Autoionization states of the positronium negative ion

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The complex-rotation method has been applied to investigate autoionization states of the positronium negative ion ($e^-e^+e^-$). Only the singlet S states are considered, but both the lowest resonance below the $n = 2$ and $n = 3$ positronium thresholds are calculated. Using the Hylleraas-type wave function with 161 terms, the resonance parameters (position and width) are determined by the complex-rotation method. The higher members of the resonances are estimated by the stabilization method but no width and "shift" are provided. In addition, by varying the mass of the positron from $1m_e$ (electron mass) to ∞, we are able to investigate the lowest resonance for systems ranging from Ps^- to H^-. From this analysis, the lowest resonance for other three-body systems ($e^-\mu^+e^-$, $\mu^-p\mu^-$, $\mu^-d\mu^-$, $\mu^-t\mu^-$) are deduced.

I. INTRODUCTION

The positronium negative ion Ps^- is one of the simplest three-body systems which interact with Coulomb forces. This system $e^-e^+e^-$ which consists of two electrons and one positron has been proven to be stable against dissociation into a free electron and a positronium atom.[1] The binding energy 0.3266 eV has been calculated variationally by several authors[2,3] and the best variational energy so far was calculated by Frost *et al.*[2] who used 50 correlation terms in the trial wave function. The positron-electron annihilation rate and the two photon angular correlations have been investigated by Ferrante.[4] The formation of the positronium negative ion has been discussed in e^+-He (Ref. 5) and Ps-H (Ref. 6) scattering calculations. Recently, the Faddeev approach has been applied to investigate the bound state of the $e^+e^-e^+$ system[7] and for e^+-Ps scattering.[8,9] Another interesting problem yet to be explored is the resonance phenomenon. If we compare the Ps^- system with the hydrogen negative ion H^-, we will find several similarities between them. For example, they both have only one bound state and the excited states of the parent atoms H and Ps are degenerate. The resonances of H^- are well documented[10] for experimental work and theoretical calculations. The mechanism responsible for the resonances in H^- below the $n=2$ threshold is due to the dipole potential created by the $2s$-$2p$ degeneracy of the hydrogen atom. Such a potential behaves like r^{-2} asymptotically[11] and is able to support an infinite number of resonances if we neglect the coupling with the hydrogen ground state. Since the dipole polarizability of the Ps atom is 8 times larger than the hydrogen counterpart, we would expect the resonances also to appear in electron-positronium scattering.

A standard method used to calculate resonances is the close-coupling approximation. However, the mixed coordinates of the scattered electron and the positronium atom would make the calculation rather difficult. A recently developed complex-rotation method[12] will simplify this problem because the asymptotic representation of the system need not always be enforced and the resonant parameters can be obtained by a simple modification of the bound-state calculational program. Although the complex-rotation method is unlike the close-coupling calculation, in that the background phase shifts are not provided, the resonance position and width can nevertheless be accurately determined.

In this work we use the complex-rotation method to investigate the autoionization states of Ps^-. Only the singlet S states will be considered but both states below the $n=2$ and $n=3$ Ps threshold will be calculated. The lowest resonances are determined by the complex rotation method and the higher members of the resonances are estimated by the stabilization method[13] in which, however, no widths and "shifts" are provided. The empirical relations between these two methods are subsequently discussed. In addition, by varying the mass of the positron m_p from $1m_e$ (the mass of electron) to ∞, we are able to examine the spectrum of resonances for systems ranging from Ps^- to H^-. In this work, only the lowest resonances are examined in detail. In particular, with a trivial change of energy scale, the resonance parameters for other similar three-particle systems ($e^-\mu^+e^-$, $\mu^-p\mu^-$, $\mu^-d\mu^-$, and $\mu^-t\mu^-$) with Coulomb interaction are deduced.

