Resonances in e^+-He^+ scattering

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(Received 3 November 1995)

The method of complex-coordinate rotation is used to investigate resonances in e^+-He^+ scattering. By using Hylleraas-type wave functions we have obtained resonance parameters for two S- and two P-wave resonances. Our resonance positions for the two S-wave states are consistent with those obtained by Bhatia and Drachman [Phys. Rev. A **42**, 5117 (1990)] who used the stabilization method. The total widths for the lowest S- and P-wave resonances are determined in the present work as 3.52 and 4.83 eV, respectively, raising the possibility that such resonances may be detectable in e^+-He^+ scattering experiments.

PACS number(s): 03.65.Nk, 31.25.−v

I. INTRODUCTION

There has been continuous interest in the investigation of atomic resonances involving positrons [1–3]. Recently, two S-wave resonances in e^+-He^+ scattering have been calculated by Bhatia and Drachman [4] using the stabilization method. They have found two resonances lying at $E_r=-0.73$ Ry and $E_r=-0.39$ Ry, respectively. One possible explanation for their existence is that these resonances are the result of the He^{2+} ion attaching to the degenerate $2s$-$2p$ excited states ($E_r=-0.125$ Ry) of the Ps atom. Since the He^{2+} ion is doubly charged, the attraction between the He^{2+} ion and the excited Ps atom is larger than that for the Ps-H^+ counterpart, and it is reasonable for the $PsHe^{2+}$ resonances to lie lower than those for the PsH^+ system. The location of the first resonance at $E_r=-0.73$ Ry is quite interesting since it lies far away from the proposed parent threshold. In fact, it lies even lower than the ground state of the Ps atom ($E_r=-0.5$ Ry). The interaction between the He^{2+} ion and the ground-state positronium atom may play a role for the existence of the lowest resonance.

In order to shed light on the mechanism for the support of such resonances, we carry out an investigation of resonances using the method of complex-coordinate rotation [5,6]. Together with the use of elaborate Hylleraas-type wave functions, we are able to determine the resonance parameters (energy and total width) for two S- and two P-wave resonances. Furthermore, by changing the charge of the positively charged particle from $Z=2$ to 1, we have examined the changes of these resonances from e^+-He^+ to e^+-H scattering.

II. HAMILTONIAN AND WAVE FUNCTIONS

The Hamiltonian for the $e^+ + He^+$ system is given by

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

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

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

where 1 and 2 denote the electron and positron, respectively, and Z is the charge of the positively charged particle. For the e^+-He^+ system, $Z=2$. Atomic units are used in the present work, with energy expressed in Rydberg units. Hylleraas-type wave functions are used here for the S-wave resonances:

$$\Psi=\sum_{k,m,n} C_{kmn}\exp[-(\alpha r_1+\beta r_2)]r_1^k r_2^m r_{12}^n, \tag{4}$$

with $\omega \geq k+m+n$, and ω, k, m, and n all being positive integers or zero.

In addition to the S-wave resonances, we have also investigated P-wave resonances by using the method of complex-coordinate rotation.

Hylleraas-type wave functions of the form

$$\Psi=\sum C_{kmn}\exp[\alpha(r_1+r_2)]r_1^{k+1}r_2^m r_{12}^n Y_{10}(\Omega_1)Y_{00}(\Omega_2) + \sum D_{kmn}\exp[\alpha(r_1+r_2)]r_2^{k+1}r_1^m r_{12}^n Y_{10}(\Omega_2)Y_{00}(\Omega_1) \tag{5}$$

are used, where Y are the usual spherical harmonics. We have used similar S- and P-wave basis sets in the earlier e^+-H resonance calculations [7–9].

In the complex-rotation method [5], the radial coordinates are rotated through an angle θ:

$$r \rightarrow r\ \exp(i\theta), \tag{6}$$

TABLE I. The first S-wave resonance in e^+-He^+ scattering ($\alpha=1.0$, $\beta=0.5$, $\theta=0.6$).

