$^{1,3}P^o$ resonance states in positronium ions

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Doubly excited $^{1,3}P^o$ autodetaching resonances in Ps^- have been calculated using the complex-rotation method, which has the advantage of giving resonance position and width at the same time. The wave function is of the Hylleraas type with number of terms up to 1330. Feshbach resonances associated with the positronium $n=4$, 5, and 6 thresholds are reported. In addition, we have also identified $^1P^o$ shape resonances associated with the positronium $n=4$ and 6 thresholds, and a $^3P^o$ shape resonance associated with the $n=5$ positronium threshold.

I. INTRODUCTION

In a continuing effort to accurately calculate resonance parameters in positronium negative ions, Ps^-, we now report results for $^{1,3}P^o$ resonances associated with the $n=4$, 5, and 6 thresholds of Ps atoms. The results are obtained by using the method of complex-coordinate rotation [1] together with employing Hylleraas-type wave functions. Studies of Ps^- are due to, in part, the observations of such a species in the laboratory by Mills [2], and the subsequent measurement of its annihilation rate [3]. Theoretical studies of various properties of Ps^- have also continuously appeared in the literature [4]. These studies include calculation of its ground-state energy [5–8] and annihilation rate [5,6,9], and the nonexistence of the $^3P^e$ state [10,11]. Resonance phenomena in Ps^- have also attracted considerable interests, as studies of resonances in two-electron systems are well documented in the literature [12]. Several methods have been used to investigate resonance phenomena in Ps^-. These methods include the complex-coordinate rotation [13,14], the close-coupling scattering approximation [15], and using adiabatic potential curves [16]. In an earlier complex-coordinate calculation for $^{1,3}P^o$ resonances, we reported results below the Ps ($n=2$) and Ps ($n=3$) thresholds [17]. The existence of such resonances is due to the dipole potential resulting from the degeneracy of ns-np states of the target positronium atom [18]. In this work, we extend the calculation to the energy regions up to the $n=6$ Ps threshold. 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 are used in the present work.

II. CALCULATIONS

The most general two-electron wave function for $^{1,3}P$ states of odd parity is [19]

$$\Phi(r_1,r_2)=-\cos(\theta_{12})(f\pm\tilde{f})D_1^{1+} -\sin(\theta_{12})(f\mp\tilde{f})D_1^{1-} , \tag{1}$$

where D are the rotational harmonics, depending on the symmetric Euler angles θ, ϕ, and ψ [20]. The trial function f is of the Hylleraas type and is given by

$$f(r_1,r_2,r_{12})=e^{-\alpha r_1-\beta r_2}r_1\sum_{l,m,n\geq 0}C_{lmn}r_1^l r_2^m r_{12}^n\pm(1\leftrightarrow 2) . \tag{2}$$

It is understood that

$$\tilde{f}(r_1,r_2,r_{12})=f(r_2,r_1,r_{12}) \tag{3}$$

and $l+m+n\leq\omega$, where ω is ≥ 0. The Hamiltonian is given by

$$H=-2\nabla_1^2-2\nabla_2^2-2\nabla_1\cdot\nabla_2-2/r_1-2/r_2+2/r_{12}=T+V , \tag{4}$$

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

In the complex-rotation method, the radial coordinates are rotated through an angle θ:

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

and the Hamiltonian can be written as

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

The eigenvalues are calculated by diagonalizing the expression

$$E=\langle\Phi H\Phi\rangle/\langle\Phi\Phi\rangle , \tag{7}$$

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

$$E_{\rm res}=E_r-i\Gamma/2\ . \tag{8}$$

The theoretical aspects of the complex-rotation method have been discussed in previous publications [1] 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 recent review [1]. Once the stabilized wave functions for a particular resonance are obtained, a straightforward 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 θ 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 $n=4$ $^1P^o(1)$ resonance, it is found that when $\theta=0.20$ rad approximately, the resonance complex eigenvalue would exhibit the most stabilized character, i.e., $\partial|E|/\partial\theta\approx$minimum. Once the optimized value for θ is obtained, we can examine the convergence behaviors for the resonance parameters for different expansion lengths. Table I shows the results when different expansion lengths are used for the $n=4$ $^1P^o(1)$ state. We estimate the resonance position as $E_r=-0.037\,780\,7\pm1\times10^{-6}$ Ry with a half-width of $3.08\times10^{-5}\pm1\times10^{-6}$ Ry. 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. Throughout the text, we believe our error estimates are quite conservative.

