Shape resonance in the Ps^- system

Sabyasachi Kar[1,*] and Y. K. Ho[2,†]

[1]*Center for Theoretical Atomic and Molecular Physics, The Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150080, People's Republic of China*

[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei, Taiwan 106, Republic of China*

(Received 18 May 2012; published 3 July 2012)

We have searched for S-wave shape resonances in the Ps^- system. The calculations are carried out in the framework of the complex-coordinate rotation method using both Hylleraas-type wave functions involving powers of interparticle coordinates, and the exponential correlated wave functions. We have located an S-wave shape resonance lying above the Ps ($N = 2$) threshold. By changing the mass of the positively charged particle from one unit of the electron mass to infinitely heavy, we have traced this resonance pole from Ps^- to H^-. Results for the shape resonance in H^- are comparable with the available results in the literature.

DOI: 10.1103/PhysRevA.86.014501 PACS number(s): 36.10.−k, 32.80.Zb, 34.80.Bm, 31.15.xt

There have been continued experimental [1–8] and theoretical investigations [9–26] on the positronium negative ion (Ps^-), one of the simplest three lepton systems interacting through Coulomb forces. The doubly excited states of Ps^- behave like an X-Y-X triatomic molecule [14,16]. The importance of investigation for such a three-body system with various angular momentum and parity states has been highlighted in earlier works [16]. In the present work, we are interested in researching S-wave shape resonance states for Ps^- and H^-. According to the Feshbach projection formalism, resonance states arising from the closed channel segment of the scattering wave functions are commonly known as Feshbach resonances or closed channel resonances, and those arising from the open channel segment of the scattering wave functions are known as shape resonances or open channel resonances. A shape resonance in e^--Ps scattering is the result of the incoming electron being temporarily trapped by a potential well formed by the attractive static and polarization potentials between the incoming electron and the Ps atom, and a repulsive angular momentum barrier. Such a potential well may be able to support both Feshbach-type resonances lying below the excitation threshold of the Ps atom, and shape resonances lying above. In the present work, we have investigated a shape resonance for the S state of Ps^- above the $N = 2$ Ps threshold using Hylleraas-type wave functions and correlated exponential wave functions. The complex-coordinate rotation method (CRM) is employed to extract resonance parameters [27]. We have found a shape resonance lying above the $N = 2$ Ps threshold that, to our knowledge, has not been reported before. We have traced this resonance pole from the positronium negative ion to the hydrogen negative ion, by varying the mass of the positively charged particle from one unit of the electron mass to infinitely heavy.

The nonrelativistic Hamiltonian (in atomic units) describing a system having two electrons and a positively charged particle having mass M is given by

$$H = T + V = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{2M}\nabla_3^2 - \frac{1}{r_{13}} - \frac{1}{r_{23}} + \frac{1}{r_{12}}, \tag{1}$$

where 1, 2, and 3 denote the two electrons 1, 2 and the positively charged particle, respectively, and r_{ij} is the relative distance between the particles i and j. For the system Ps^-, $M = 1$ and for the system H^-, $M \to \infty$.

For S states we have used the following Hylleraas-type wave functions to describe the proposed systems:

$$\Psi_{kmn} = \sum_{kmn} C_{kmn}\{\exp[-\alpha(r_{13} + r_{23})]r_{12}^k r_{13}^m r_{23}^n + (1 \leftrightarrow 2)\}. \tag{2}$$

In Eq. (1) we also have $k + m + n \leqslant \Omega$, where Ω,l,m, and n are positive integers or zero. In the present work, wave functions with up to $\Omega = 21$ ($N_b = 1078$) are used. We have also carried out calculations using exponential correlated wave functions,

$$\Psi = \sum_i C_i\{\exp[(-\alpha_i r_{13} - \beta_i r_{23} - \gamma_i r_{12})\omega] + (1 \leftrightarrow 2)\}; \tag{3}$$

the nonlinear variational parameters α_i, β_i, and γ_i are generated in a quasirandom manner:

$$X_i = \left[\frac{1}{2}i(i+1)\sqrt{p_X}\right](A_{2,X} - A_{1,X}) + A_{1,X}, \tag{4}$$

where $[x]$ designates the fractional part of x; $[A_{1,X}, A_{2,X}]$, with $(X = \alpha, \beta, \gamma)$, are real variational intervals which need to be optimized. p_α, p_β, and p_γ are some prime numbers. So the number of parameters depends on the size of the basis. However, we have effectively optimized six parameters, $A_{1,\alpha}$, $A_{2,\alpha}$, $A_{1,\beta}$, $A_{2,\beta}$, $A_{1,\gamma}$, and $A_{2,\gamma}$. Here ω is an overall scaling factor.