ω	M	E_r (Ry)	$\Gamma/2$ (Ry)
11	364	−0.741274	0.129816
12	455	−0.740854	0.129405
13	560	−0.741088	0.129472
14	680	−0.740969	0.129424
15	816	−0.741021	0.129435
16	969	−0.740993	0.129429

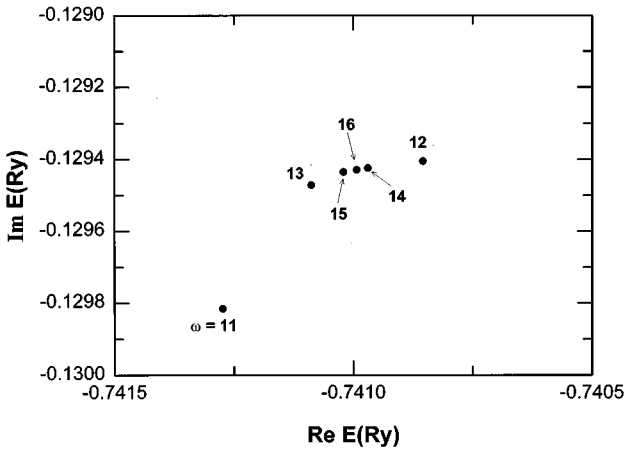

FIG. 1. Convergence behavior for the lowest S-wave resonance in e^+-He^+ scattering as different expansion lengths (ω) are used (α=1.0, β=0.5, θ=0.6).

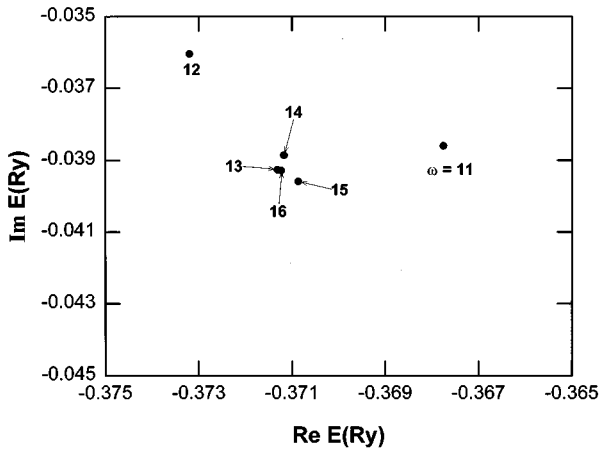

FIG. 2. Convergence behavior for the second S-wave resonance in e^+-He^+ scattering as different expansion lengths (ω) are used (α=0.4, β=0.25, θ=0.6).

and the Hamiltonian is transformed into

$$H = T\ \exp(-2i\theta) + V\ \exp(-i\theta). \tag{7}$$

The eigenvalues are calculated by diagonalizing the expression

$$E = \langle \Phi H \Phi \rangle / \langle \Phi \Phi \rangle. \tag{8}$$

Since the rotated Hamiltonian is complex, complex eigenvalues are obtained. A complex resonance energy is given by

$$E_{\rm res} = E_r - i\Gamma/2, \tag{9}$$

with E_r the resonance energy and Γ the width.

The theoretical aspects of the complex-rotation method have been discussed in previous publications [5] 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 calculation 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 [5]. A resonance complex eigenvalue is deduced by the stabilization condition with respect to the changes of the nonlinear parameters in Eqs. (4) and (5), and of θ. The optimization of such parameters is usually performed with a smaller basis set, typically with M=680 (ω=14). Convergence behaviors can be examined by using different expansion lengths. Up to M=969 (ω=16) terms are used in the present calculations for S-wave resonances, and M=2660 (ω=18) terms for P-wave resonances.

TABLE II. The second S-wave resonance in e^+-He^+ scattering (α=0.4, β=0.25, θ=0.6).

