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Triply excited autodissociating resonant states in the positron-helium system

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In this paper, we present a complex-coordinate rotation calculation for high-lying S-wave resonances in positron-helium scattering. Highly correlated Hylleraas wave functions containing all six interparticle coordinates are used. A total of seven resonances, including their positions and widths, are reported, where the lowest one, denoted as $e^+\mathrm{He}(2s^2)$, is formed by a positron attaching to the doubly excited $2s^2\ {}^1S^e$ state of helium, and the other six resonances, denoted as $\mathrm{Ps}^-\mathrm{He}^{2+}$ (nS) with n from 2 to 7, are located in the Rydberg series converging to the $\mathrm{Ps}^- + \mathrm{He}^{2+}$ threshold. Our results are compared with those available in the literature. The calculated energies for $\mathrm{Ps}^-\mathrm{He}^{2+}$ (nS) with n from 2 to 7 show a good fit to a quantum defect formula that describes the interaction between the positively charged He^{2+} ion and the negatively charged Ps^- ion. The $3S$ state in this Rydberg series provides an alternative designation for the previously identified $e^+\mathrm{He}(3s^2)$ state in the literature.

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I. INTRODUCTION

It has been shown that a positron can bind the doubly excited states of a two-electron system such as the hydrogen negative ion, H^- [1], or the helium atom [2,3], to form a quasibound resonance state. Since these states are located in the scattering continua between the positron and the target (H^- or He), they would manifest themselves as resonances in positronium-hydrogen and positron-helium scattering, respectively. Recently, Mitroy and coworkers have reported calculations of resonances in the positron-helium system around and below the doubly excited states of He, with two S-wave resonances each below the $2s^2\ {}^1S^e$ and $3s^2\ {}^1S^e$ thresholds [2,3]. Subsequently, an attempt to search for such resonances was carried out in a laboratory [4]. Although these resonances were not found, an estimate on the upper limit of the cross sections was made. The objective of the present paper is to carry out calculations of triply excited resonances in the positron-helium system, in the energy region around the doubly excited states of atomic helium. Resonance parameters of both position and width for some S-wave resonances will be obtained by using the method of complex-coordinate rotation [5] and by employing elaborated Hylleraas-type wave functions in which all six interparticle coordinates are included (see Ref. [6], for example). In addition to the two S-wave resonances calculated earlier in Refs. [2,3], we will calculate additional resonances approaching the $\mathrm{Ps}^- + \mathrm{He}^{2+}$ threshold from below. An interpretation of our results will be given, and hopefully our findings will shed light for further experimental activities to observe such resonances.

There have been considerable interests in theoretical investigations of atomic resonances involving positrons, including those in positron-helium scattering around the energy region of the excited Ps ($N = 2$) and ($N = 3$) thresholds [7–11]. Other recent theoretical investigations on positronic resonances are positron scattering with Li [12–19], Na [12,20–23], K [12,20,24], and Cu [25]. Investigations on shape resonances in positron–alkaline-earth scattering were also reported in the literature [26–29]. The experimental investigations on resonances in positron-atom and positron-molecule scattering were described in Refs. [30,31]. It should be mentioned that, given the resolution of the present positron beams, it is unlikely that the narrow resonances in positron-alkali metals could be observed. Nevertheless, it remains a challenging endeavor for experimentalists for years to come. A ${}^1P^o$ shape resonance in the positronium negative ion was observed in a photoionization experiment from the ground state of the Ps^- ion [30,32]. Earlier reviews focusing mainly on theoretical developments of atomic resonances involving positrons are available in the literature [33,34]. The outline of the present paper is as follows. After the introduction in Sec. I, we describe the Hamiltonian and wave functions used in this paper in Sec. II. Section III shows the calculational details and discusses the results. Then in Sec. IV, we summarize our paper and draw a concluding remark.

