High-angular-momentum resonances in positron scattering by a He⁺ ion

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The method of complex-coordinate rotation is applied to investigate resonances in positron scattering by helium ions. Here we present results for high-angular-momentum states (L=2-6). Together with the earlier values for the L=0 and 1 states, these stabilized complex eigenvalues exhibit a regular pattern. We also calculate some narrow S-wave resonances below the excited positronium (N=2) threshold. Our converged results for the first S state lying above the He⁺ (n=5) threshold differ substantially from the calculation by Igarashi and Shimamura [Phys. Rev. A 56, 4733 (1997)].

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I. INTRODUCTION

There has been continuous interest in the investigation of atomic resonances involving positrons and positronium atoms [1-4]. Recent theoretical studies in this area include those for Ps-H [5–7], Ps-Li [8], Ps-Na and Ps-K [9], and Ps-Rb and Ps-Cs [10], as well as Ps-Ps scattering [11]. The resonance energies and widths for some resonances in positron scattering by hydrogen atoms [12] and by lithium atoms [13] have also been calculated. Resonances in other positronrelated systems, such as antiprotons on positronium [14], are also of recent interest. From the experimental side, an attempt has been made recently to observe resonances in positron scattering by some atoms and molecules [15]. Theoretical studies of positron scattering by He⁺ ion are controversial. Using the stabilization method, Bhatia and Drachman [16] located two S-wave resonances in e^+ -He⁺ scattering. Such resonances were later confirmed in a complex-coordinate-rotation calculation [17]. Also in Ref. [17], the widths for the S-wave resonances were reported, together with two new P-wave resonances. In a later study using the hyperspherical close-coupling method, Igarashi and Shimamura [18] were unable to reproduce these resonances, and presented an argument against the existence of these states. Instead, they reported some narrow S-wave resonances lying just below the positronium Ps(n=1) formation and the excited Ps(n=2) thresholds. Bransden *et al.* [19] carried out a calculation for scattering of positrons by He⁺ ions but no resonances were reported. Other recent work on this system includes a calculation using the algebraic coupled-state variational method [20]. However, again no resonance investigation was carried out in Ref. [20]. Because of the controversial issues raised by Igarashi and Shimamura [18], it is the purpose of this paper to present an investigation of resonances in positron scattering by helium ions. Here, we have calculated high-partial-wave $(L \ge 2)$ resonances for this system. We have also repeated and extended the earlier calculations for the L=0 and 1 states, and found that our earlier results [17], for all practical purposes, have not changed. In this work, we further present an investigation of the narrow S-wave resonances reported in Ref. [18]. For the lowest resonance, considerable differences between the values of [18] and our converged results are found.

The organization of the paper is as follows. In Sec. II we present the Hamiltonian and wave functions used in the work. In Sec. III we show the calculations and discuss our present results. Section IV gives a summary and some concluding remarks.

II. HAMILTONIAN AND WAVE FUNCTIONS

The total Hamiltonian H for the e^+ -He⁺ system, with the energy expressed in Rydberg units, is given by

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

with

$$T = -\nabla_1^2 - \nabla_2^2 \tag{2}$$

and

$$V = -\frac{2Z}{r_1} + \frac{2Z}{r_2} - \frac{2}{r_{12}},\tag{3}$$

where the indices 1 and 2 refer to the coordinates of the electron and the positron. Throughout this work the infinite nuclear mass is used. In the present work, Z=2.

The basis set is constructed using Hylleraas coordinates:

$$\{\chi_{ijk}(\alpha,\beta) = r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2} y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2)\}, \qquad (4)$$

where $y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2)$ is the vector coupled product of solid spherical harmonics for the electron and the positron forming an eigenstate of total angular momentum *L* defined by

$$y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2) = \sum_{m_1 m_2} \langle l_1 l_2 m_1 m_2 | LM \rangle Y_{l_1 m_1}(\hat{r}_1) Y_{l_2 m_2}(\hat{r}_2),$$
(5)

and $\bar{r}_{12} = |\bar{r}_1 - \bar{r}_2|$ is the distance between the electron and the positron. The explicit form for the wave function is

$$\Psi(\overline{r}_1,\overline{r}_2) = \sum_{ijk} a_{ijk} x_{ijk}(\alpha,\beta), \qquad (6)$$

and $i+j+k+L \leq \Omega$ with *i*, *j*, and *k* being positive integers and zero.