II. CALCULATIONS AND RESULTS

The Hamiltonian of the positronium negative ion is

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

where T and V are kinetic energy and potential energy operators, respectively, and

$$T = -\frac{1}{m_1}\nabla_1^2 - \frac{1}{m_2}\nabla_2^2 - \frac{1}{m_p}\nabla_p^2, \tag{2}$$

$$V = -\frac{2}{r_{1p}} - \frac{2}{r_{2p}} + \frac{2}{r_{12}}. \tag{3}$$

Atomic units are used in this work and the energy is in rydbergs. The subscripts 1, 2, and p refer to the electrons 1, 2, and positron, respectively, and r_{1p} denotes the distance between electron 1 and positron, etc. Hylleraas-type wave functions of the form

$$\Psi = \sum_{k,l,m\geq 0} C_{klm} \exp[-\alpha(r_{1p}+r_{2p})] r_{12}^k (r_{1p}^l r_{2p}^m + r_{1p}^m r_{2p}^l), \tag{4}$$

are employed to represent this system, where $(k+l+m) \leq \omega$ and $l \geq m$ with ω is a positive integer. Since the total wave function is in an S state, we are able to express the kinetic operator T in terms of distance coordinates, and Eq. (2) becomes[14]

$$\begin{aligned} T = &-\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\left(\frac{\partial^2}{\partial r_{12}^2}+\frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right) - \left(\frac{1}{m_1}+\frac{1}{m_p}\right)\left(\frac{\partial^2}{\partial r_{1p}^2}+\frac{2}{r_{1p}}\frac{\partial}{\partial r_{1p}}\right) \\ &-\left(\frac{1}{m_2}+\frac{1}{m_p}\right)\left(\frac{\partial^2}{\partial r_{2p}^2}+\frac{2}{r_{2p}}\frac{\partial}{\partial r_{2p}}\right) - \frac{1}{m_1}\cos\theta_{12,1p}\frac{\partial^2}{\partial r_{12}\partial r_{1p}} \\ &-\frac{1}{m_2}\cos\theta_{12,2p}\frac{\partial^2}{\partial r_{12}\partial r_{2p}} - \frac{1}{m_p}\cos\theta_{1p,2p}\frac{\partial^2}{\partial r_{1p}\partial r_{2p}}, \end{aligned} \tag{5}$$

where

$$\cos\theta_{1p,2p} = (r_{1p}^2 + r_{2p}^2 - r_{12}^2)/2r_{1p}r_{2p} \quad \text{etc.}$$

A. Complex-rotation method

A method for calculating autoionization states is the complex-rotation method. This method rotates the Hamiltonian $H(r)$ into a complex energy plane by transforming $r \to re^{i\theta}$ where $\theta \geq 0$ and real. The resonance parameters E_r and Γ are determined by solving a complex eigenvalue problem

$$\langle \Psi | H(r,\theta) - W | \Psi \rangle = 0. \tag{6}$$

For the systems with Coulomb interaction,

$$H(r,\theta) = Te^{-2i\theta} + Ve^{-i\theta} \quad \text{and} \quad W = E_r - \tfrac{1}{2}i\Gamma. \tag{7}$$

The resonance eigenvalue is determined by observing where the rotational paths slow down at the same position in the complex energy plane for different nonlinear parameters.[15,16] In this work, up to 161 terms ($\omega = 10$) are used. The results are shown in Figs. 1 and 2 for the lowest state below the $n=2$ and $n=3$ positronium excitation thresholds respectively. The nonlinear parameters α are chosen in the neighborhood of $1/2n$ for state below the nth excited threshold.[16] Since the rotational paths slow down at slightly different positions for different nonlinear parameters, we assign these small differences as estimated error. The resonance parameters are $E_r = -0.152061 \pm 0.000002$ Ry and $\Gamma = (8.55 \pm 0.20) \times 10^{-5}$ Ry (Ref. 17) for the state below the $n=2$ threshold and $E_r = -0.070685 \pm 0.000010$ Ry and $\Gamma = (1.45 \pm 0.10) \times 10^{-4}$ Ry for the state below the $n=3$ threshold. It is interesting to note that the lowest resonance determined at $\omega = 9$ ($N = 125$ terms) is $E_r = -0.152061 \pm 0.000004$ Ry, and $\Gamma = (8.6 \pm 0.4) \times 10^{-5}$

