PHYSICAL REVIEW A **84**, 034503 (2011)

Higher-lying resonances in Ps-H scattering below the e^+-H$^-$ threshold

Z.-C. Yan[1] and Y. K. Ho[2,*]

[1]*Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada E3B 5A3*

[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, Republic of China*

(Received 3 March 2011; published 29 September 2011)

In this work, we perform a study on high-lying S-wave resonances in Ps-H scattering below the e^+-H$^-$ threshold. The method of complex-coordinate rotation is applied together with highly correlated wave functions containing all six interparticle distances. Using such Hylleraas bases up to 6412 terms, the energy positions up to the 8S state and the widths up to the 7S state in the Rydberg series converging to the H$^-$ threshold are determined. The energies of 4S to 7S states from the present calculations are fitted into the quantum defect formula, from which the energies of higher members in the Rydberg series can be deduced.

DOI: 10.1103/PhysRevA.84.034503 PACS number(s): 36.10.Dr, 31.15.vj, 34.80.Uv

I. INTRODUCTION

The positronium hydride PsH, which has been observed in the laboratory [1], is a four-body exotic system made up of two electrons, one positron, and one proton. Because of its interesting structure containing a positron, PsH provides a unique opportunity for us to study the correlation between electron and positron, in addition to the electron-electron correlation, which has generated considerable theoretical studies. Theoretical calculations have shown that PsH has a true bound state of S symmetry (see [2,3] and references therein) stable against dissociation into Ps and H. Besides the bound state, there also exist other Rydberg states, caused by the Coulomb interaction between the positron and the negatively charged ion H$^-$ [4]. Such Rydberg states in the continuum would appear as resonance states in Ps-H scattering (see the energy levels in Fig. 1). The importance of the H$^-$ configuration was confirmed in a complex-rotation calculation when the explicit electron-electron correlation was included in the wave functions [5]. Later, resonances in Ps-H scattering were investigated using the close-coupling method by including explicitly the H$^-$ channel [6]. Complex-rotation calculations were also carried out for S, P, D, F, and G states using fully correlated Hylleraas basis functions in which all the six interparticle distances were contained [1,7–9]. Triply excited S-wave resonances in Ps-H scattering lying below the doubly excited $2s^2\,{}^1S^e$ state were calculated [10]. An investigation on nonresonance Ps-H scattering was also performed [11]. Recently, an effective potential approach was used by Di Rienzi and Drachman [12] to study higher-lying resonances in Ps-H scattering below the Ps$^-$-H$^+$ threshold, and the resonance energies for the Rydberg series of S, P, and D symmetries were located. We have also calculated the high-lying S-wave resonances in the same energy region of the Ps-H system using the complex-rotation method [13]. The subject of atomic resonance involving positron and positronium has been discussed in several review articles [14–21]. In order to shed light on the importance of the H$^-$ ion and better understand the Rydberg series between the positron and the hydrogen negative ion, we now carry out an investigation on high-lying S-wave resonances in Ps-H scattering converging on the e^+-H$^-$ threshold. We apply the method of complex-coordinate rotation, together with highly correlated Hylleraas wave functions.

II. HAMILTONIAN AND WAVE FUNCTIONS

We set up the coordinate system by choosing the hydrogen nucleus as the origin, which embodies the H$^-$ + e^+ channel. Atomic units are used throughout. The Hamiltonian for the PsH system is

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

$$T = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 - \tfrac{1}{2}\nabla_3^2, \tag{2}$$

$$V = -\frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_3} + \frac{1}{r_{12}} - \frac{1}{r_{23}} - \frac{1}{r_{31}}, \tag{3}$$

where indices 1 and 2 refer to the two electrons, index 3 refers to the positron (see Ref. [22]), and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. The wave function for the electron spin singlet state is expanded in terms of Hylleraas coordinates:

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

where

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

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

All terms in Eq. (5) are included such that

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

where Ω is an integer. The total number of terms in the wave functions is $N = 6412$ for the case of $\Omega = 11$.