The present calculations have been performed within the framework of the complex-coordinate rotation method. In the complex-rotation method [27], the radial coordinates are transformed by

$$r \to r\exp(i\theta), \tag{5}$$

where θ is real and positive, and the transformed Hamiltonian (1) becomes

$$H \to T\exp(-2i\theta) + V\exp(-i\theta), \tag{6}$$

where T and V are the kinetic and the potential energies. Under such a transformation, one needs to calculate the

*skar@hit.edu.cn
†ykho@pub.iams.sinica.edu.tw

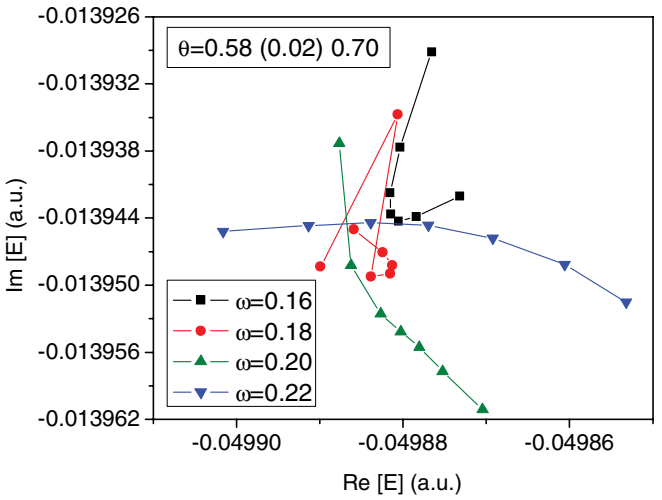

FIG. 1. (Color online) The rotational paths for an S-wave shape resonance of Ps^- in the energy plane for four different values of the scaling factor ω.

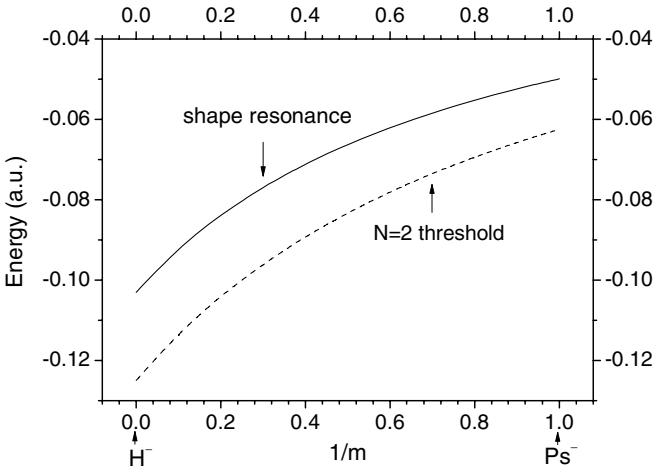

FIG. 2. Resonance energies of the three-body systems vs the inverse of the mass of the positively charged particle along with the $N = 2$ threshold energies of the two-body subsystems. Unit of M is the electron mass.

matrix element for the kinetic energy term in Eq. (1) and the potential energy term in Eq. (1) separately, and then scale them according to Eq. (6). Resonances can be examined once the complex eigenvalue problem is diagonalized with the wave functions in Eqs. (2) and (3). Resonance poles can be identified by observing the stabilized complex eigenvalues $E(\theta, \alpha)$ [in the case of Eq. (2)] or $E(\theta, \omega)$ [in the case of Eq. (3)]. The complex resonance energy is given by

$$E_{\rm res} = E_r - i\Gamma/2, \tag{7}$$

where E_r is the resonance energy, and Γ is the width. The resonance parameters are determined by locating stabilized roots with respect to variation of the nonlinear parameters in the wave functions and of the rotational angle.

Using the complex-coordinate rotation method, we have located an S-wave shape resonance lying above the Ps ($N = 2$) threshold. Figure 1 shows rotational paths for this shape resonance obtained using 700-term exponential correlated wave functions [Eq. (3)]. For the exponential wave functions, we have examined the convergence of our calculations using 500, 600, and 700 terms. Similar stabilized behavior for varying rotational angles using a Hylleraas-type basis [see Eq. (2)] has also been observed. Employing the wave functions in Eqs. (2) and (3), we have obtained the resonance parameters $(E_r, \Gamma/2)$ in atomic units as $(-0.049\,8788, 0.013\,9470)$ and $(-0.049\,881, 0.013\,948)$, respectively. From the minimal change of the resonance complex eigenvalue with respect to the changing θ, we estimate the uncertainty of this resonance is about 5×10^{-6} for each of the real and imaginary parts. This stabilized complex eigenvalue has never been reported in the literature, to the best of our knowledge. Furthermore, by changing the mass of the positively charged particle from one unit of the electron mass to infinitely heavy, we have traced this resonance pole from the positronium negative ion to the hydrogen negative ion. For H^-, the counterpart of this shape resonance is found to have resonance parameters $E_r = -0.103\,035\,69$ a.u. and $\Gamma/2 = 0.015\,627\,29$ a.u. using the wave functions (2), and

TABLE I. Resonance parameters $(E_r, \Gamma/2)$ in terms of the mass of the positively charged particle along with the $N = 2$ threshold energies of the two-body subsystems. The uncertainties are estimated as 5×10^{-6} for each of the real and imaginary parts of the complex eigenvalues.