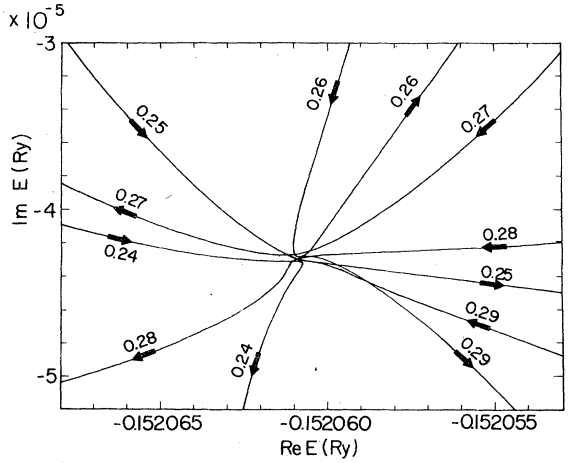

FIG. 1 Lowest resonance $^1S^e$ of Ps^- below the $n=2$ threshold by the complex-rotation method ($N=161$, $\omega=10$). The nonlinear parameter is shown next to each rotational path and the arrow indicates the direction of the path as the angle θ increases. The paths are nearly stationary for $\theta = 0.2$–0.35 rad when they come across the resonance position.

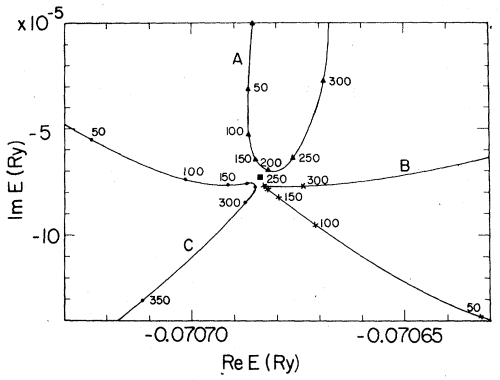

FIG. 2. Autoionization state $^1S^e$ of Ps^- below the $n=3$ threshold by the complex-rotation method ($N=161$, $\omega=10$). The rotational angle θ is shown in mrad near each eigenvalue. The nonlinear parameters for different curves are A, $\alpha=0.15$; B, $\alpha=0.175$; C, $\alpha=0.195$.

Ry. It indicates the final results have converged within the stated errors. For the $n=3$ state, there is an uncertainty of 12% in the width for $\omega=9$. By increasing to $\omega=10$, the error for the width is reduced to about 7% and the position changes only slightly.

It should be mentioned that the resonance state below the $n=2$ threshold has been investigated independently by Arifov *et al.*[18] using the "core pair" approximation. They obtained a resonant position at −0.152 Ry which agrees with the present calculation in the first three digits. However, the width of that state was not calculated.

B. Stabilization method

Another method for locating resonances is the stabilization method.[13] The resonance eigenvalue is insensitive to a change of expansion lengths or nonlinear parameters. In Fig. 3(a), we plot the eigenvalues 8 to 21 against the nonlinear parameter for a given N (161 terms). It is clear that the eigenvalue at −0.152 Ry is stable and the "avoided crossings" occur near $\alpha=0.215$ and 0.3. Usually, we take the middle of the plateau as the resonance position. For an accurate calculation, one must include the "shift."[19] To calculate the shift and the width, the continuum wave functions must be used. Again, the mixed coordinates of the electron and the Ps atom will make an accurate calculation rather difficult. Anyway, it is interesting to point out the empirical relation between the complex-rotation method (Fig. 1) and the stabilization method [Fig. 3(a)]. From $\alpha=0.13$ to $\alpha=0.21$, the 10th eigenvalue is stable. As α increases, the 9th eigenvalue becomes stable. The plateau extends from $\alpha=0.22$ to 0.295. In the later plateau, the rotational paths start rotating