Table II shows the similar convergence behavior for the $n=4$ $^1P^o(2)$ resonance once the optimized nonlinear parameters $\alpha=\beta=0.09$ and optimized rotational angle $\theta=0.2$ are obtained. It is seen that the convergence character is somewhat slow so we extend the calculation to $N=1330$ terms ($\omega=18$) in order to have a better estimate on the accuracy of the width. Table III summarizes the result for the $n=4$ $^1P^o(3)$ state. For the $^1P^o$ resonances below the $n=4$ Ps threshold, we have identified a total of six resonances. 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 $E=-0.031\,25$ Ry. The convergence behavior for this shape resonance is shown here in Table IV, and we estimate that it would lie at $E_r=-0.030\,975\pm5\times10^{-6}$ Ry, about 0.000 24 Ry above the $n=4$ threshold. We conclude that such a stabilized

TABLE I. Convergence behaviors for the $n=4$ $^1P^o(1)$ resonance in Ps^- ($\alpha=\beta=0.12$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
12	455	0.037 780 98	3.164×10^{-5}
13	560	0.037 781 33	3.030×10^{-5}
14	680	0.037 780 42	3.098×10^{-5}
15	816	0.037 781 08	3.100×10^{-5}
16	969	0.037 780 89	3.075×10^{-5}
17	1140	0.037 780 74	3.078×10^{-5}

TABLE II. Convergence behaviors for the $n=4$ $^1P^o(2)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
15	816	0.034 080 9	2.90×10^{-7}
16	969	0.034 082 7	1.46×10^{-6}
17	1140	0.034 082 4	1.16×10^{-6}
18	1330	0.034 082 4	1.24×10^{-6}

TABLE III. Convergence behaviors for the $n=4$ $^1P^o(3)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
14	680	0.033 073 5	1.511×10^{-5}
15	816	0.033 076 5	2.191×10^{-5}
16	969	0.033 077 2	1.992×10^{-5}
17	1140	0.033 076 9	1.961×10^{-5}
18	1330	0.033 076 7	1.981×10^{-5}

TABLE IV. A $^1P^o$ shape resonance lying above the $n=4$ Ps threshold ($\alpha=\beta=0.08$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
15	816	0.030 962	0.000 027 5
16	969	0.030 966	0.000 029 7
17	1140	0.030 975	0.000 030 1

TABLE V. Convergence behaviors for the $n=5$ $^1P^o(1)$ resonance in Ps^- ($\alpha=\beta=0.12$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
13	560	0.024 920 54	2.176×10^{-5}
14	680	0.024 926 33	2.933×10^{-5}
15	816	0.024 925 97	3.057×10^{-5}
16	969	0.024 925 77	3.041×10^{-5}
17	1140	0.024 925 90	3.061×10^{-5}

TABLE VI. Convergence behaviors for the $n=5$ $^1P^o(2)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
15	816	0.022 415 9	1.461×10^{-5}
16	969	0.022 436 4	3.054×10^{-6}
17	1140	0.022 431 2	2.68×10^{-6}
18	1330	0.022 432 0	1.93×10^{-6}

TABLE VII. Convergence behaviors for the $n=5$ $^1P^o(3)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
15	816	0.022 086 3	0.000 029 9
16	969	0.022 088 0	0.000 033 6
17	1140	0.022 087 5	0.000 031 5
18	1330	0.022 087 4	0.000 031 3

TABLE VIII. Convergence behaviors for the $n=5$ $^1P^o(4)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
14	680	0.021 660 66	0.000 137 37
15	816	0.021 660 15	0.000 135 88
16	969	0.021 661 07	0.000 136 17
17	1140	0.021 660 34	0.000 135 87
18	1330	0.021 660 93	0.000 135 84

TABLE IX. $^1P^o$ resonances associated with $n=4$, 5, and 6 positronium thresholds.

	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
	$N=4$	
$^1P^o(1)$	$0.037\,780\,7\pm1\times10^{-6}$	$0.000\,030\,8\pm1\times10^{-6}$
$^1P^o(2)$	$0.034\,082\,5\pm1\times10^{-6}$	1.3×10^{-6}
$^1P^o(3)$	$0.033\,077\pm1\times10^{-6}$	$0.000\,019\,6\pm1\times10^{-6}$
$^1P^o(4)$	$0.032\,322\pm5\times10^{-6}$	$4.7\times10^{-6}\pm5\times10^{-6}$
$^1P^o(5)$	$0.031\,760\pm5\times10^{-6}$	$1.7\times10^{-5}\pm5\times10^{-6}$
$^1P^o(6)$	$0.031\,605\pm2\times10^{-6}$	$2.5\times10^{-6}\pm2\times10^{-6}$
$^1P^o$	$0.030\,975\pm1\times10^{-5}$ [a]	$0.000\,030\pm1\times10^{-5}$
	$N=5$	
$^1P^o(1)$	$0.024\,925\,5\pm1\times10^{-6}$	$0.000\,030\,5\pm1\times10^{-6}$
$^1P^o(2)$	$0.022\,431\pm5\times10^{-6}$	2.7×10^{-6}
$^1P^o(3)$	$0.022\,087\,5\pm1\times10^{-6}$	$0.000\,031\,5\pm1\times10^{-6}$
$^1P^o(4)$	$0.021\,660\pm1\times10^{-6}$	$0.000\,136\pm1\times10^{-6}$
	$N=6$	
$^1P^o(1)$	$0.017\,595\pm5\times10^{-6}$	$0.000\,055\pm5\times10^{-6}$
$^1P^o(2)$	$0.015\,925\pm1\times10^{-5}$	$1.6\times10^{-5}\pm1\times10^{-5}$
$^1P^o(3)$	$0.015\,890\pm2\times10^{-6}$	$0.000\,062\,0\pm2\times10^{-6}$
$^1P^o(4)$	$0.015\,804\pm5\times10^{-6}$	$0.000\,060\pm5\times10^{-6}$
$^1P^o$	$0.013\,750\pm5\times10^{-6}$ [a]	$0.000\,026\pm5\times10^{-6}$