State	L	(l_1, l_2)	Ω	Total N
S	0	(0,0)	20	1771
Р	1	(1,0);(0,1)	21	$2 \times 1771 = 3542$
D	2	(2,0);(1,1);(0,2)	20	3×1330=3990
F	3	(3,0);(2,1);(1,2);(0,3)	19	$4 \times 969 = 3876$
G	4	(4,0);(3,1);(2,2);(1,3);(0,4)	19	$5 \times 816 = 4080$
Н	5	(5,0);(4,1);(3,2);(2,3);(1,4);(0,5)	19	$6 \times 680 = 4080$
Ι	6	(6,0);(5,1);(4,2);(3,3);(2,4);(1,5);(0,6)	19	7×560=3920

TABLE I. States with total angular momentum L.

The basic integrals that appear in our calculations are of the form

$$I(a,b,c;\alpha,\beta) = \int d\hat{r}_1 d\hat{r}_2 y_{l_1' l_2'}^{L'M'} (\hat{r}_1,\hat{r}_2)^* \\ \times y_{l_1 l_2}^{LM} (\hat{r}_1,\hat{r}_2) r_1^a r_2^b r_{12}^c e^{-\alpha r_1 - \beta r_2}.$$
(7)

For the nonrelativistic eigenvalue problem, it is only necessary to consider the case of $c \ge -1$ in Eq. (7). The detailed evaluation of Eq. (7) can be found in Ref. [21]. The final result is

$$I(a,b,c;\alpha,\beta) = \sum_{qk} C_{cqk} G(q) I_R(a,b,c;\alpha,\beta,q,k), \quad (8)$$

where the angular part G(q) is

$$G(q) = (-1)^{L+q} (l_1, l_2, l'_1, l'_2)^{1/2} \begin{pmatrix} l'_1 & l_1 & q \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} l'_2 & l_2 & q \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} L & l_1 & l_2 \\ q & l'_2 & l'_1 \end{pmatrix} \delta_{MM'} \delta_{LL'}, \quad (9)$$

and the radial part I_R is

$$I_{R}(a,b,c;\alpha,\beta;q,k) = \frac{s!}{(\alpha+\beta)^{s+1}} \left[\frac{1}{a+3+q+2k} \times_{2}F_{1} \left(1,s+1;a+4+q+2k;\frac{\alpha}{\alpha+\beta} \right) + \frac{1}{b+3+q+2k} {}_{2}F_{1} \left(1,s+1;b+4 + q+2k;\frac{\beta}{\alpha+\beta} \right) \right],$$
(10)

with $_{2}F_{1}(a;b;c;x)$ being the hypergeometric function and s=a+b+c+5, and

$$C_{cqk} = \frac{2q+1}{c+2} \binom{c+2}{2k+1} \prod_{t=0}^{s_{qc}} \frac{2k+2t-c}{2k+2q-2t+1}, \quad (11)$$

with $S_{qc} = \min[q-1, \frac{1}{2}(c+1)]$. It should be pointed out that in Eq. (8) the range of q is limited by the triangular rule of the 3-j symbols in Eq. (9): where

$$q_m \leqslant q \leqslant q_M, \tag{12}$$

(10)

$$q_m = \max(|l_1 - l_1'|, |l_2 - l_2'|), \tag{13}$$

$$q_M = \min(l_1 + l'_1, l_2 + l'_2). \tag{14}$$

Thus, the summation over q in Eq. (8) is always finite.

