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# Doubly excited $^3P^e$ resonant states in $Ps^-$

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Doubly excited $^3P^e$ resonant states in $Ps^-$ are calculated using a method of complex-coordinate rotation. Resonance parameters (both resonance positions and widths) for doubly excited states associated with the $n=2$, 3, 4, 5, and 6 thresholds of positronium atoms are evaluated using elaborate Hylleraas-type functions. In addition to ten Feshbach-type resonances lying below various Ps thresholds, we have identified three shape resonances, one each lying above the $n=2$, 4, and 6 Ps thresholds. It is further noted that the energy levels for the present $^3P^e$ states are nearly degenerate with respect to the previously calculated $^1P^o$ states. Such a symmetric character suggests that the highly and doubly excited $Ps^-$, similar to its counterpart in $H^-$, would exhibit rovibrational behaviors analogous to those of *XYX* triatomic molecules.

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## I. INTRODUCTION

The positronium ion, Ps−, is a three-particle system that consists of two electrons and a positron interacting through Coulomb forces. There have been continuous investigations of various properties of this system [1]. The studies are due in part to the observation of such a species in the laboratory by Mills [2] and the subsequent measurement of its annihilation rate [3]. Furthermore, $Ps^-$ is a member of a family of three-body systems, and the recent theoretical studies of such systems include the investigations of the underlying symmetries of the Hamiltonian. In $H^-$ and He, for example, it was revealed that high-lying doubly excited $H^-$ and He would behave very much like a linear XYX triatomic molecule. The energy levels for the doubly excited two-electron systems reveal molecular rotational and vibrational characters [4]. In order to have a better understanding of the underlying symmetry of the Hamiltonian and the molecular characters of the $e^-e^+e^-$ system, calculations of high-lying doubly excited states for various partial waves and parities are needed. In previous investigations, resonances for $^{1,3}S^e$ [5] and $^{1,3}P^o$ states have been calculated up to the Ps ($n=6$) threshold [6]. For *D*-wave resonances, only one resonance below the Ps ($n=2$) threshold was calculated [7]. In the present work we present a calculation of $^3P^e$ resonances up to the Ps ($n=6$) threshold. Hylleraas- type wave functions are used in this work. Investigations of a $^3P^e$ bound state in $Ps^-$ were carried out by Mills [8] and by Bhatia and Drachman [9]. It was found that in contrast to the $H^-$ case, there is no $^3P^e$ bound state (below the $n=2$ threshold) in $Ps^-$. By analyzing the adiabatic hyperspherical potential curves, Botero [7] indicated that a shape resonance lying above the $n=2$ Ps threshold would exist. In our present work we also carry out an investigation of such a shape resonance. Resonance parameters for position and width are reported.

## II. CALCULATIONS

In this work the method of complex-coordinate rotation [10] is used to calculate resonance parameters. The advantage of using this method is that resonance parameters can be obtained by using bound-state-type wave functions and no asymptotic wave functions are necessarily used. Such an advantage becomes apparent when we are calculating a resonance in which many channels are open. The calculation of the resonance position and total width for a many-channel resonance is as straightforward as that for an elastic resonance. Elaborate Hylleraas-type wave functions [9,11] are used in the present work,

$$\Psi(r_1,r_2)=(\sin\theta_{12})r_1r_2 \times \sum_{l,m,n} C_{lmn}[r_1^l r_2^m e^{-(\alpha r_1+\beta r_2)} + (1\leftrightarrow 2)]r_{12}^n \mathcal{D}_1^{0+} , \tag{1}$$

where the $\mathcal{D}$ functions involve the symmetric Euler angles describing the orientation in space of the coordinate vectors and $l+m+n\le\omega$, with $\omega$ a positive integer or zero. The Hamiltonian is given by

$$H=-2\nabla_1^2-2\nabla_2^2-2\nabla_1\cdot\nabla_2-2/r_1-2/r_2+2/r_{12} = T+V , \tag{2}$$

where $r_1$ and $r_2$ are the coordinates of electrons with respect to the positron, and $r_{12}=|\bar{r}_1-\bar{r}_2|$.