III. CALCULATIONS AND RESULTS

For calculating the S-wave autodissociating resonant states, we use the method of complex-coordinate rotation [23,24]. In

---

[*] ykho@pub.iams.sinica.edu.tw

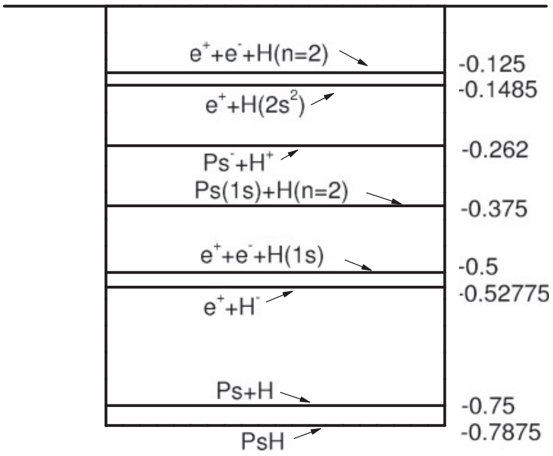

FIG. 1. Energy levels for the Ps-H system (in a. u.).

this method, all radial coordinates r are rotated by an angle θ according to

$$r \to re^{i\theta}. \tag{8}$$

The Hamiltonian is thus transformed into

$$H(\theta) = Te^{-2i\theta} + Ve^{-i\theta}, \tag{9}$$

where T and V are those given by Eqs. (2) and (3), respectively. Complex eigenvalues are obtained by diagonalizing the transformed Hamiltonian, which can be written as

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

where E_r is the resonance position and Γ the resonance width. In our wave functions, we choose the values of the nonlinear parameters around $\alpha = 0.95$ and $\beta = 0.95$, and let γ vary ranging from 0.31 to 0.11. We can also consider γ as a variational parameter to determine the stabilized complex resonance eigenvalues. The physical picture is that the wave functions are designed to simulate the positron moving away from the field of H^- when γ is systematically decreased from $\gamma = 0.31$. We have obtained resonance energies and widths for the $2s$ to $7s$ states, as well as the energy for the $8s$ state. The results are shown in Table I. In Table II, we show a comparison of the lowest three resonances with earlier calculations [6,25–27]]. The resonance energies are converted to eV and are measured from the ground-state energy of the hydrogen atom. It is seen that the complex-rotation results compared well with the close-coupling results [6], as well as with our earlier calculations using the stabilization method [25], showing reasonably good agreements. For high-lying resonances, however, no data are available in the literature for comparison. We notice that some resonance structures for high-lying resonances are available in Ref. [6]. Next, based on our resonance energies, we calculate the binding energies ΔE, relative to the H^- ground-state energy of −0.527 751 016 54 a.u. [28]. We then fit the binding energies of $n = 4$ to 7 into the quantum defect formula

TABLE I. S-wave resonances in the Ps-H system below the e^+-H^- threshold.

State E_r (a.u.) (actual calculations)	$\Gamma/2$(a.u.)	E_r (a. u.) (Fitted values, see text)
(1S) −0.789 196 7147[a]		−0.750′896
(2S) −0.602 78	0.001 753	−0.607 95
(3S) −0.568 2	0.000 92	−0.568 64
(4S) −0.552 48	0.000 52	−0.552 48
(5S) −0.544 33	0.000 36	−0.544 30
(6S) −0.539 63	0.000 21	−0.539 60
(7S) −0.536 5	0.000 12	−0.536 65
(8S) −0.534 5		−0.534 68

E(infinite) =-0.527 751 016 54 a.u. [28,29]

[a] Value taken from Ref. [2].