	Hylleraas-type wave functions [Eq. (2)]		Exponential correlated wave functions [Eq. (3)]		$N = 2$ threshold energy of
M	E_r (a.u.)	$\Gamma/2$ (a.u.)	E_r (a.u.)	$\Gamma/2$ (a.u.)	the two-body subsystem
∞	− 0.103 035 69	0.015 627 29	− 0.103 0357	0.015 6273	− 0.125
10	− 0.092 406 31	0.016 344 05	− 0.092 4064	0.016 3440	− 0.113 636 3636
5	− 0.083 909 59	0.016 598 93	− 0.083 9098	0.016 5990	− 0.104 166 6667
3.33	− 0.076 947 92	0.016 570 03	− 0.076 9480	0.016 5703	− 0.096 131 6397
2.5	− 0.071 185 99	0.016 368 03	− 0.071 1860	0.016 3687	− 0.089 285 7143
2	− 0.066 293 52	0.016 058 68	− 0.066 2940	0.016 0587	− 0.083 333 3333
1.67	− 0.062 141 27	0.015 688 66	− 0.062 1412	0.015 6892	− 0.078 183 5206
1.43	− 0.058 470 86	0.015 273 29	− 0.058 4731	0.015 2760	− 0.073 559 6708
1.25	− 0.055 245 57	0.014 835 58	− 0.055 2470	0.014 8341	− 0.069 444 4444
1.11	− 0.052 386 03	0.014 387 72	− 0.052 3872	0.014 3892	− 0.065 758 2938
1	− 0.049 878 73	0.013 947 05	− 0.049 881	0.013 948	− 0.0625

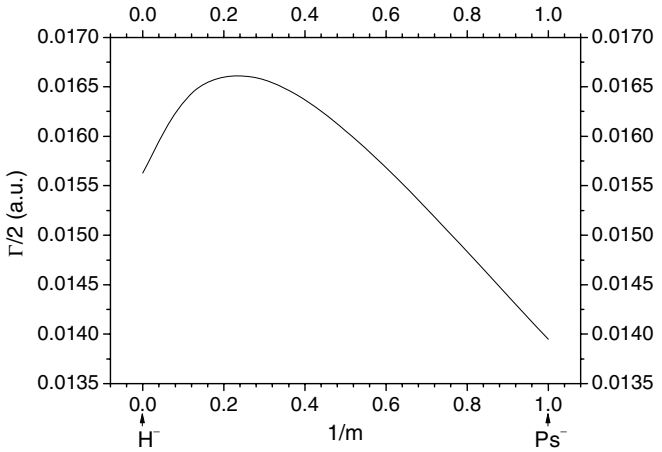

FIG. 3. Resonance widths vs the inverse of the mass (in atomic units) of the positively charged particle. Unit of M is the electron mass.

$E_r = -0.103\,0357$ a.u. and $\Gamma/2 = 0.015\,6273$ a.u. using the exponential correlated wave functions (3). Our finding for the H^- ion is consistent with the result ($E_r = -0.103\,035\,676$ a.u. and $\Gamma/2 = 0.015\,627\,312$ a.u.) reported in Ref. [28] using the same CRM but with a Sturmian-type basis in perimetric coordinates. We present our calculated results in Table I, and Figs. 2 and 3, along with the $N = 2$ threshold energies of the two-body subsystems consisting of the positively charged particles with mass M, and one of the two electrons. It appears that our calculations using the two different wave functions in Eqs. (2) and (3) yield similar results, and they agree quite well with those in Ref. [28]. It was conjectured [28] that the new shape resonance is due to a nonadiabatic coupling between different binding and antibinding adiabatic potentials which correspond to a mixing of different (K, T) approximate quantum numbers as defined by the group theoretical method [29,30], and by using the hyperspherical coordinate approach [31]. As for the Ps^- shape resonance reported in the present work, there appear to be no other calculations reported in the literature. It is hoped that our present finding will stimulate further investigations on this type of newfound shape resonance. For example, resonances may be analyzed by calculating the time-delay or lifetime matrix [32]. A peak structure in the eigenvalues of the time-delay matrix would reveal the existence of a resonance pole in the S matrix. Such an independent investigation on the shape resonance reported here is encouraged.