In the complex-rotation method, the radial coordinates are rotated through an angle $\theta$

$$r\rightarrow r\exp(i\theta) \tag{3}$$

and the Hamiltonian can be written as

$$H=T\exp(-2i\theta)+V\exp(-i\theta)\ . \tag{4}$$

The eigenvalues are calculated by diagonalizing the expression

$$E=\langle \Phi H \Phi \rangle / \langle \Phi\Phi \rangle\ , \tag{5}$$

wherein the wave function is real. Since the rotated Hamiltonian is complex, complex eigenvalues are obtained. The resonance parameters are determined by finding a root which is stable with respect to the variation of the nonlinear parameters $\alpha$, $\beta$, and the angle $\theta$, provided it is greater than $\arg(E_{\text{res}})/2$. The complex resonance energy is given by

$$E_{\text{res}}=E_r-i\Gamma/2\ . \tag{6}$$

The theoretical aspects of the complex rotation method have been discussed in previous publications [10] and will not be repeated here. Instead we only briefly describe the computational procedures. First, we use the stabilization method to obtain optimized wave functions with which complex-coordinate calculations will then be carried out. The use of the stabilization method as a first step for the method of complex-coordinate rotation has been demonstrated in a review [10]. Once the stabilized wave functions for a particular resonance are obtained, a staightforward complex rotation method is applied, and the so-called "rotational paths" are examined after the complex transformation $r \rightarrow r\exp(i\theta)$ is made. We then determine the optimized $\theta$ by examining the resonance complex eigenvalue when it exhibits the most stabilized characters. This is usually done by employing smaller basis expansion sets. For example, for the $n=3$ $^3P^e(1)$ resonance, it is found that when $\alpha=0.22$ and $\theta=0.3$ radians approximately, the resonance complex eigenvalue would exhibit the most stabilized character, i.e., $\partial|E|/\partial\theta \approx$ minimum. Once the optimized value for $\theta$ is obtained, we can examine the convergence behaviors for the resonance parameters for different expansion lengths $N$.

### III. RESULTS AND DISCUSSIONS

Table I shows the results when different expansion lengths are used for the $n=3$ $^3P^e(1)$ state. We estimate the resonance position as $E_r=-0.063\,261\,3(1)$ Ry, and $\Gamma/2=0.000\,179\,1(1)$ Ry, with the number(s) inside the parentheses representing the uncertainty in the last digit(s) quoted. It should also be mentioned that the present calculation is not a bound calculation. The error estimates for the resonance parameters are based on the stabilized behaviors of such parameters.

TABLE I. Doubly excited $^3P^e$ states of Ps$^-$ below the Ps ($n=3$) threshold ($\alpha=\beta=0.22$, $\theta=0.30$).

| $\omega$ | $N$ | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|---|
| | | $^3P^e(1)$ | |
| 14 | 444 | −0.063 261 20 | 0.000 179 15 |
| 15 | 525 | −0.063 261 42 | 0.000 179 18 |
| 16 | 615 | −0.063 261 38 | 0.000 179 04 |
| 17 | 715 | −0.063 261 31 | 0.000 179 09 |
| 18 | 825 | −0.063 261 35 | 0.000 179 12 |
| | | $^3P^e(2)$ | |
| 14 | 444 | −0.056 210 88 | 0.000 031 16 |
| 15 | 525 | −0.056 210 58 | 0.000 028 77 |
| 16 | 615 | −0.056 210 02 | 0.000 027 90 |
| 17 | 715 | −0.056 209 77 | 0.000 027 51 |
| 18 | 825 | −0.056 209 48 | 0.000 027 37 |

TABLE II. Doubly excited $^3P^e$ states of Ps$^-$ associated with the Ps ($n=4$) threshold ($\alpha=\beta=0.22$, $\theta=0.3$).

