of the Ps-H system, we now carry out an investigation of high-lying S-wave resonances in Ps-H scattering below the Ps^--H^+ threshold. We use the method of complex-coordinate rotation together with highly correlated Hylleraas wave functions containing all six interparticle coordinates to describe the system.

The study of the positronium-hydrogen system is part of the recent experimental and theoretical investigation of few-body exotic systems involving antimatter. For example, there has been renewed interest in carrying out experimental studies around the world [16–18] on the positronium negative ion, a three-lepton system consisting of two electrons and one positron, following the earlier works of Mills [19]. Also, with the improved technique for storing positrons [20], the positronium molecule Ps_2, arguably the first observed "molecule" containing antimatter, has recently been produced in the laboratory [21]. Atomic data involving positron-atom scattering and annihilation have played a role in the interpretation of the origin of positron-electron annihilation with γ rays at 511 keV observed around the center of our galaxy, the Milky Way [22]. The subject of atomic resonances involving positrons and positronium has been discussed in several reviews [23–29]. Our present work on PsH will help to shed light on the investigations of high-lying Rydberg states in Ps_2 [14]. The general layout of the present paper is as follows. We describe the Hamiltonian and wave functions in Sec. II, and calculations and results in Sec. III. We make final remarks and conclusions in Sec. IV.

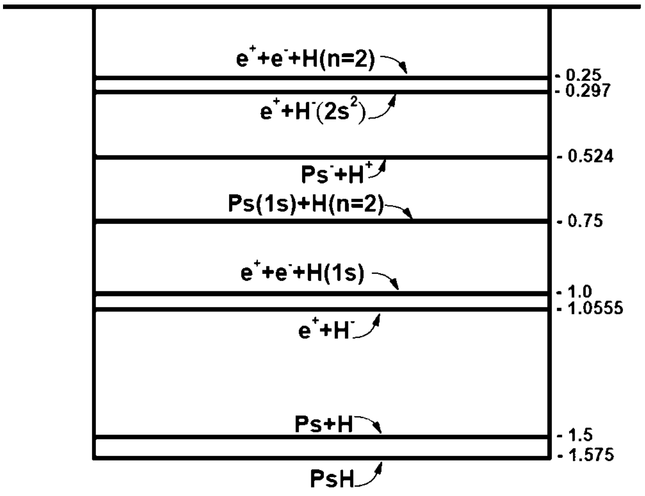

FIG. 1. Energy levels (in Ry) of positronium-hydrogen system.

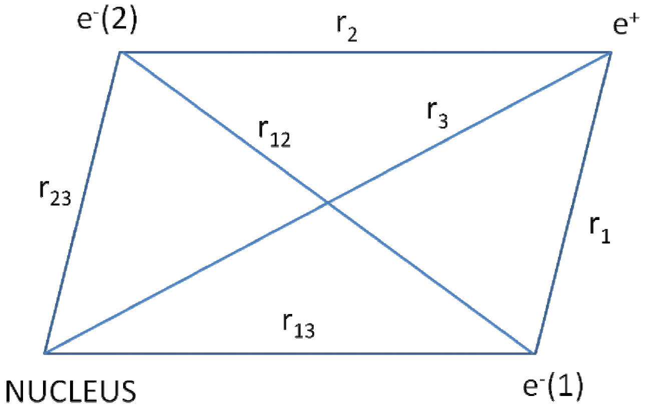

FIG. 2. (Color online) Coordinates for the Ps-H system. In the present work, we use the positron as the origin of the coordinate system in order to emphasize on the configuration of the Ps^- ion.

II. HAMILTONIAN AND WAVE FUNCTIONS

In order to emphasize the $\mathrm{Ps}^- + \mathrm{H}^+$ channel, we take the positron as the origin of our coordinate system (see Fig. 2). Assuming that the proton mass is infinite, then the Hamiltonian for the PsH system is [30] (in Rydberg units throughout)

$$H = T + V, \tag{1}$$

with

$$T = -2\nabla_1^2 - 2\nabla_2^2 - \nabla_3^2 - 2\sum_{i>j\geq 1}^{3} \boldsymbol{\nabla}_i \cdot \boldsymbol{\nabla}_j \tag{2}$$

and

$$V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_3} + \frac{2}{r_{12}} - \frac{2}{r_{23}} - \frac{2}{r_{31}}, \tag{3}$$

where indices 1,2 refer to the two electrons, and index 3 refers to the proton. The wave function can be expanded according to