[a] Shape resonance.

TABLE X. Convergence behaviors for the $n=4$ $^3P^o(1)$ resonance in Ps^- ($\alpha=\beta=0.12$, $\theta=0.25$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
13	560	0.040 169 68	0.000 118 0
14	680	0.040 167 21	0.000 120 5
15	816	0.040 167 56	0.000 119 5
16	969	0.040 167 55	0.000 119 9

TABLE XI. Convergence behaviors for the $n=4$ $^3P^o(2)$ resonance in Ps^- ($\alpha=\beta=0.12$, $\theta=0.25$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
13	560	0.034 631 9	0.000 131 8
14	680	0.034 840 8	0.000 115 8
15	816	0.034 842 1	0.000 116 0
16	969	0.034 842 5	0.000 116 7
17	1140	0.034 842 1	0.000 117 0

TABLE XII. Convergence behaviors for the $n=4$ $^3P^o(3)$ resonance in Ps^- ($\alpha=\beta=0.12$, $\theta=0.25$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
11	364	0.034 262 3	0.000 169 6
12	455	0.034 261 0	0.000 164 4
13	560	0.034 259 1	0.000 165 5
14	680	0.034 259 2	0.000 165 2
15	816	0.034 259 4	0.000 165 0
16	969	0.034 259 3	0.000 165 1

TABLE XIII. Convergence behaviors for the $n=5$ $^3P^o(1)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
14	680	0.025 985 0	0.000 113 7
15	816	0.025 931 4	0.000 105 7
16	969	0.025 964 7	0.000 099 7
17	1140	0.025 965 1	0.000 106 5

TABLE XIV. Convergence behaviors for the $n=5$ $^3P^o(2)$ resonance in Ps^- ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
12	455	0.023 291 3	5.70×10^{-5}
13	560	0.023 295 0	4.69×10^{-5}
14	680	0.023 296 8	5.54×10^{-5}
15	816	0.023 299 1	5.13×10^{-5}
16	969	0.023 300 8	5.12×10^{-5}
17	1140	0.023 299 9	5.16×10^{-5}

TABLE XV. A $^3P^o$ shape resonance lying above the $n=5$ Ps threshold ($\alpha=\beta=0.09$, $\theta=0.20$).

ω	N	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
12	455	0.019 656 9	0.000 074 5
13	560	0.019 672 2	0.000 058 0
14	680	0.019 681 8	0.000 049 1
15	816	0.019 689 0	0.000 042 6
16	969	0.019 695 6	0.000 037 3
17	1140	0.019 702 0	0.000 034 2
18	1330	0.019 707 8	0.000 032 9

TABLE XVI. $^3P^o$ resonances associated with $n=4$, 5, and 6 positronium thresholds.