ω	M	E_r (Ry)	$\Gamma/2$ (Ry)
11	364	−0.36775	0.03860
12	455	−0.37320	0.03605
13	560	−0.37131	0.03927
14	680	−0.37117	0.03886
15	816	−0.37086	0.03959
16	969	−0.37123	0.03929

III. CALCULATIONS AND RESULTS

Table I and Fig. 1 show the convergence behavior for the lowest S-wave resonance. The optimized parameters are determined as α=1.0, β=0.5, and θ=0.6. From the results when different expansion lengths are used, we determine the resonance parameters as $E_r = -0.74099 \pm 0.00005$ Ry and $\Gamma/2 = 0.12943 \pm 0.00005$ Ry. The total width of this resonance is very broad. It means that the resonance pole is quite far away from the real axis. The relatively large value of θ is therefore needed in order for the cut that starts from the He^+ (N=2) threshold to be rotated far away from the resonance pole.

Table II and Fig. 2 show the convergence behavior for the second S-wave resonance. The optimized parameters for this state are α=0.4, β=0.25, and θ=0.6. With the use of up to M=969 terms (ω=16) wave functions, we have determined the resonance parameters as $E_r = -0.3712 \pm 0.0005$ Ry and $\Gamma/2 = 0.0393 \pm 0.0005$ Ry. This resonance lies at a position not very far above the He^+ (N=3) threshold. Again, the relatively large value of θ is therefore needed in order for the

TABLE III. The first P-wave resonance in e^+-He^+ scattering (α=0.9, θ=0.6).

ω	M	E_r (Ry)	$\Gamma/2$ (Ry)
10	572	−0.708989	0.177219
11	728	−0.708643	0.178179
12	910	−0.708628	0.177241
13	1120	−0.708828	0.177434
14	1360	−0.708671	0.177616
15	1632	−0.708655	0.177490
16	1938	−0.708726	0.177511
17	2280	−0.708694	0.177540
18	2660	−0.708688	0.177517

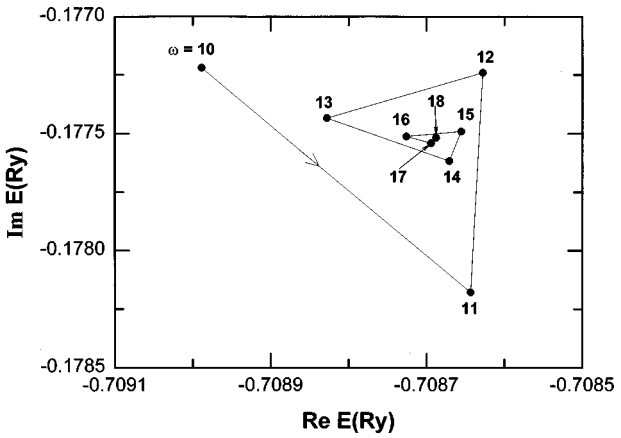

FIG. 3. Convergence behavior for the lowest P-wave resonance in e^+-He^+ scattering as different expansion lengths (ω) are used ($\alpha=0.9$, $\theta=0.6$).

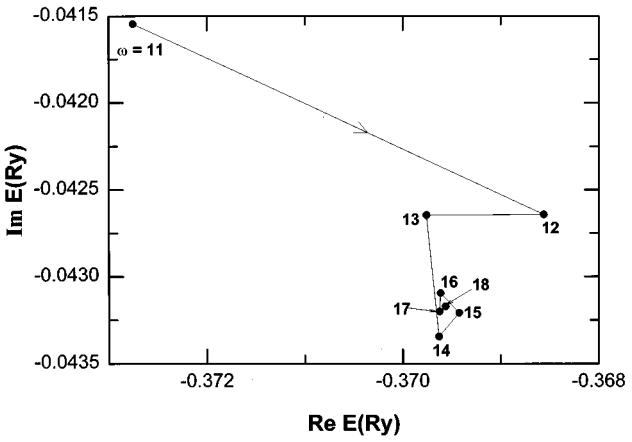

FIG. 4. Convergence behavior for the second P-wave resonance in e^+-He^+ scattering as different expansion lengths (ω) are used ($\alpha=0.40$, $\theta=0.6$).

cut that starts from the He^+ ($N=3$) threshold to be rotated away from the resonance pole. It is noted that our S-wave resonance positions of -0.74099 and -0.3712 Ry are consistent with those of -0.73 and -0.39 Ry obtained by Bhatia and Drachman using the stabilization method [4]. No widths were, however, reported in Ref. [4].