III. CALCULATIONS AND RESULTS

We first investigate the D-wave resonances. For a state with total angular momentum L=2, we have three basic possible combinations to which the individual angular momenta (l_1, l_2) are coupled. The possible values for (l_1, l_2) are (2, 0), (1, 1), and (0, 2) (see Table I). The higher harmonics are taken care of by the r_{ii} terms. For each summation in Eq. (6), we employ basis sets ranging from $\Omega = 16$ to 19, which correspond to 680 and 1140 terms. The total numbers of terms, after adding up the three sums, are N = 2040 and 3420 for $\Omega = 16$ and 19, respectively. In the method of complexcoordinate rotation [1,22], the radial coordinate r_{ii} between the charged particles *i* and *j* is transformed into $r_{ij}e^{i\theta}$, where θ is the rotational angle. A complex eigenvalue that can be considered as a resonance eigenvalue is one that exhibits stabilized character with respect to changes of θ , as well as to changes of α and β in the wave functions [see Eq. (4)]. Furthermore, the resonance eigenvalue also shows convergence behaviors when the size of the basis set is increased.

Table II shows the convergence and stabilized behaviors for the lowest *D*-wave resonance below the Ps(n=1) threshold. In this example, we use $\Omega = 16$, 17, 18, and 19, which correspond to total numbers of terms of 2040, 2448, 2907, and 3420, respectively. In Table II, we also use wave functions with parameters of $\alpha = 0.8$ and $\beta = 0.5$ calculated at θ = 0.65. Furthermore, when we change the θ value from θ

TABLE II. Stabilization of the first *D*-wave eigenvalue obtained using wave functions with $\alpha = 0.8$, $\beta = 0.5$, and $\theta = 0.65$.

Ω	Ν	E_r (Ry)	$\Gamma/2$ (Ry)
16	$3 \times 680 = 2040$	-0.629 16	0.311 61
17	$3 \times 816 = 2448$	-0.62898	0.311 50
18	$3 \times 969 = 2907$	-0.62877	0.311 77
19	$3 \times 1140 = 3420$	-0.62881	0.311 67



FIG. 1. Resonance poles for e^+ -He⁺ scattering, showing the two groups of resonance poles lying below and above the Ps(n = 1) threshold.

=0.45 to 0.70, the complex eigenvalue exhibits stabilized behavior, i.e., $\partial |E|/\partial \theta$ is approximately a minimum, with $E = E_r - i\Gamma/2$, at about $\theta = 0.65$. From Table II, we have deduced that the resonance parameters for the lowest D-wave resonance lying below the Ps(n=1) threshold are $E_r =$ -0.6288 Ry and $\Gamma/2=0.3117$ Ry. We should mention that this eigenvalue also shows stabilized behavior when the values of the nonlinear parameters are changed, but within the neighborhood of the above mentioned α and β values. In Table III and Fig. 1, we summarize the stabilized complex eigenvalues lying below the positronium Ps(n=1) threshold. Here the L=0 and 1 results are taken from Ref. [17]. The D-wave results are from the present calculations. We should mention that in the present work we have extended the investigation of the L=0 and 1 states by increasing the sizes of the basis sets. Basically, the L=0 and 1 complex eigenvalues remain stabilized. For this group of resonances, we have not found stabilized complex eigenvalues for the F-wave states. We should also point out that, at this juncture, the physical





FIG. 3. Enlarged scale for the resonance poles in e^+ -He⁺ scattering lying above the Ps(n=1) threshold.

reasons behind such resonances are yet to be understood.

Figure 1 also shows the results for the second group of resonances which lie above the Ps(n=1) threshold. For this group of resonances, the authors in Ref. [18] were unable to reproduce our earlier L=0 and 1 results. Here, we also extend our earlier calculations by employing larger expansion sets for the basis wave functions. For example, we use Ω = 20, which corresponds to N = 1771 and 3542 terms for the S and P states, respectively. Again, for all practical purposes, the stabilized behaviors for these two states have not changed. Furthermore, in the present work we carry out calculations for high-angular-momentum states. Table IV shows the stabilized behaviors for a D-state resonance pole. Based on examination of changes of the complex eigenvalue with respect to changes of θ , we determine the resonance energy and Γ [full width at half maximum (FWHM)] as $E_r =$ -0.3665 Ry and $\Gamma/2=0.050$ 84 Ry. We next calculate F states. Similarly for F states, the possible values for (l_1, l_2) are (3,0), (2,1), (1,2), and (0,3). For each sum we use



FIG. 4. Comparison of the S-wave resonance poles below the Ps(n=2) threshold (open circles, present calculations; closed circles, Ref. [18]).