| $\omega$ | $N$ | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|---|
| | | $^3P^e(1)$ | |
| 14 | 444 | −0.037 789 222 4 | 0.000 015 070 2 |
| 15 | 525 | −0.037 789 242 9 | 0.000 015 066 7 |
| 16 | 615 | −0.037 789 242 1 | 0.000 015 056 7 |
| 17 | 715 | −0.037 789 235 1 | 0.000 015 056 9 |
| 18 | 825 | −0.037 789 235 9 | 0.000 015 062 0 |
| | | $^3P^e(2)$ | |
| 14 | 444 | −0.033 088 136 | $8.481\times10^{-6}$ |
| 15 | 525 | −0.033 087 705 | $8.809\times10^{-6}$ |
| 16 | 615 | −0.033 087 607 | $8.943\times10^{-6}$ |
| 17 | 715 | −0.033 087 573 | $8.985\times10^{-6}$ |
| 18 | 825 | −0.033 087 579 | $9.004\times10^{-6}$ |
| | | Shape resonance | |
| 14 | 444 | −0.030 956 4 | 0.000 032 0 |
| 15 | 525 | −0.030 960 8 | 0.000 030 7 |
| 16 | 615 | −0.030 964 8 | 0.000 030 5 |
| 17 | 715 | −0.030 968 4 | 0.000 031 0 |
| 18 | 825 | −0.030 971 5 | 0.000 032 2 |

Table I also shows the similar convergence behavior for the $n=3$ $^3P^e(2)$ resonance at the optimized nonlinear parameters $\alpha=\beta=0.22$ and $\theta=0.3$. We estimate that the resonance parameters for the $n=3$ $^3P^e(2)$ state are

TABLE III. Doubly excited $^3P^e$ states of Ps$^-$ associated with the Ps ($n=5$) threshold ($\alpha=\beta=0.22$, $\theta=0.3$).

| $\omega$ | $N$ | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|---|
| | | $^3P^e(1)$ | |
| 14 | 444 | −0.024 931 815 | 0.000 025 068 |
| 15 | 525 | −0.024 931 645 | 0.000 025 536 |
| 16 | 615 | −0.024 931 667 | 0.000 025 463 |
| 17 | 715 | −0.024 931 665 | 0.000 025 479 |
| 18 | 825 | −0.024 931 660 | 0.000 025 473 |
| | | $^3P^e(2)$ | |
| 14 | 444 | −0.022 121 37 | 0.000 024 6 |
| 15 | 525 | −0.022 096 86 | 0.000 021 4 |
| 16 | 615 | −0.022 096 94 | 0.000 025 3 |
| 17 | 715 | −0.022 097 06 | 0.000 025 8 |
| 18 | 825 | −0.022 097 16 | 0.000 026 2 |
| | | $^3P^e(3)$ | |
| 14 | 444 | −0.021 657 603 | 0.000 133 91 |
| 15 | 525 | −0.021 659 698 | 0.000 132 72 |
| 16 | 615 | −0.021 659 985 | 0.000 132 23 |
| 17 | 715 | −0.021 660 040 | 0.000 132 07 |
| 18 | 825 | −0.021 660 014 | 0.000 132 02 |

TABLE IV. Convergence behaviors for doubly excited $^3P^e$ states of $Ps^-$ associated with the Ps ($n=6$) threshold. Nonlinear parameters used: $^3P^e(1)$, $\alpha=\beta=0.2$; $^3P^e(2)$, $\alpha=\beta=0.2$; $^3P^e(3)$, $\alpha=\beta=0.2$; $^3P^e$ shape resonance, $\alpha=\beta=0.15$. In all cases, $\theta=0.3$.

| $\omega$ | $N$ | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|---|
| | | $^3P^e(1)$ | |
| 15 | 525 | −0.017 598 2 | 0.000 051 9 |
| 16 | 615 | −0.017 596 9 | 0.000 054 0 |
| 17 | 715 | −0.017 596 1 | 0.000 053 3 |
| | | $^3P^e(2)$ | |
| 15 | 525 | −0.015 898 | 0.000 077 |
| 16 | 615 | −0.015 901 | 0.000 061 |
| 17 | 715 | −0.015 894 | 0.000 058 |
| | | $^3P^e(3)$ | |
| 15 | 525 | −0.015 801 1 | 0.000 050 6 |
| 16 | 615 | −0.015 820 3 | 0.000 057 5 |
| 17 | 715 | −0.015 810 8 | 0.000 057 1 |
| | | $^3P^e$ shape resonance | |
| 14 | 444 | −0.013 761 1 | 0.000 024 0 |
| 15 | 525 | −0.013 761 0 | 0.000 021 9 |
| 16 | 615 | −0.013 760 6 | 0.000 019 9 |