II. HAMILTONIAN AND WAVE FUNCTION

The Hamiltonian for the positron-helium system is (in atomic units throughout) given as

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

$$T = -\frac{1}{2}\left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2\right), \tag{2}$$

$$V = -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{Z}{r_3} + \frac{1}{r_{12}} - \frac{1}{r_{23}} - \frac{1}{r_{31}}, \tag{3}$$

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where indices 1 and 2 refer to the two electrons, index 3 refers to the positron, and $Z = 2$ for the helium nucleus. The wave function is expanded in Hylleraas coordinates:

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \sum_{i=1}^{N} a_i \psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) \pm (1 \leftrightarrow 2), \tag{4}$$

where

$$\psi_i = r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha r_1 - \beta r_2 - \gamma r_3} \mathcal{Y}^{LM}_{(\ell_1 \ell_2)\ell_{12},\ell_3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3), \tag{5}$$

$$\begin{aligned} \mathcal{Y}^{LM}_{(\ell_1 \ell_2)\ell_{12},\ell_3} = & \sum_{m_i} \langle \ell_1 m_1; \ell_2 m_2 | \ell_1 \ell_2; \ell_{12} m_{12} \rangle \\ & \times \langle \ell_{12} m_{12}; \ell_3 m_3 | \ell_{12} \ell_3; LM \rangle \\ & \times Y_{\ell_1 m_1}(\boldsymbol{r}_1) Y_{\ell_2 m_2}(\boldsymbol{r}_2) Y_{\ell_3 m_3}(\boldsymbol{r}_3). \end{aligned} \tag{6}$$

All terms in (5) are included such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leqslant \Omega, \tag{7}$$

where Ω is an integer. The total number of terms is $N = 6412$ in the wave-function expansion. Computational details for evaluating the matrix elements of the Hamiltonian can be found in Ref. [6].

III. CALCULATIONS AND RESULTS

For calculations of the S-wave autodissociating resonant states, we use the method of complex-coordinate rotation [5]. The radial coordinates are transformed according to

$$r \rightarrow r e^{i\theta} \tag{8}$$

where r is the distance between two charged particles. The transformed Hamiltonian can be written as

$$H(\theta) = T e^{-2i\theta} + V e^{-i\theta}, \tag{9}$$

where T and V are given by Eqs. (2) and (3), respectively, and θ is a positive number. Complex eigenvalues are obtained by diagonalizing the transformed Hamiltonian, and the complex resonance energy is given by

$$E_{\text{res}} = E_r - i\Gamma/2, \tag{10}$$

where E_r is the resonance position and Γ is the resonance width. To investigate the resonance associated with the doubly excited $2s^2\,{}^1S^e$ state of He, in our wave functions we choose the nonlinear parameters $\alpha = 0.95$ and $\beta = 0.95$ and let γ vary ranging from 0.5 to 0.9. The nonlinear parameter γ can be considered as a variational parameter to determine the stabilized complex resonance eigenvalues. The physical picture is that the wave functions are used to simulate the positron attaching to the doubly excited helium atom.

Figure 1 shows the rotational paths near the pole of the first resonance state for different wave functions. From the most stabilized region in the complex energy plane we determine the resonance parameters (E_r, $\Gamma/2$) in atomic units for this resonance as (−0.794892, 0.001296), which is compared to the result of (−0.79484, 0.00124) by Mitroy's group [2] using the complex rotation method with explicitly correlated Gaussians (ECGs) of 1428 terms. Later this group [3] also reported the result of (−0.79527, 0.00066) using stochastic variational method together with the complex rotation method (SVM-CR). Our results are summarized in Table I. The state denoted as e^+He $(2s^2\,{}^1S^e)$ in the positron-helium system is most likely the result of the positron attaching to the doubly excited $2s^2\,{}^1S^e$ state of He, in a manner similar to the counterpart in the PsH system where the positron is attached to the doubly excited state $2s^2\,{}^1S^e$ of the H$^-$ ion [1]. Table I also shows the results for the e^+He $(2s^2\,{}^1S^e)$ state obtained from CI and SVM resonance energy (only) calculations in Ref. [2] based on projection methods, and the energy-only projection result for the e^+He $(3s^2\,{}^1S^e)$ state with CI basis.