TABLE III. Resonances in e^+ -He⁺ scattering lying below the Ps(n=1) threshold.

State	L	E_r (Ry)	Γ/2 (Ry)
S	0	-0.7410^{a}	-0.1294^{a}
Р	1	-0.7087^{a}	-0.1775^{a}
D	2	-0.6288^{b}	-0.3117^{b}

^aTaken from Ref. [17].

^bPresent calculations.

TABLE VII. Stabilization of the second S-wave resonance be-
low and approaching the Ps(n=2) threshold ($\alpha = \beta = 0.2$). $\boxed{\Omega \quad N \quad \theta \quad E_r (Ry) \quad \Gamma/2 (Ry)}$

_	Ω	Ν	θ	E_r (Ry)	Γ/2 (Ry)
_	17	1140	0.30	-0.134 880 0	7.990×10^{-4}
	18	1330	0.30	-0.1348722	7.971×10^{-4}
	19	1540	0.30	-0.1348623	7.932×10^{-4}
=	20	1771	0.30	-0.134 863 3	7.910×10^{-4}
	17	1140	0.35	-0.1348600	7.940×10^{-4}
	18	1330	0.35	-0.1348637	7.917×10^{-4}
	19	1540	0.35	-0.1348664	7.922×10^{-4}
	20	1771	0.35	-0.1348644	7.920×10^{-4}

TABLE IV. Stabilization of the second *D*-wave eigenvalue obtained using wave functions with $\alpha = 0.8$, $\beta = 0.5$, and $\theta = 0.65$.

Ω	Ν	E_r (Ry)	Γ/2 (Ry)
16	$3 \times 680 = 2040$	-0.367 32	0.050 89
17	$3 \times 816 = 2448$	-0.36643	0.050 80
18	$3 \times 969 = 2907$	-0.36658	0.050 83
19	$3 \times 1140 = 3420$	-0.36651	0.050 84

TABLE VIII. Comparison of S-wave resonances below the Ps(n=2) threshold.

Pres	sent	Ref. [18]		
E_r (Ry)	$\Gamma/2$ (Ry)	E_r (Ry)	$\Gamma/2$ (Ry)	
-0.150 803 5	5.348×10^{-4}	-0.151 19	1×10^{-13}	
-0.134864	7.92×10^{-4}	-0.13484	6.8×10^{-4}	
-0.128 653	3.89×10^{-4}	-0.128 64	3.6×10^{-4}	

TABLE V. Resonances in e^+ -He⁺ scattering in the region above the positronium Ps(n=1) formation threshold.

State	L	E_r (Ry)	Γ/2 (Ry)
S	0	-0.3712^{a}	$-0.039 3^{a}$
Р	1	-0.36956^{a}	-0.04317^{a}
D	2	-0.36651^{b}	$-0.050 84^{b}$
F	3	-0.36238^{b}	-0.06273^{b}
G	4	-0.35485^{b}	$-0.075\ 30^{b}$
Н	5	-0.33420^{b}	$-0.095\ 57^{b}$

^aTaken from Ref. [17].

^bPresent calculations.

TABLE IX. *P*- and *D*-wave resonances below the Ps(n=2) threshold.

State	L	E_r (Ry)	Γ/2 (Ry)
Р	1	-0.1497250	4.465×10^{-4}
Р	1	-0.134210	6.66×10^{-4}
Р	1	-0.128572	4.1×10^{-4}
Р	1	-0.127948	3.8×10^{-4}
D	2	-0.147564	3.23×10^{-4}
D	2	-0.132930	4.30×10^{-4}
D	2	-0.127 92	2.6×10^{-4}

TABLE X. Resonances in e^+ -He⁺ scattering in the energy region between the He⁺(n=5) and Ps(n=2) thresholds.

the $Ps(n =$	2) threshold	$(\alpha = \beta = 0.24, \ \theta = 0.35)$).
Ω	Ν	E_r (Ry)	Γ/2 (Ry)
16	969	-0.150 805 84	0.000 535 91
17	1140	-0.15080370	0.000 534 62
18	1130	-0.15080362	0.000 534 70
19	1540	-0.15080358	0.000 534 78
20	1771	-0.15080356	0.000 534 76