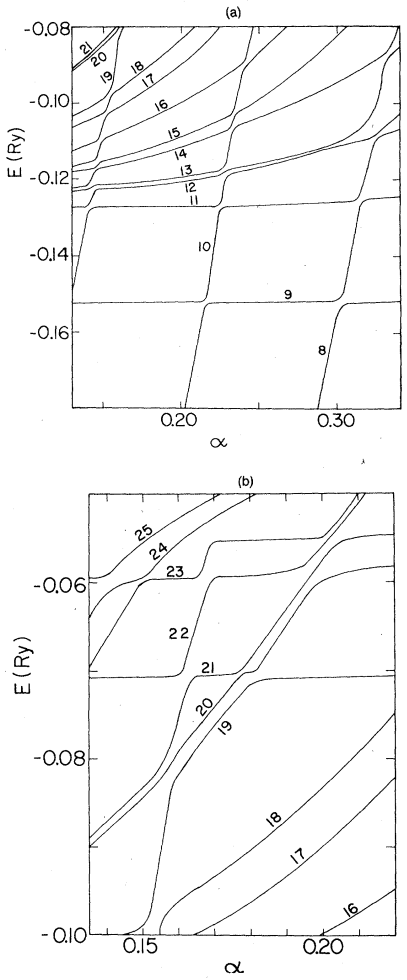

FIG. 3. Autoionization states of Ps^- by the stabilization method ($N=161$, $\omega=10$). The eigenvalues are plotted against the nonlinear parameters α with the number shown next to each eigenvalue. (a) States below the $n=2$ threshold. There are two stabilized eigenvalues below the $n=2$ threshold for the range of α examined here. The first one at $E_r=-0.152061$ Ry is examined by the complex-rotation method in Fig. 1. The second at $E_r=-0.1272$ Ry represents the higher resonance converging on the $n=2$ threshold. (b) States below the $n=3$ threshold. There are two stabilized eigenvalues for the range of α considered here. The first one at $E_r=-0.070685$ Ry is examined by the complex-rotation method (Fig. 2). The second one at $E_r=-0.05954$ Ry represents the higher resonance converging on the $n=3$ threshold.

from the left-hand side of the resonance position (see Fig. 1) and then when α passes 0.255 approximately, the paths simply rotate from the right-hand side. This kind of behavior also occurs in the case of the former plateau from $\alpha=0.13$ to 0.21 (although it is not shown in Fig. 1 for clarity), and so on.

In Fig. 3(a), the eigenvalue at $E_r=-0.1272$ Ry is

TABLE I. Resonances in e^--Ps scattering. The resonance positions are measured from the ground state of the positronium atom. The rydberg [1 Ry = 13.605 826 eV, see B. N. Taylor, W. H. Parker, and D. N. Langenberg, Rev. Mod. Phys. 41, 375 (1969)] is used for energy conversion.

E_r (eV)	Γ (eV)
below the $n=2$ threshold	
$^1S^e(1)$ 4.734 00 ± 0.000 03	$(1.16\times10^{-3})\pm(0.03\times10^{-3})$
$^1S^e(2)$ 5.0723	
below the $n=3$ threshold	
$^1S^e(1)$ 5.841 19 ± 0.000 14	$(1.97\times10^{-3})\pm(0.14\times10^{-3})$
$^1S^e(e)$ 5.9928	

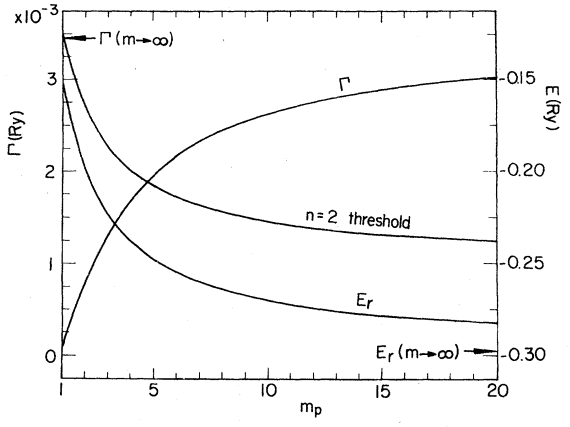

FIG. 4. Resonance of $e^-e^+(m_p)e^-$ systems below the $n=2$ threshold of the $e^-e^+(m_p)$ atoms. Resonance parameters are plotted against the mass of the positron m_p. Here we only show results ofr $1m_e$ to $20m_e$ in which the width changes drastically. As we increase m_p to ∞, both position and width curves are continuous and approaching the H^- limit

also found to be stable. It represents a higher resonant state converging on the $n=2$ Ps threshold. Unfortunately, when we examine this state in the complex-rotation method, we fail to observe a clear cut "slow down" behavior; hence we prefer not to report the width of the higher member of the series. This is similar to the H^- case in that the configuration of the second resonance is $2s3s$.[20] The use of Eq. (4) with only one nonlinear parameter with limited expansion length fails to represent this state adequately, even though 161 terms are employed. Furthermore, the calculation of the width is more sensitive to the trial wave function used. Perhaps a more sophisticated wave function or a bigger expansion length will provide a better result.