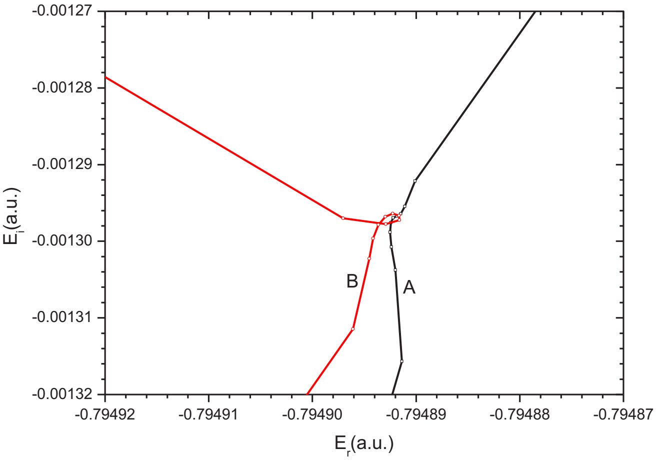

FIG. 1. Stabilized complex eigenvalue $E_{\text{res}} = E_r + iE_i$ near the pole of the e^+He$(2s^2\,{}^1S^e)$ resonance state, showing $E_r = -0.794892$ a.u. and $\Gamma/2 = 0.001296$ a.u. The set for the nonlinear parameters (α,β,γ) used in the wave function Eq. (5) is (0.95, 0.95, 0.65) for curve A and (0.95, 0.95, 0.55) for curve B.

From Table I, it is observed that the e^+He$(2s^2)$ state reported in Ref. [3] differs considerably from our present results. Here, we provide a possible explanation. The results reported in Ref. [3] as shown in Table I were obtained using the method of complex scaling. In the complex scaling method a resonance pole is determined when the variation of the complex eigenvalue exhibits stabilized behavior with respect to changes of θ [see Eq. (7) in Ref. [3]]. From Fig. 3 in Ref. [3], two arrows were shown to indicate the possible positions of the resonance pole. The authors then chose $\theta = 0.275$, from which the complex pole was deduced at $(E_r, E_i) = (-0.79527, -0.00066)$. However, had they chosen $\theta = 0.135$, the other optimized θ value (see Fig. 3 in Ref. [3]), the resonance pole (read by eye) would become (−0.79494, −0.00115) approximately, and such a value would be in line with our present result (−0.794892, −0.001296), and also in line with the result (−0.79484, −0.00124) in Ref. [2]. In any case, we encourage further investigations on this resonance state for such an interesting e^+-He system.

Figure 2 shows the rotational paths near the pole of the second resonance reported in this paper. We obtained $E_r = -0.75678$ a.u. and $\Gamma/2 = 0.00533$ a.u. This resonance was not calculated in Refs. [2,3]. At first, the origin of this resonance state is not clear notwithstanding that there is a nearby

TABLE I. Summary of resonance energies E_{res} and half widths in atomic units.

State	Method	E_{res}	$\Gamma/2$
$e^+\mathrm{He}(2s^2\,{}^1S^e)$	CR(Hy)	-0.794892 ± 0.000010[a]	0.001296 ± 0.000010[a]
	SVM-CR	-0.79527[b]	0.00066[b]
	SVM-CR	-0.79494[b,d]	0.00115[b,d]
	Projection(SVM)	-0.795210[c]	
	Projection(CI)	-0.795058[c]	
	CR(ECG)	-0.79484[c]	0.00124[c]
$\mathrm{Ps}^-\mathrm{He}^{2+}(2S)$	CR(Hy)	-0.75678 ± 0.00010[a]	0.00533 ± 0.00010[a]
$\mathrm{Ps}^-\mathrm{He}^{2+}(3\mathrm{S})$	CR(Hy)	-0.48307 ± 0.00015[a]	0.00338 ± 0.00015[a]
$e^+\mathrm{He}(3s^2\,{}^1S^e)$	SVM-CR	-0.48432[b]	0.00539[b]
	Projection(CI)	-0.481643[c]	

[a] Present paper.
[b] Mitroy and Grineviciute [3].
[c] Bromley *et al.* [2].
[d] Taking from Fig. 3 in Ref. [3]; see text for explanation and discussion.

threshold of $\mathrm{Ps}(1S) + \mathrm{He}^+(2S)$ with the threshold energy of -0.75 a.u. Further discussion about this resonance state will be given later in the text.