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \sum_{i=1}^{N} a_i \psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \pm (1 \leftrightarrow 2), \tag{4}$$

where ψ_i is a general term in the Hylleraas basis set, which has the form

$$r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} \mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \tag{5}$$

with

$$\begin{aligned}\mathcal{Y}^{LM}_{(\ell_1\ell_2)\ell_{12},\ell_3} = \sum_{m_i} &\langle \ell_1 m_1; \ell_2 m_2 | \ell_1 \ell_2; \ell_{12} m_{12}\rangle \\ &\times \langle \ell_{12} m_{12}; \ell_3 m_3 | \ell_{12}\ell_3; LM\rangle \\ &\times Y_{\ell_1 m_1}(\mathbf{r}_1) Y_{\ell_2 m_2}(\mathbf{r}_2) Y_{\ell_3 m_3}(\mathbf{r}_3),\end{aligned} \tag{6}$$

being a vector-coupled product of spherical harmonics for the two electrons and the proton to form an eigenstate of total angular momentum L and component M. All terms in (5) are included such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega, \tag{7}$$

where Ω is an integer. However, terms that may potentially cause near linear dependences are excluded. For example, if $\ell_1 = \ell_2$ and $\alpha \approx \beta$, then terms with $j_1 > j_2$ are omitted, as well as terms with $j_1 = j_2$ when $j_{23} > j_{31}$. The computational details for evaluating necessary integrals can be found in [31]. In the present work, we use wave functions with $\Omega = 9$, 10, and 11, corresponding to the total numbers of terms of 2625, 4172, and 6412, respectively. Our final results are based on the total number of terms $N = 6412$ in the wave functions.

III. CALCULATIONS AND RESULTS

For calculations of the S-wave autodissociating resonant states, we use the method of complex-coordinate rotation [32,33]. The radial coordinates are transformed according to

$$r \rightarrow r e^{i\theta}, \tag{8}$$

where r is the distance between two charged particles. The transformed Hamiltonian can be written as

$$H(\theta) = T e^{-2i\theta} + V e^{-i\theta}, \tag{9}$$

where T and V are those given by Eqs. (2) and (3), respectively. Complex eigenvalues are obtained by diagonalizing the transformed Hamiltonian, and the complex resonance energy is given by

$$E_{\mathrm{res}} = E_r - i\Gamma/2, \tag{10}$$

where E_r is the resonance position and Γ is the resonance width. In our wave functions, we choose the nonlinear parameters $\alpha = 0.49$, $\beta = 0.49$, and let γ have values ranging from 0.24 to 0.50. The nonlinear parameter γ can be considered as a variational parameter to determine the stabilized complex resonance eigenvalues. The physical picture is that the wave functions are used to simulate the positronium negative ion moving away from the field of the H^+ positive ion when the value of γ is systematically decreased from $\gamma = 0.50$. We have found stabilized complex eigenvalues (i.e., $\partial|E|/\partial\theta = \text{minimum}$) which are summarized in Table I. In particular, we have obtained the resonance positions and widths for the four resonances, denoted as the $2S$, $3S$, $4S$, and $5S$, respectively. As for the lowest resonance in this Rydberg series, the $1S$ state, we have been unable to obtain a stabilized imaginary part of the complex eigenvalue. We can only estimate that the real part (resonance energy) is stabilized around $E_r = -1.1062$ Ry. Since this state lies below the ground state energy of the hydrogen atom (see Fig. 1), perhaps we need to employ different wave functions to simulate the configuration of this state. In Table I, we also present results for other high-lying states. The resonance energies up to the $8S$ state have been calculated. Again, for the states of $6S$–$8S$, we have been unable to obtain well-converged values for the imaginary parts. In Table I, we compare our results with those of Ref. [14]. For a given state, the results shown in the second row (inside the parentheses) are expressed in eV, with the resonance energies measured from the Ps-H scattering threshold. It is seen that our resonance energies are consistently lower than those of Ref. [14], which

TABLE I. *S*-wave resonances in the Ps-H system below the Ps$^-$-H$^+$ threshold. For a given state, the results shown in the second row (inside the parentheses) are expressed in eV, with the resonance energies measured from the Ps-H scattering threshold.

State	E_r (Ry) (Present)	$\Gamma/2$ (Ry) (Present)	E_r (Ry) [14]
(1*S*)	−1.1062		−0.899
	(5.358)		(8.177)
(2*S*)	−0.78218	0.00135	−0.751
	(9.7665)	(0.0367)	(10.191)
(3*S*)	−0.6902	0.006	−0.670
	(11.018)	(0.163)	(11.293)
(4*S*)	−0.6416	0.0026	−0.624
	(11.679)	(0.071)	(11.919)
(5*S*)	−0.6068	0.0022	−0.596
	(12.153)	(0.060)	(12.300)
(6*S*)	−0.5832		
	(12.474)		
(7*S*)	−0.5684		
	(12.675)		
(8*S*)	−0.5582		
	(12.814)		
Infinite	−0.524 010 14 Ry [34]		
	(13.279)		

indicates that the Feshbach shifts, the interaction between the open and closed channels omitted in Ref. [14], are negative for their reported *S*-wave resonances. The largest discrepancy between the present work and Ref. [14] is for the 1*S* state. The degree of agreement with [14] becomes better as we move up to the higher members of the Rydberg series. As for the uncertainties of our values, we estimate that they are about a few parts in the last digits for the real and imaginary parts of the complex resonance eigenvalues. In particular, the 2*S* state is the most accurate in our calculation, followed by the 4*S* and 5*S* states. As for the 3*S* state, since the absolute error is a few parts in the last digit, we estimate the imaginary part to be 0.006 ± 0.002 Ry. The reason for such a large uncertainty is that this 3*S* state is located at −0.6902 Ry which is not too far away from the Ps(1*S*)+H(n=2) threshold with the threshold energy of −0.75 Ry (see Fig. 1). In the complex-rotation calculation, this complex resonance eigenvalue interferes with the scattering cut that originates from the Ps(1*S*)+H(n=2) branch point, resulting in the difficulty in obtaining a more converged result.