$E_r=-0.056\,209\,5(10)$ and $\Gamma/2=0.000\,027\,4(10)$ Ry. Table II summarizes the result for the $n=4$ $^3P^e$ states below the $n=4$ Ps threshold; we have identified a total of three resonances in this energy region. We will summarize them later in the text. In addition to these Feshbach-type resonances lying below the $n=4$ Ps threshold, we have also identified a stabilized complex eigenvalue lying "above" the $n=4$ threshold. Recall that the energy level of the Ps ($n=4$) threshold is $E=-0.03125$ Ry. The convergence behavior for this resonance is also shown here in Table II, and we estimate that it would lie at $E_r=-0.030\,972(5)$ Ry, about 0.000 278 Ry above the $n=4$ threshold. We conclude

TABLE V. The $^3P^e$ shape resonance lying above the $n=2$ Ps threshold ($\alpha=\beta=0.5$).

| $\omega$ | $N$ | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|---|
| | | $\theta=0.6$ | |
| 15 | 525 | −0.124 375 5 | 0.000 255 5 |
| 16 | 615 | −0.124 383 6 | 0.000 252 8 |
| 17 | 715 | −0.124 391 2 | 0.000 251 9 |
| 18 | 825 | −0.124 398 1 | 0.000 252 5 |
| | | $\theta=0.7$ | |
| 15 | 525 | −0.124 382 3 | 0.000 270 5 |
| 16 | 615 | −0.124 387 3 | 0.000 267 2 |
| 17 | 715 | −0.124 391 7 | 0.000 265 4 |
| 18 | 825 | −0.124 395 7 | 0.000 264 9 |
| | | $\theta=0.8$ | |
| 15 | 525 | −0.124 388 8 | 0.000 283 1 |
| 16 | 615 | −0.124 393 9 | 0.000 274 6 |
| 17 | 715 | −0.124 394 2 | 0.000 271 3 |
| 18 | 825 | −0.124 392 5 | 0.000 271 0 |

TABLE VI. Comparison of the $^3P^e$ shape resonance lying above the $n=2$ Ps threshold.

| | Present calculation Complex-coordinate rotation | Hyperspherical coordinate[a] |
|---|---|---|
| $E_r$ (Ry) | $-0.124\,40\pm3\times10^{-5}$ | −0.124 26 |
| $\Gamma/2$ (Ry) | $0.000\,27\pm3\times10^{-5}$ | 0.000 36 |

[a] Reference [7].

TABLE VII. Doubly excited $^3P^e$ state of $Ps^-$ associated with various positronium thresholds $n$. The number(s) inside the parentheses represents the uncertainty in the last digit(s) quoted.

| State | $E$ (Ry) | $\Gamma/2$ (Ry) |
|---|---|---|
| | $n=2$ | |
| $^3P^e$ | −0.124 40(3)[a] | 0.000 27(3) |
| | $n=3$ | |
| $^3P^e(1)$ | −0.063 261 3(1) | 0.000 179 1(1) |
| $^3P^e(2)$ | −0.056 209 5(10) | 0.000 027 4(10) |
| | $n=4$ | |
| $^3P^e(1)$ | −0.037 789 236(10) | 0.000 015 06(1) |
| $^3P^e(2)$ | −0.033 087 6(1) | $9.0(1)\times10^{-6}$ |
| $^3P^e$ | −0.030 972(5)[a] | 0.000 032(5) |
| | $n=5$ | |
| $^3P^e(1)$ | −0.024 931 66(10) | 0.000 025 47(10) |
| $^3P^e(2)$ | −0.022 097 2(5) | 0.000 026 2(5) |
| $^3P^e(3)$ | −0.021 660 0(1) | 0.000 132 0(1) |
| | $n=6$ | |
| $^3P^e(1)$ | −0.017 596(1) | 0.000 053(1) |
| $^3P^e(2)$ | −0.015 894(10) | 0.000 058(10) |
| $^3P^e(3)$ | −0.015 811(10) | 0.000 057(10) |
| $^3P^e$ | −0.013 761(10)[a] | 0.000 020(10) |

[a] A shape resonance as it lies above threshold.