Figure 3 shows the rotational paths near the pole of the third resonance reported here. Our results of ($E_r = -0.48307$, $\Gamma/2 = 0.00338$) a.u. are compared with (-0.48432, 0.00539) a.u. obtained in Ref. [3] and with $E_r = -0.481643$ a.u. in Ref. [2]. This state was classified as e^+He ($3s^2\,{}^1S^e$) in Refs. [2,3]. However, based on the fact that the location of this state is quite farther away from the helium doubly excited ($3s^2\,{}^1S^e$) state, as compared to the other e^+He ($2s^2\,{}^1S^e$) state relative to the doubly excited He ($2s^2\,{}^1S^e$) state, as shown in Fig. 4, the formation of this state can be due to other mechanisms. In Table I, we compare our present results with earlier calculations. The energy of the doubly excited $2s^2\,{}^1S^e$ state in He is $E_r = -0.777818$ a.u. as reported in Ref. [35]. Our first resonance lies at $E_r = -0.794892$ a.u., about 0.017072 a.u. below the two-electron doubly excited threshold. The energy of the doubly excited $3s^2\,{}^1S^e$ state in He is -0.35354 a.u. [36]. Our third resonance is located at $E_r = -0.48307$ a.u., about 0.12953 a.u. lower than that of the $3s^2\,{}^1S^e$ doubly excited threshold. Thus this resonance state, also calculated in Refs. [2,3], is not due to the "parent" $3s^2\,{}^1S^e$ state as it lies quite far below the two-electron doubly excited threshold (see Fig. 4).

In order to shed light on the nature of these resonances in the positron-helium system, we carried out further calculations for higher-lying states. For the wave functions of the higher-lying states, we chose the nonlinear parameters $\alpha = 0.49$ and $\beta = 0.49$ and let γ vary from 0.24 to 0.50. The nonlinear parameter γ can be considered as a variational parameter to determine the stabilized complex resonance eigenvalues. The physical picture is that the wave functions are used to simulate the positronium negative ion moving away from the field of the He^{2+} positive ion when γ is systematically decreased from $\gamma = 0.50$ to about 0.24. In Table II, we show our results with six resonance states, including the two states displayed in Table I [excluding the $e^+\mathrm{He}(2s^2)$ state]. These resonances may be attributed to the $\mathrm{Ps}^-\mathrm{He}^{2+}(nS)$ Rydberg series, a result

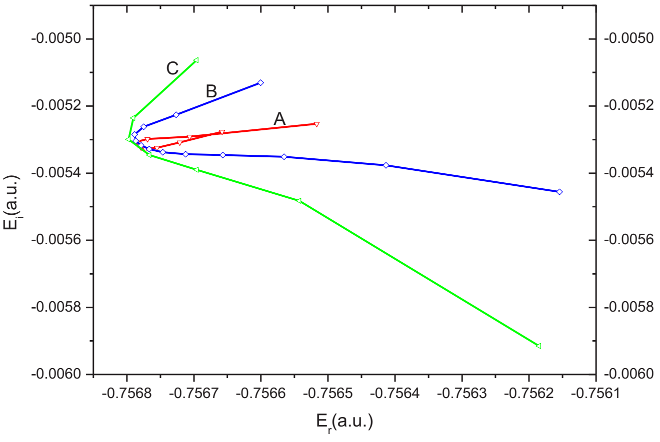

FIG. 2. Stabilized complex eigenvalue $E_{\mathrm{res}} = E_r + i E_i$ near the pole of the $\mathrm{Ps}^-\mathrm{He}^{2+}(2S)$ resonance state, showing $E_r = -0.75678$ a.u. and $\Gamma/2 = 0.00533$ a.u. The set for the nonlinear parameters (α,β,γ) used in the wave function Eq. (5) is (0.91, 0.91, 0.27) for curve A, (0.91, 0.91, 0.25) for curve B, and (0.91, 0.91, 0.29) for curve C.

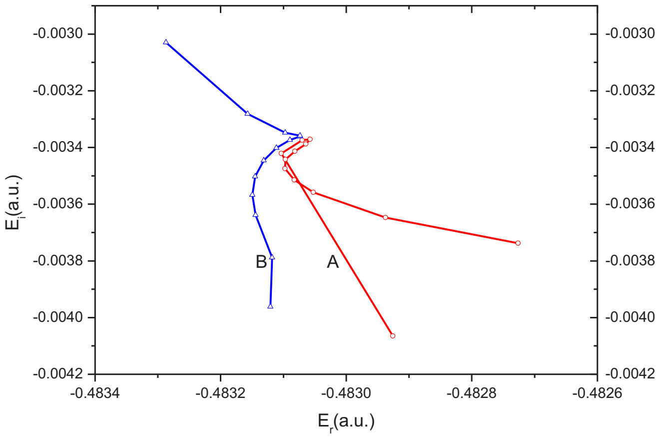

FIG. 3. Stabilized complex eigenvalue $E_{\mathrm{res}} = E_r + i E_i$ near the pole of the $\mathrm{Ps}^-\mathrm{He}^{2+}(3S)$ state, showing $E_r = -0.48307$ a.u. and $\Gamma/2 = 0.00338$ a.u. The set for the nonlinear parameters (α, β, γ) used in the wave function Eq. (5) is (0.63, 0.63, 0.40) for curve A and (0.63, 0.63, 0.45) for curve B.