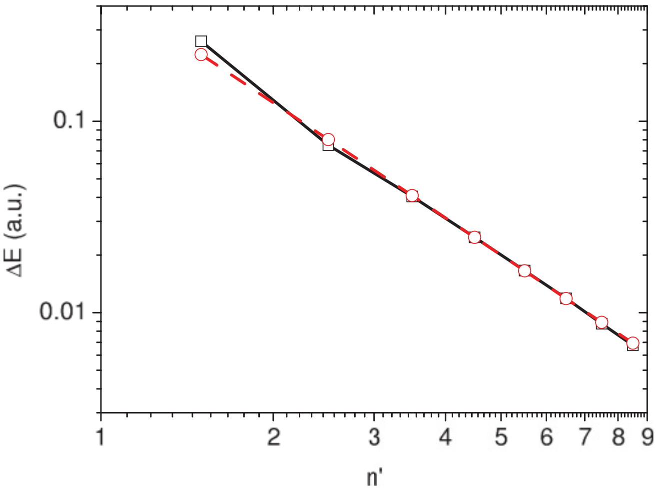

FIG. 2. (Color online) Fitting of the binding energies relative to the H^- threshold (in red circles) for the $n = 4$ to 7 S states into the Rydberg quantum defect formula of Eq. (11), yielding $\delta = -0.49690$. The fitted parameter is then used in Eq. (11) to calculate the first eight members of the Rydberg series, showing a comparison with the actual calculations (in black squares).

$$\Delta E = (1/2)Z^2/(n - \delta)^2 \ \ (\text{in a.u.}), \tag{11}$$

where the quantum defect δ is to be deduced from the fitting with $Z = 1$ for the H^- ion. We obtain $\delta = -0.496\,90$. Figure 2 shows a log-log plot for ΔE vs n', with $n' = n\ \delta$, the effective principal quantum number. The straight line connecting the members of the Rydberg series shows the typical characteristic of Coulomb interaction. Using the fitted δ, the resonance energies for higher members ($N > 8$) of the Rydberg series can be deduced. Also in Fig. 2, we use the fitted δ in Eq. (11) to calculate the energy levels of the lowest eight members of the Rydberg series, including the ground state (in this case n' $= 1-\delta$) of positronium hydride [2]. The fitted energies are also shown in Table I. It shows that with slight deviation form the actual calculations (black solid line) for the lower-lying members in this Rydberg series, the phenomenon that the calculated energies, including resonances and the ground state, seem to follow the pattern set by the quantum defect Rydberg formula is quite remarkable. In addition to the energies for the higher-lying members of the Rydberg series, we can also estimate the widths for such members if they share the same lower-lying open channels to which such resonance states can be autodissociated. For example, the 4S to 8S states

TABLE II. Resonances in Ps-H scattering. Energies (measured from the ground-state energy of the H atom) and widths (inside the parentheses) are in eV. The $2S$ to $4S$ states are resonances and the $1S$ state (not shown here) is the ground state of PsH.

	Complex- rotation	Stabilization method	22 Ps 1H + H$^-$	Optical potential	Five-state coupled- channel
	Present calculations	[25]	[6]	[26]	[27]
$2S$	4.006	4.007	4.141	4.021	4.01
	(0.0954)	(0.0969)	(0.071)	(0.0259)	(0.15)
$3S$	4.947	4.953	4.963		
	(0.0501)	(0.0574)	(0.033)		
$4S$	5.375	5.376	5.388		
	(0.0283)	(0.0278)	(0.032)		

calculated in the present work lie between the [H(1s)+Ps(2s)] and the [H(1s)+Ps(3s)] thresholds with threshold energies of -0.5625 and -0.52778 a.u., respectively. The widths for such resonances follow approximately the scaling law $\Gamma_n = 2\,A/(n{-}\delta)^3$, where A can be determined from the calculated widths. Using the widths for the $5S$, $6S$, and $7S$ states, we determine A as 0.0552. The widths for higher members n (but below the [H(1s)+Ps(3s)] threshold) can be estimated using the scaling law with the abovementioned determined A value. However, for the even higher-lying resonance states in PsH that are located above the [H(1s)+Ps(3s)] threshold, the scaling constant A would be different, since an additional channel is now open. Estimation of the widths for such higher-lying resonances is outside the scope of our present investigation.

IV. SUMMARY AND CONCLUSION

In summary, we have performed a complex-coordinate rotation calculation for the high-lying S-wave resonances in Ps-H scattering, using highly correlated Hylleraas wave functions. The energy positions for the $2S$ to $8S$ states in the Rydberg series converging to the H$^-$-e^+ threshold have been determined, together with the widths for $2S$ to $7S$ states. The energies of $4S$ to $7S$ in the Rydberg series are used to fit into the quantum defect formula with high reliability. From the quantum defect results, the energy levels for higher members of the Rydberg series can be estimated. This work has also shown the importance of the H$^-$ ion. Using the calculated resonance energies to fit into the quantum defect formula for a Rydberg series converging on the H$^-$ threshold, we have shown that the resonances reported in the present work are the results of a Rydberg series due to the Coulomb interaction between a positively charged positron and the negatively charged H$^-$ ion, which supports Drachman's explanation about the physical nature for such resonances in Ps-H scattering [4].