Next, from the resonance energies, we calculate the binding energies ΔE, relative to the Ps$^-$ energy of −0.524 010 14 Ry [34–36]. We then fit the binding energies of n=5–8 to the Rydberg quantum defect formula of the type

$$\Delta E = \frac{P}{2(n-\mu)^2}, \tag{11}$$

where the quantum defect μ and the constant P are parameters to be deduced from the fitting, which are P=4.8913 and μ=−0.433 28. The fitting is quite good as the χ^2 is very small (on the order of 10^{-7}) and the square of the correlation coefficient (ρ^2) is very close to 1. We then use the fitted parameters P and μ to calculate ΔE and extend the calculation down to n=1. In Fig. 3 we plot the binding energy ΔE vs the principal quantum number n. The red circles connected by the red dotted line are from the calculated values using the fitted P and μ. The squares connected by the blue solid line are from our present complex-rotation calculations. The triangles connected by the green dash-dotted line are from Ref. [14]. In Fig. 3, the binding energies vs n are plotted on a log-log scale, giving evidence of the $1/n^2$ behavior for a typical Rydberg series. The higher members of the Rydberg series can be estimated from Eq. (11) using the fitted parameters P and μ.

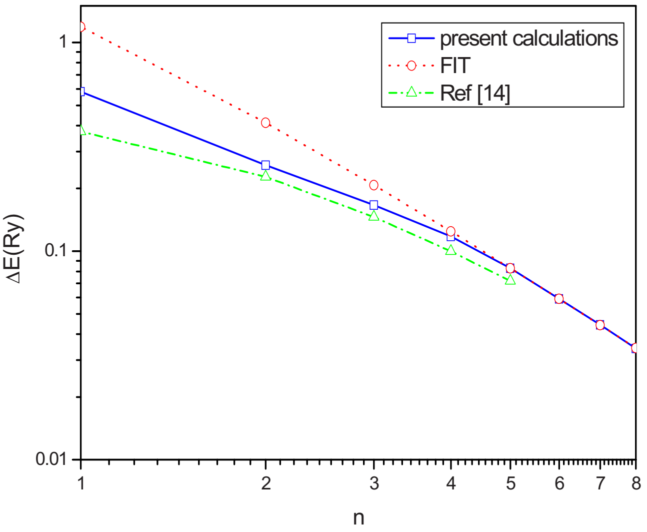

FIG. 3. (Color online) Binding energy ΔE (relative to the Ps$^-$ threshold) vs principal quantum number n. The red circles for the 5*S*–8*S* states are fitted to the quantum defect formula (11), and the red dashed line is extended down to n=1. The squares connected by the blue solid line are from our present complex-rotation calculations. The triangles connected by the green dashed-dotted line are from Ref. [14].

IV. DISCUSSION AND CONCLUSIONS

In summary, we have carried out a complex-coordinate-rotation calculation of high-lying *S*-wave resonances in Ps-H scattering, using highly correlated Hylleraas wave functions. The energy positions for the 1*S*–8*S* states in the Rydberg series converging to the Ps$^-$+H$^+$ threshold have been determined, together with the widths for 2*S*–5*S*. The energies of 5*S*–8*S* states of the Rydberg series have been used to fit into the quantum defect formula with high reliability. From the quantum defect formula, the energy levels for higher members of the Rydberg series can be estimated.

Next, let us comment on the general trend for the resonances in Ps-atom scattering. If the atom denoted by *A* and an extra electron can form a negative ion A^- (for example, the hydrogen atom and an extra electron to form the ion H$^-$), then resonances would exist in Ps-*A* scattering lying below the e^+-A^- threshold, a result of the Rydberg states formed between the positron and the negatively charged A^- ion. If such Rydberg states are located in the scattering continua as shown in earlier work [4–11], they would manifest themselves as resonances in Ps-A scattering (see Fig. 1). Furthermore, as demonstrated in Ref. [14] and in the present work, high-lying resonances in Ps-A scattering could still exist in higher-energy regions lying below the Ps$^-$-A^+ threshold, a result of the Rydberg states formed between the positively charged A^+ ion and the negatively charged Ps$^-$ ion. Members of the Rydberg series located in the scattering continua would appear as resonances due to the interactions between the open and closed channels (see Fig. 1). We should mention that such high-lying resonances lying below the Ps$^-$ $+A^+$ threshold would exist whether or not the A^- ion exists. To conclude, the resonances discussed in this work are the results of theoretical investigations which have yet to be observed experimentally. However, with the recent advances in storing positrons [20] and in producing positronium beams for atomic collision purposes [37], it is hoped that our results will provide useful input into the experimental search for resonances in positronium-atom scattering.

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