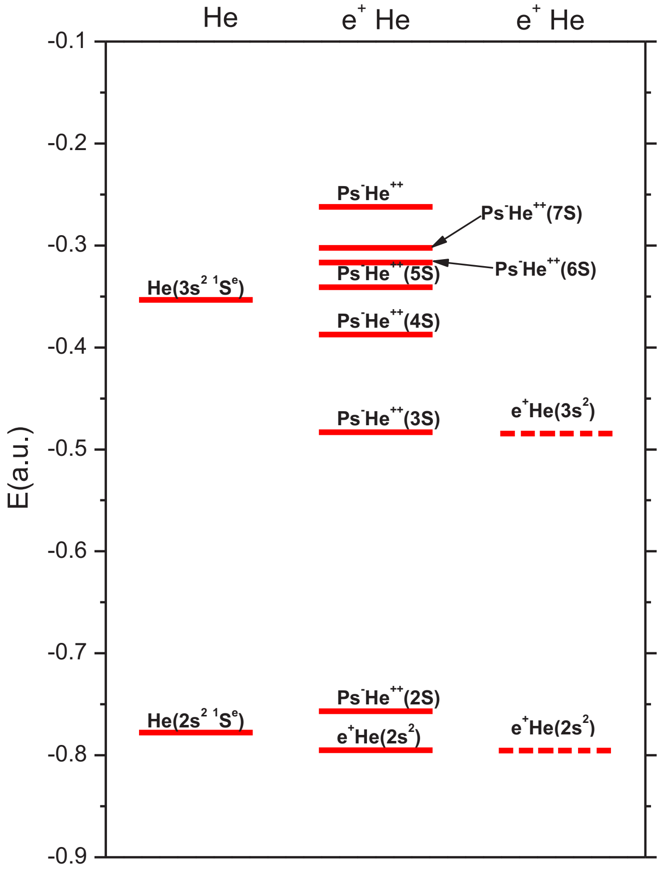

FIG. 4. Energy levels for the e^+He($2s^2$) state and Rydberg states in the Ps$^-$He^{2+}(nS) series with $n = 2$ to 7. Under the heading e^+-He, the solid line is from the present calculation. The two dashed lines are from the SVM-CR results in Ref. [2] for the e^+He($2s^2$) state and in Ref. [3] for the e^+He($3s^2$) state, respectively.

of the positive He^{2+} ion interacting with the negative Ps$^-$ ion. Since these states are embedded in the positron-helium scattering continua, they would manifest themselves as resonances in the e^+-He scattering. These states in Ps$^-$He^{2+} are similar to those resonant Rydberg states in the Ps$^-$H$^+$ [37,38] and e^+Ps$^-$ [39] systems. Next, from the resonance energies, we calculated the binding energies ΔE, relative to the energy of the Ps$^-$ ion, with $E_{\rm inf} = -0.262005$ a.u. [40–42]. We then fit the binding energies of the $n = 2-7$ states to the Rydberg quantum defect formula:

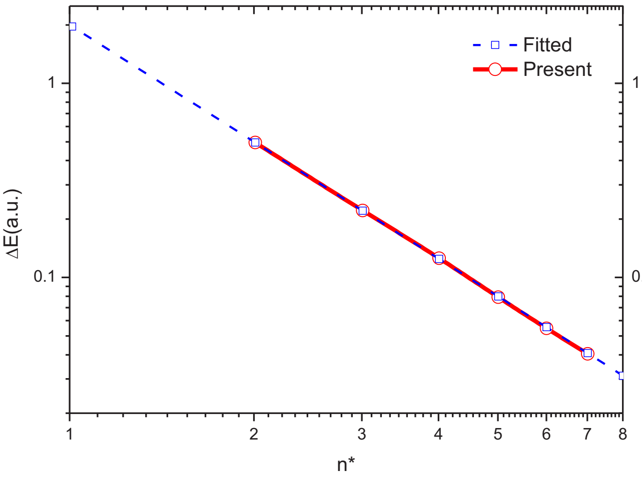

FIG. 5. Fitting of the Rydberg states of the Ps$^-$He^{2+} system, in logarithmic scale. The circles are from the present *ab initio* calculations, and the squares are from the data fitted to the quantum defect formula. n^* is the effective quantum number.