Table III and Fig. 3 show the convergence behavior for the lowest P-wave resonance in e^+-He^+ scattering. The optimized parameters are determined at $\omega=11$ ($M=728$ terms) as $\alpha=0.9$ and $\theta=0.6$. With the use of expansion lengths up to $M=2\times1330=2660$ terms ($\omega=18$), we determined the resonance parameters for the lowest P-wave resonance state as $E_r=-0.70869\pm0.00004$ Ry and $\Gamma/2=0.17752\pm0.00004$ Ry. Table IV and Fig. 4 show the results for the second P-wave resonance in e^+-He^+ scattering. We use $\alpha=0.4$ and $\theta=0.6$ and expansion lengths of $M=2660$ ($\omega=18$) terms. The resonance position is determined as $E_r=-0.36956\pm0.00010$ Ry, and $\Gamma/2=0.04317\pm0.00010$ Ry. We summarize our results in Table V.

In order to shed light on the ''mechanism'' of the resonances, we have investigated the changes of such resonances as the charge of the infinitely heavy nucleus is changed from $Z=2$ to 1 for the systems (e^+,e^-,Z), where Z is the charge of the positively charged particle. By changing Z from $Z=2$ to $Z=1$, we have investigated systems from e^+- He^+ to e^+-H. Figures 5 and 6 show the results for S-wave and P-wave resonances, respectively. For the S-wave case, a resonance starts to appear at approximately $Z=1.48$. It lies below the Ps ($N=1$) threshold but above the $N=2$ threshold of the (e^-,Z) parent atom. As Z is increased further, such a resonance stays in the energy region between these two thresholds. As for the second S-wave resonance, we are able to trace its movement from $Z=2$ to $Z=1$ as they lie below the Ps ($N=2$) threshold. Our finding indicates that the second S-wave resonance with $E_r=-0.37$ Ry in e^+-He^+ scattering is a result of the degeneracy of the Ps ($N=2$) $2s$-$2p$ states, just like the resonance of $E_r=-0.150279$ Ry lying below the Ps ($N=2$) threshold in e^+-H scattering [7]. For the lowest resonance, while our work indicates that the Ps ($N=2$) is not responsible for such a resonance, we still could not conclusively point out the mechanism supporting its existence. One possible explanation is that when Z is larger than approximately 1.48, the interaction between the charged particle and the positronium atom in its ground state is quite strong, and the resulting attractive polarization potential is strong enough to support a stabilized state. Furthermore, this lowest resonance lies at a position above the parent (e^-,Z) $N=2$ threshold. The opening of such an autoionization route may be the major reason that its autoionization width is so huge ($\Gamma=0.2588$ Ry$\approx$3.52 eV for the S-wave and $\Gamma=0.355$ Ry$\approx$4.83 eV for the P-wave). In the present work, we have also investigated the changes of the P-wave resonances as Z changes. Figure 6 shows the results for the Z dependence of these resonances. It is seen that their movements are very similar to those for the S-wave resonances.

TABLE IV. The second P-wave resonance in e^+-He^+ scattering ($\alpha=0.4$, $\theta=0.6$).

ω	M	E_r (Ry)	$\Gamma/2$ (Ry)
11	728	-0.372754	0.041546
12	910	-0.368563	0.042640
13	1120	-0.369759	0.042646
14	1360	-0.369631	0.043346
15	1632	-0.369425	0.043209
16	1938	-0.369615	0.043096
17	2280	-0.369625	0.043201
18	2660	-0.369563	0.043172

TABLE V. S- and P-wave resonances in e^+-He^+ scattering.