TABLE VI. Stabilization of the first S-wave resonance below

State	L	E_r (Ry)	Γ/2 (Ry)
S	0	-0.150804	5.35×10^{-4}
P	1	-0.1497247	4.46×10^{-4}
D	2	-0.147564	3.23×10^{-4}
F	3	-0.144382	2.40×10^{-4}
G	4	-0.140333	2.22×10^{-4}
Н	5	-0.135625	2.91×10^{-4}
Ι	6	-0.13045	5.2×10^{-4}

 $\Omega = 19$. The total number of terms (N) is therefore 4×969 = 3876. Figure 2 shows the θ trajectory for the *F*-wave resonance pole lying above the Ps(n=1) threshold. Shown here are the resonance poles calculated using θ values ranging from $\theta = 0.55$ to 0.7. Curve A represents the values calculated using the wave functions with expansion $\Omega = 17$ (N =2720). Curves B and C denote $\Omega = 18$ (N=3260) and Ω = 19 (N = 3876), respectively. Here, we use wave functions with parameters of $\alpha = 0.4$ and $\beta = 0.25$. We further deduce the parameters for the stabilized complex eigenvalue as E_r = -0.362 38 Ry and $\Gamma/2=$ 0.062 73 Ry. Other high-angularmomentum states are similarly calculated. Our results are summarized in Table V and in Figs. 1 and 3. In Fig. 1, we show both groups of resonances lying below and above the Ps(n=1) threshold. In Fig. 3, we show an enlargement for the second group of resonance poles. It seems that each group of resonances follows a regular pattern, indicating that each of them belongs to some kind of "family of resonances."

Next, we carry out an investigation of the narrow S-wave resonances reported in Ref. [18]. Igarashi and Shimamura found a narrow S-wave resonance lying below the positronium Ps(n=1) formation threshold. However, we have carried out an extensive search for such a resonance and found no resonances lying immediately below the Ps(n=1) threshold. As for the resonance below the Ps(n=2) threshold, we have calculated three S-wave resonances. Table VI shows the convergence for the lowest eigenvalue, and the resonance parameters for this state are determined as $E_r =$ $-0.150\,803\,5\,\text{Ry}$ and $\Gamma/2 = 5.348 \times 10^{-4}\,\text{Ry}$. Table VII shows the convergence behavior for the second S wave below the Ps(n=2) threshold. In Table VIII and Fig. 4 we show the comparison between our S-wave results and those of Ref. [18]. It is seen that while their second and third S-wave resonances agree reasonably well with our results, their $\Gamma/2$ value for the lowest resonance $(1 \times 10^{-13} \text{ Ry})$ differs substantially from our result of 5.348×10^{-4} Ry. In Ref. [18], the authors explained that the lowest S-wave resonance is a shape resonance lying above the He^+ (n=5) threshold. The autoionization for such a shape resonance is by tunneling. The process would take a long time, and hence the width would be narrow. However, this resonance is located quite far above the proposed threshold, as seen in Fig. 4, and as such it is usually near the top of the potential barrier. Normally, the lifetime for such a resonance should not be too long as it could tunnel out quite rapidly, and the $\Gamma/2$ value should not be as narrow as 10^{-13} Ry. Our converged result of $\Gamma/2 = 5.348 \times 10^{-4}$ Ry for the $\Gamma/2$ value is consistent with the above explanation.

In the present work, we also carry out calculations for P and D states below the Ps(n=2) threshold. We report the results for four such P-wave resonances and three D-wave resonances in Table IX. To our knowledge, no P- and D-wave resonances in this region have been reported in the literature until now.

We next continue to calculate high-angular-momentum states in the energy region below the Ps(n=2) threshold. Using the wave functions described in Table I, we obtained



FIG. 5. Resonance poles for e^+ -He⁺ scattering between the He⁺(n=5) and Ps(n=2) thresholds.

resonance energies and widths for the D, F, G, H, and I states. Results are shown in Table X and in Fig. 5, together with the lowest members of the S and P states. From Fig. 5, it seems that these resonances follow a regular pattern. Again, to our knowledge, these high-angular-momentum states have not been found before.