TABLE VIII. Symmetry between doubly excited $^3P^e$ and $^1P^o$ states in $Ps^-$. (Energy levels are given in rydbergs.)

| $^1P^o$ [a] | | $^3P^e$ |
|---|---|---|
| | $n=3$ | |
| −0.063 244 7 | | −0.063 261 3 |
| | $n=4$ | |
| −0.037 780 7 | | −0.037 789 236 |
| −0.033 077 | | −0.033 087 6 |
| −0.030 975[b] | | −0.030 972[b] |
| | $n=5$ | |
| −0.024 922 5 | | −0.024 931 66 |
| −0.022 087 5 | | −0.022 097 2 |
| −0.021 660 | | −0.021 660 0 |
| | $n=6$ | |
| −0.017 595 | | −0.017 596 |
| −0.015 890 | | −0.015 894 |
| −0.015 804 | | −0.015 811 |
| −0.013 750[b] | | −0.013 761[b] |

[a] Reference [6].

[b] Shape resonance.

that such a stabilized complex eigenvalue would lead to a shape resonance in $e^-$- Ps scattering. It is noted that the counterpart of this shape resonance in $\mathrm{H}^-$ would lie below the hydrogen threshold [12]. Table III shows the convergence behaviors for the $^3P^e$ resonances below the $n=5$ Ps threshold, and Table IV shows the $^3P^e$ resonance below the $n=6$ Ps threshold. Again, in addition to the Feshbach resonances we have identified a stabilized complex eigenvalue lying above the $n=6$ Ps threshold (the energy level for the $n=6$ Ps states is $E=-0.013\,889$ Ry). Our resonance energy of $E=-0.013\,761$ Ry lies at about 0.000 128 Ry above the $n=6$ threshold. It is noted that the counterpart of this $^3P^e$ shape resonance in $\mathrm{H}^-$ would lie below the $n=6$ hydrogen threshold and becomes a Feshbach resonance [12].

The possible bound $^3P^e$ state of $\mathrm{Ps}^-$ below the $n=2$ Ps threshold was investigated by Mills [8] and by Bhatia and Drachman [9] using a variational method. They concluded that such a bound state in $\mathrm{Ps}^-$, in contrast to its counterpart in $\mathrm{H}^-$, does not exist. Botero [7], by examining the adiabatic curves that were obtained using hyperspherical coordinates, calculated the energy level for such a state and found it lying above the $n=2$ threshold to become a shape resonance. In this work we also investigate such a shape resonance. The optimized nonlinear parameters are found to be $\alpha=\beta=0.5$ and $\theta=0.8$. The convergence behaviors using different expansion lengths are shown here in Table V. We conclude that the resonance parameters for this resonance are $E_r=-0.124\,40(3)$ Ry and $\Gamma/2=0.000\,27(3)$ Ry. A comparison with the results obtained in Ref. [7] is shown in Table VI. Table VII summarizes results for all the doubly excited intrashell states associated with the $n=2$, 3, 4, 5, and 6 positronium thresholds, respectively.

One of the vibrational characters of an *XYX* molecule is that the $^3P^e$ and $^1P^o$ states are nearly degenerate. In Table VIII we show the comparison between the present $^3P^e$ results and the previously calculated $^1P^o$ states [6]. It is noted that the $^3P^e$ and $^1P^o$ states are highly symmetrical. It is further noted that the $^3P^e$ states lie slightly lower than the $^1P^o$ counterparts. This suggests that the $e^-e^+e^-$ system would exhibit the vibrational characters similar to those for an *XYX* molecule. Of course in order to have a better understanding of the symmetry character of the $\mathrm{Ps}^-$ Hamiltonian, accurate calculations for highly excited autoionizing states with higher angular momenta for $\mathrm{Ps}^-$ are needed. It is hoped that our recent investigation on doubly excited $\mathrm{Ps}^-$ would stimulate other theoretical studies, as well as further experimental investigations on this purely leptonic three-particle system.

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