E_r (Ry)	$\Gamma/2$ (Ry)
S wave	
-0.74099 ± 0.00005	0.12943 ± 0.00005
-0.3712 ± 0.0005	0.0393 ± 0.0005
P wave	
-0.70869 ± 0.00004	0.17752 ± 0.00004
-0.36956 ± 0.00010	0.04317 ± 0.00010

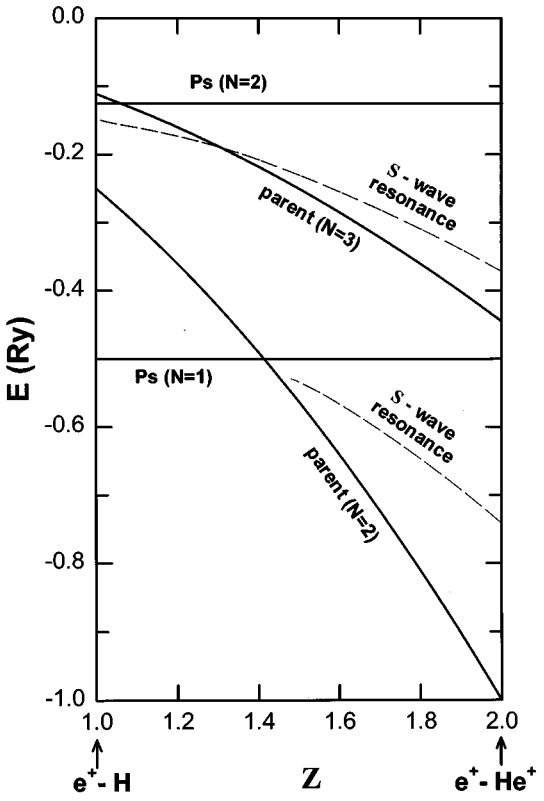

FIG. 5. S-wave resonances in (e^+,e^-,Z) systems. Z is changed from $Z=1$ to $Z=2$, as the system is changed from e^+-H to e^+-He^+. Solid lines are for the threshold energies of the Ps atom and the (e^-,Z) parent atom. Dashed lines are for resonance positions.

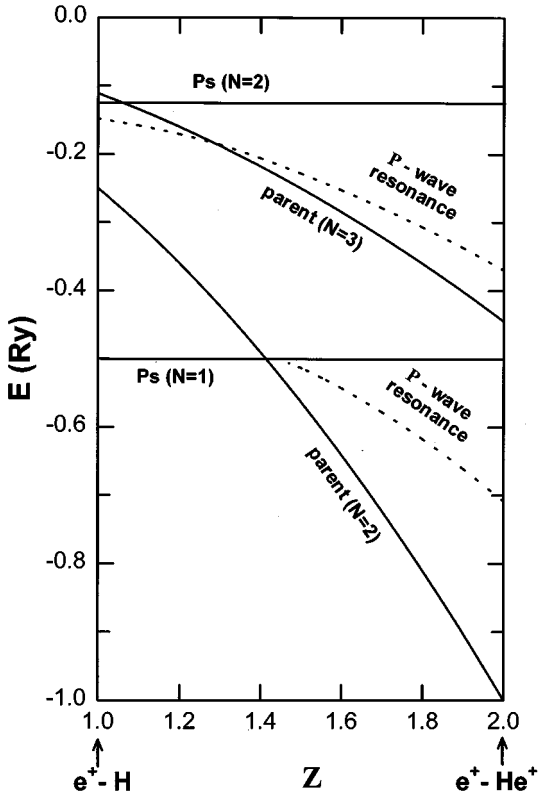

FIG. 6. P-wave resonances in (e^+,e^-,Z) systems. Z is changed from $Z=1$ to $Z=2$, as the system is changed from e^+-H to e^+-He^+. Solid lines are for the threshold energies of the Ps atom and the (e^-,Z) parent atom. Dashed lines are for resonance positions.

In summary, we have carried out a calculation of S- and P-wave resonances in e^+-He^+ scattering using a method of complex-coordinate rotation. Our results indicate that the widths of these resonances are extremely broad, raising the possibilities that they may be detectable in e^+-He^+ scattering experiments.

ACKNOWLEDGMENTS

This work was supported by National Science Council with Grant No. 85-2112-M-001-016. The use of computing facilities at the National Center for High-Performance Computing is gratefully acknowledged.

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