	$-E_r$ (Ry)	$\frac{1}{2}\Gamma$ (Ry)
	$N=4$	
$^3P^o(1)$	$0.040\,167\,5\pm1\times10^{-6}$	$0.000\,119\,9\pm1\times10^{-6}$
$^3P^o(2)$	$0.034\,842\pm2\times10^{-6}$	$0.000\,116\pm2\times10^{-6}$
$^3P^o(3)$	$0.034\,259\,5\pm1\times10^{-6}$	$0.000\,165\pm1\times10^{-6}$
$^3P^o(4)$	$0.032\,982\,4\pm3\times10^{-7}$	$1.3\times10^{-6}\pm3\times10^{-7}$
$^3P^o(5)$	$0.032\,549\pm1\times10^{-6}$	$0.000\,043\pm1\times10^{-6}$
	$N=5$	
$^3P^o(1)$	$0.025\,965\pm5\times10^{-6}$	$0.000\,106\pm5\times10^{-6}$
$^3P^o(2)$	$0.023\,299\,8\pm1\times10^{-6}$	$0.000\,051\pm1\times10^{-6}$
$^3P^o(3)$	$0.022\,965\pm5\times10^{-6}$	$0.000\,113\pm5\times10^{-6}$
$^3P^o(4)$	$0.021\,817\pm1\times10^{-6}$	$1.3\times10^{-6}\pm1\times10^{-6}$
$^3P^o(5)$	$0.021\,36\pm2\times10^{-5}$	$0.000\,066\pm2\times10^{-5}$
$^3P^o(6)$	$0.020\,914\pm5\times10^{-6}$	$0.000\,026\pm5\times10^{-6}$
$^3P^o$	$0.019\,708\pm5\times10^{-6}$ [a]	$0.000\,033\pm5\times10^{-6}$
	$N=6$	
$^3P^o(1)$	$0.018\,125\pm1\times10^{-5}$	$0.000\,075\pm1\times10^{-5}$
$^3P^o(2)$	$0.016\,760\pm1\times10^{-6}$	$0.000\,011\pm1\times10^{-6}$
$^3P^o(3)$	$0.016\,25\pm3\times10^{-5}$	$6.0\times10^{-5}\pm3\times10^{-5}$
$^3P^o(4)$	$0.015\,548\pm2\times10^{-6}$	$6.0\times10^{-6}\pm2\times10^{-6}$
$^3P^o(5)$	$0.015\,110\pm5\times10^{-6}$	$1.3\times10^{-5}\pm5\times10^{-6}$
$^3P^o(6)$	$0.014\,801\,5\pm1\times10^{-6}$	$0.000\,101\pm1\times10^{-6}$

[a] Shape resonance.

complex eigenvalue would lead to a shape resonance in e^--Ps scattering, or in photoionization cross sections of Ps^-. It is noted that the counterpart of this shape resonance in H^- would lie below the hydrogen threshold [21]. It seems that this case is similar to that for the $n=2$ $^3P^e$ state. The bound $^3P^e$ state in Ps^- does not exist [10,11], but in H^- it lies below the $n=2$ threshold. Furthermore it was found by Bhatia and Drachman [22] that the energy contribution due to the mass polarization term would not decrease sufficiently enough to lead to a bound state for Ps^- when the mass of the positively charged proton is reduced to that of a positron. An independent investigation of the effect for such a mass polarization term on the $^1P^o$ shape resonance is of interest.

Tables V–VIII show the convergence behaviors for the $^1P^o$ resonances below the $n=5$ Ps threshold. We summarize all the $^1P^o$ resonances in Table IX. Also in Table IX, we show the $^1P^o$ resonances below the $n=6$ Ps threshold. The estimated errors for such resonances are somewhat larger than those below the $n=4$ and 5 thresholds. Again, in addition to these Feshbach resonances, we have identified a stabilized complex eigenvalue lying above the $n=6$ Ps threshold, recalling that the energy level for the $n=6$ Ps states is of $E=-0.013\,889$ Ry. Our resonance energy of $E=-0.013\,750$ Ry lies at about 0.000 139 Ry above the $n=6$ threshold. It is noted that the counterpart of this $^1P^o$ shape resonance in H^- would lie below the $n=6$ hydrogen threshold and becomes a Feshbach resonance [21].

In the present work we also report resonance parameters for $^3P^o$ resonances associated with the $n=4$, 5, and 6 Ps thresholds. Tables X–XII show convergence behaviors for the first three resonances below the $n=4$ threshold. We have identified a total of five $^3P^o$ resonances in this energy region and they are summarized later in the text. Tables XIII and XIV show Feshbach resonances below the $n=5$ threshold, and a total of six Feshbach resonances are identified in this energy region. In addition, we have also found a stabilized complex eigenvalue lying above the $n=5$ threshold. The convergence behavior for this shape resonance is shown in Table XV. Recalling that the $n=5$ Ps states having an energy of $E=-0.02$ Ry, our stabilized eigenvalue would lie at $E=-0.019\,708$ Ry, about 0.000 292 Ry above the threshold. We conclude that such a stabilized eigenvalue would lead to a shape resonance in e^--Ps scattering. The counterpart of this $^3P^o$ shape resonance in H^- was not, however, calculated in Ref. [21]. We summarize all the $^3P^o$ resonances in Table XVI, including six members of Feshbach-type resonances that lie below the $n=6$ Ps threshold. The estimated errors for the $n=6$ resonances are somewhat larger than those for the $n=4$ and 5 resonances.

In summary, we have carried out an accurate calculation for $^{1,3}P^o$ resonance states in Ps^- below the $n=4$, 5, and 6 Ps thresholds. A total of 31 Feshbach-type resonances (those below various Ps thresholds) are reported. We have also found three shape resonances, two for $^1P^o$ and one for $^3P^o$, as they lie immediately above their respective thresholds. All of our calculations for Ps^- would provide motivation and useful references for future theoretical and experimental investigations for such a purely leptonic three-particle system.

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