IV. SUMMARY AND DISCUSSION

In this work we have presented an investigation of resonances in positron scattering by helium ions. We found stabilized complex eigenvalues for high-angular-momentum states. States ranging from L=2 to 6 were calculated. Together with the earlier results for the L=0 and 1 states, such complex eigenvalues can be grouped together, forming a regular pattern. We also carried out a calculation on some narrow S-wave resonances reported in Ref. [18]. For the width lowest of the S-wave resonance, we found substantial disagreement between the value of [18] and our converged result. Furthermore, other angular-momentum states (up to L=6) immediately below the Ps(n=2) threshold were also calculated. We believe that these resonance states are a result of the induced dipole potential between the proton and the excited positronium atom in the n=2 state. As for the stabilized complex eigenvalues below and above the Ps(n=1)threshold (see Fig. 1), although our calculations are extensive and that the existence of such complex eigenvalues is conclusive, we have not provided an explanation for the physical mechanism behind the existence of such states. In this regard, future work should be concentrated on the understanding of the physical nature of these resonances. Nevertheless, hopefully our present work will stimulate further investigations on this intriguing three-body atomic system.

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- [1] Y. K. Ho, Phys. Rep. 99, 1 (1983).
- [2] R. J. Drachman, in *Atomic Physics with Positrons*, edited by J.
 W. Humberston and E. A. G. Armour (Plenum, New York, 1987), p. 203.
- [3] Y. K. Ho, Hyperfine Interact. 73, 109 (1992); Chin. J. Phys. (Taipei) 35, 97 (1997).
- [4] R. J. Drachman, Nucl. Instrum. Methods Phys. Res. B 143, 1 (1998).
- [5] J. E. Blackwood, M. T. McAlinden, and H. R. J. Walters, Phys. Rev. A 65, 030502(R) (2002); C. P. Campbell, M. T. McAlinden, F. G. R. S. MacDonald, and H. R. J. Walters, Phys. Rev. Lett. 80, 5097 (1998).
- [6] Z.-C. Yan and Y. K. Ho, Phys. Rev. A 57, R2270 (1998); 59, 2697 (1999); Y. K. Ho and Z.-C. Yan, J. Phys. B 31, L877 (1998); Phys. Rev. A 62, 052503 (2000).
- [7] J. Di Rienzi and R. J. Drachman, Phys. Rev. A 65, 032721 (2002).
- [8] P. K. Biswas, Phys. Rev. A 61, 012502 (2000).
- [9] S. K. Adhikari and P. J. Mandal, J. Phys. B 34, 1361 (2001).
- [10] S. K. Adhikari, Phys. Lett. A 283, 224 (2001).
- [11] J. Usukura and Y. Suzuki, Few-Body Syst., Suppl. 13, 56

(2001).

- [12] Z.-C. Yan and Y. K. Ho, J. Phys. B 35, 1875 (2002).
- [13] U. Roy and Y. K. Ho, J. Phys. B 35, 2149 (2002).
- [14] C. Y. Hu, D. Caballero, and Z. Papp, Phys. Rev. Lett. 88, 063401 (2002).
- [15] J. P. Sullivan, S. J. Gilbert, S. J. Buckman, and C. M. Surko, J. Phys. B 34, L467 (2001).
- [16] A. K. Bhatia and R. J. Drachman, Phys. Rev. A 42, 5117 (1990).
- [17] Y. K. Ho, Phys. Rev. A 53, 3165 (1996).
- [18] A. Igarashi and I. Shimamura, Phys. Rev. A 56, 4733 (1997).
- [19] B. H. Bransden, C. J. Noble, and R. J. Whitehead, J. Phys. B 34, 2267 (2001).
- [20] T. T. Gien, J. Phys. B 34, L535 (2001).
- [21] Z.-C. Yan and G. W. F. Drake, Chem. Phys. Lett. 259, 96 (1996).
- [22] W. P. Reinhardt, Annu. Rev. Phys. Chem. 33, 223 (1982); B. R. Junker, Adv. At. Mol. Phys. 18, 208 (1982); M. Bylicki, Adv. Quantum Chem. 32, 207 (2001); N. Moiseyev, Phys. Rep. 302, 212 (1998).