ACKNOWLEDGMENTS

Z.C.Y. is supported by NSERC, ACEnet, SHARCnet, and WestGrid of Canada. Y.K.H. is supported by the NSC of Taiwan, ROC. We are grateful to an anonymous referee for valuable suggestions.

---

[1] D. M. Schrader, Finn M. Jacobsen, N. P. Frandsen, and U. Kikkelsen, Phys. Rev. Lett. **69**, 57 (1992).

[2] Z.-C. Yan and Y. K. Ho, Phys. Rev. A **59**, 2697 (1999).

[3] J. Mitroy, Phys. Rev. A **73**, 054502 (2006).

[4] R. J. Drachman, Phys. Rev. A **19**, 1900 (1979).

[5] Y. K. Ho, Phys. Rev. A **17**, 1675 (1978)

[6] C. P. Campbell *et al.*, Phys. Rev. Lett. **80**, 5097 (1998); Jennifer E. Blackwood, Mary T. McAlinden, and H. R. J. Walters, Phys. Rev. A **65**, 030502(R) (2002).

[7] Z.-C. Yan and Y. K. Ho, Phys. Rev. A **57**, R2270 (1998).

[8] Y. K. Ho and Z.-C. Yan, J. Phys. B **31**, L877 (1998).

[9] Y. K. Ho and Z.-C. Yan, Phys. Rev. A **62**, 052503 (2000).

[10] Y. K. Ho, Phys. Rev. A **41**, 68 (1990).

[11] P. Van Reeth and J. W. S. Humberston, J. Phys. B **36**, 1923 (2003).

[12] J. Di Rienzi and R. J.Drachman, Phys. Rev. A **76**, 032705 (2007).

[13] Z.-C. Yan and Y. K. Ho, Phys. Rev. A **78**, 012711 (2008).

[14] R. J. Drachman, in *Atomic Physics with Positrons*, edited by J. W. Humberston and E. A. G. Armour (Plenum, New York, 1987), p. 203.

[15] Y. K. Ho, in *Annihilation in Gases and Galaxies,* Edited by R. J. Drachman, NASA Conf. Publ. No. 3058 (NASA, Washington, DC, 1990), p. 243.

[16] J. W. Humberston, Adv. Atom. Mole. Opt. Phys. **32**, 205 (1994).

[17] Y. K. Ho, Hyperfine Inter **73**, 109 (1992); **89**, 401 (1994).

[18] Y. K. Ho, Chin. J. Phys. **35**, 97 (1997).

[19] R. J. Drachman, Nucl. Inst. Meth. B **143**, 1 (1998).

[20] H. R. J. Walters, A. C. H. Yu, S. Sahoo *et al.*, Nucl. Inst. Meth. B **221**, 149 (2004).

[21] Y. K. Ho, Nucl. Inst. Meth. B **266**, 516 (2008).

[22] Z.-C. Yan and G. W. F. Drake, J. Phys. B **30**, 4723 (1997).

[23] Y. K. Ho, Phys. Rep. **99**, 1 (1983), and references therein.

[24] W. P. Reinhardt, Annu. Rev. Phys. Chem. **33**, 223 (1982).

[25] Z.-C. Yan and Y. K. Ho, J. Phys. B **36**, 4417 (2003).

[26] J. Di Rienzi and R J Drachman, Phys. Rev. A **65**, 032721 (2002); **66**, 054702 (2002).

[27] S. K. Adhikari, Phys. Rev. A **63**, 054502(2001).

[28] A. M. Frolov and V. H. Smith Jr., J. Phys. B **36**, 4837 (2003).

[29] S. Kar, and Y. K. Ho, New J. Phys. **7**, 141 (2005).