In Fig. 3(b), we plot the eigenvalues 16 to 25 against the nonlinear parameter α. The first stabilized eigenvalue for the $n=3$ series has been examined by the complex-rotation method in Fig. 2. Another stabilized eigenvalue at $E_r=-0.05954$ Ry represents the higher member of the series converging on the $n=3$ Ps threshold. Once again, this eigenvalues does not exhibit clear cut slowing down behavior in the complex-rotation method. This is similar to the H^- case[16] in that the configuration of this resonance is $3s4s$. As a result, the wave function we use in this work is not adequate to represent this particular state.

We summarize the above autoionization states in Table I with the energy unit converted to eV. The resonant positions are measured from the ground state of the positronium atom.

C. Resonance parameters for Ps^- to H^-

With the Hamiltonian expressed in the distance coordinates and the trial wave function taken as Eq. (4), it is straightforward to examine autoionization states of all $e^-e^+(m_p)e^-$ systems with any value of m_p. In particular, we vary m_p from $1m_e$ to ∞ such that systems from Ps^- to H^- are examined. We have obtained continuous functions both in resonance position and width. In Fig. 4 we show only the lowest resonance for $1m_e$ to $20m_e$ in which the width changes drastically. The entire curves for position and width, actually, are continuous and approaching the H^- limit.[21]

The other three-body systems for which the odd particle is heavier than other two identical particles and with Coulomb interaction can be similarly

TABLE II. Resonances of three-body systems with Coulomb interaction below the $n=2$ threshold.

System [a]	Target	Dissociation energy of target atom (eV)	E_r (eV) [b]	Γ (eV)
$e^-\mu^+e^-$	μ^+e^-	13.540	9.530	0.0462
$\mu^-p\mu^-$	$P\mu$	2528.53	1776.01	7.12
$\mu^-d\mu^-$	$d\mu$	2663.24	1872.29	8.31
$\mu^-t\mu^-$	$t\mu$	2711.28	1904.44	8.67

[a] Masses (in m_e) used in computing energy levels; $m_\mu=206.77$; $m_p=1836.12$; $m_d=3670.4$; $m_t=5496.8$ and 1 Ry = 13.605 826 eV.

[b] Resonance positions are measured from the ground states of target atoms.

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, deteuron, and triton, respectively. Resonance parameters of these systems can be obtained by the same technique as described previously or just deduced from Fig. 4. For example, the mass ratio of p/μ^- is 8.88. With a trivial change of energy scale, we are able to obtain the resonance parameters at $m_p = 8.88 m_e$ for the $\mu^-p\mu^-$ system. The results are shown in Table II with the energy unit already converted to eV. They are measured up from the ground state of the parent atoms $e^-\mu$, $p\mu$, etc. For each system, only the lowest resonance below the $n=2$ threshold is given. The resonance below the $n=3$ thresholds will be straightforward as in the H^- (Ref. 16) and Ps^- cases.

III. DISCUSSIONS

In this work, we have investigated the autoionization states of the positronium negative ion ($e^-e^+e^-$). The lowest resonance below the $n=2$ and $n=3$ positronium thresholds have been examined by the complex-rotation method and the stabilization method, in that the empirical relation between these two methods are discussed. The existence of these resonances is conclusive. It would be desirable to have these resonances verified experimentally. However, we realize the tremendous difficulty of this problem. For instance, the lifetimes of the target positronium atom are short. They are 1.4×10^{-7} and 1.25×10^{-10} sec for orthopositronium (spins of e^- and e^+ are parallel) and parapositronium (spins are antiparallel), respectively. Recent experiments[22] indicate that the positronium formation cross section is comparable to the elastic cross section for positron collisions with certain rare gases. The technical problem, however, is that we may not have enough positronium atoms for the scattering process. Another difficulty is that the widths of these resonances are very narrow. The lowest resonance is about 40 times smaller than the hydrogen counterpart. The verification of these resonances will be a challenging problem for experimentalists for some time to come. However, since the lifetimes of the positronium atom and the positronium negative ion[23] are longer than those of autoionization states, it means the observation of these resonances is nevertheless possible in principle.

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