Y.K.H. is supported by NSC of Taiwan.

[1] A. P. Mills Jr., Phys. Rev. Lett. **46**, 717 (1981); **50**, 671 (1983).
[2] U. I. Uggerhøj, Phys. Rev. A **73**, 052705 (2006).
[3] F. Fleischer, K. Degreif, G. Gwinner, M. Lestinsky, V. Liechtenstein, F. Plenge, and D. Schwalm, Phys. Rev. Lett. **96**, 063401 (2006).
[4] D. B. Cassidy and A. P. Mills Jr., Nature **449**, 195 (2007).
[5] C. M. Surko, Nature **449**, 153 (2007).
[6] Y. Nagashima and T. Sakai, New J. Phys. **8**, 319 (2006); Y. Nagashima, T. Hakodate, A. Miyamoto, and K. Michishio, *ibid.* **10**, 123029 (2008).
[7] K. Michishio, T. Tachibana, H. Terabe, A. Igarashi, K. Wada, T. Kuga, A. Yagishita, T. Hyodo, and Y. Nagashima, Phys. Rev. Lett. **106**, 153401 (2011), and references therein.
[8] H. Ceeh, C. Hugenschmidt, K. Schreckenbach, S. A. Gärtner, P. G. Thirolf, F. Fleischer, and D. Schwalm, Phys. Rev. A **84**, 062508 (2011).
[9] Y. K. Ho, Phys. Rev. A **19**, 2347 (1979); Phys. Lett. A **102**, 348 (1984).
[10] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **28**, 2523 (1983); **32**, 3745 (1985).
[11] S. J. Ward, J. W. Humberston, and M. R. C. McDowell, J. Phys. B **20**, 127 (1987).
[12] J. Botero, Phys. Rev. A **35**, 36 (1987); Z. Phys. D **8**, 177 (1988).
[13] A. K. Bhatia and Y. K. Ho, Phys. Rev. A **42**, 1119 (1990); Y. K. Ho and A. K. Bhatia, *ibid.* **44**, 2890 (1991); **45**, 6268 (1992).
[14] J. M. Rost and D. Wintgen, Phys. Rev. Lett. **69**, 2499 (1992).
[15] Y. K. Ho and A. K. Bhatia, Phys. Rev. A **47**, 1497 (1993); **50**, 2155 (1994).
[16] Y. Zhou and C. D. Lin, Phys. Rev. Lett. **75**, 2296 (1995).
[17] R. Krivec, V. B. Mandelzweig, and K. Varga, Phys. Rev. A **61**, 062503 (2000).
[18] A. M. Frolov and V. H. Smith Jr., J. Phys. B **36**, 4837 (2003).
[19] A. Igarashi and I. Shimamura, J. Phys. B **37**, 4221 (2004).
[20] G. W. F. Drake and M. Grigorescu, J. Phys. B **38**, 3377 (2005).
[21] S. Kar and Y. K. Ho, Phys. Rev. A **71**, 052503 (2005); **71**, 032502 (2006); Chem. Phys. Lett. **424**, 403 (2006).
[22] Y. K. Ho, in *Proceedings of NASA GSFC Science Symposium on Atomic and Molecular Physics (NASA/CP-2006-214146)*, edited by A. K. Bhatia (Goddard Space Flight Center, Greenbelt, MD, 2007), p. 111.
[23] Y. K. Ho, Nucl. Instrum. Methods Phys. Res., Sect. B **266**, 516 (2008), and references therein.
[24] J. Zs. Mezei, A. T. Kruppa, and K. Varga, Few-Body Syst. **41**, 233 (2007).
[25] S. Kar and Y. K. Ho, Few-Body Syst. **46**, 173 (2009); Eur. Phys. J. D **57**, 13 (2010); Comput. Phys. Commun. **182**, 119 (2011).
[26] N. Blinov and A. Czarnecki, Phys. Rev. A **85**, 012522 (2012).
[27] Y. K. Ho, Phys. Rep. **99**, 1 (1983), and references therein.
[28] A. Burgers and E. Lindroth, Eur. Phys. J. D **10**, 327 (2000).
[29] D. R. Herrick and O. Sinanoglu, Phys. Rev. A **11**, 97 (1975).
[30] D. R. Herrick, Adv. Chem. Phys. **52**, 1 (1983).
[31] Z. Chen and C. D. Lin, Phys. Rev. A **42**, 18 (1990).
[32] A. Igarashi and I. Shimamura, Phys. Rev. A **70**, 012706 (2004).