$$\Delta E = (\mu/2)Z_1{}^2(Z_2')^2/(n^*)^2 \quad (\text{in a.u.}) \tag{11}$$

with $\Delta E = E_{\rm inf} - E_{\rm ns}$, $Z_2' = -(1-\sigma)$, and $n^* = n - \delta$. Here, μ is the reduced mass of the Ps$^-$ ion relative to the infinitely heavy nucleus of the He^{2+} ion, which is $\mu = 3m_{\rm e}$, with $m_{\rm e}$ being the mass of the electron. $Z_1 = 2$ is the charge of the He^{2+} ion, and Z_2' is the effective charge of Ps$^-$ as felt by the He^{2+} ion, in comparison to the net charge -1 of Ps$^-$, due to mutual screening of the two electrons with the screening factor σ. n^* is the effective quantum number, with δ being the quantum defect. Both σ and δ are to be determined by the fitting process. The Ps$^-$ as a whole would appear as a "particle" with the effective charge Z_2'. The fitting with chi square $= 5.769 \times 10^{-7}$ and r square $= 0.99998$ gives $\sigma = 0.42195$ and $\delta = -0.01279$. As r square is very close to 1.0, it indicates that the fitting is quite good. From the fitted σ value, we obtain the effective charge for the Ps$^-$ ion as 0.67805. Using the fitted σ and δ values, we calculate the "fitted" energy levels for the 1S to 7S states, and show them in Fig. 5 and Table II. Figure 5 shows ΔE versus n^*, the effective quantum number, in log-log scale. Also from Table II, comparing the fitted resonance energy

TABLE II. Present results of resonance energies and half widths of Rydberg states in the Ps$^-$He^{2+} system, in atomic units. E_r(fitted) is defined as $E_{\rm inf}$ – fitted[ΔE]. The estimated uncertainties for the 2S and 3S states are given in Table I, and those for the 4S to 7S states are about five parts in the fourth digit after the decimal for both the real and imaginary parts for each of these states.

State	E_r (*ab initio*)	$\Gamma/2$	ΔE	Fitted[ΔE]	E_r(fitted)
Ps$^-$He^{2+}(1S)				1.95453	−2.21654
Ps$^-$He^{2+}(2S)	−0.75678	0.00533	0.494775	0.49487	−0.75687
Ps$^-$He^{2+}(3S)	−0.48307	0.00338	0.221065	0.22087	−0.48288
Ps$^-$He^{2+}(4S)	−0.38750	0.00411	0.125495	0.12451	−0.38651
Ps$^-$He^{2+}(5S)	−0.34105	0.00295	0.079045	0.07979	−0.34179
Ps$^-$He^{2+}(6S)	−0.31667	0.00360	0.054695	0.05545	−0.31746
Ps$^-$He^{2+}(7S)	−0.30237	0.00360	0.040365	0.04077	−0.30277
Ps$^-$ + He^{2+}	−0.262005		0.0		

levels with those obtained by the actual *ab initio* calculations, the difference for any given nS state ($n = 2\text{–}7$) is no more than 0.001 a.u. Based on the quality of such a fit, and the stabilized behaviors in the complex eigenvalue calculations, we estimate the uncertainties for the nS states with $n = 4\text{–}7$ that are about five parts in the fourth digit after the decimal, for both the real and imaginary parts of these complex resonance states. As for the fitted $1S$ state shown in Table II, caution should be made when one interprets such results. It should be mentioned that a brief attempt to search for this state was unsuccessful. No stabilized complex eigenvalue near the fitted $1S$ state was obtained using the present wave functions that were optimized around the configurational space near the doubly excited threshold of He, and around the region below the $\mathrm{Ps^-He^{2+}}$ threshold. The $1S$ state, if it existed, would be around the region near the singly excited states of He. The optimized wave functions are hence different from those used in the present paper. An extensive search for the fitted $1S$ state is of future interest, but it is outside the scope of the present investigation. It should be noted that the nonlinear parameters (α, β, γ) used for the two lowest states, the $2S$ and $3S$ states, in the $\mathrm{Ps^-He^{2+}}$ Rydberg series as shown in Table II are somewhat different from those for higher-lying states. This is because for the $2S$ and $3S$ states there exist some nearby channels from the helium atom. So, in a sense, the physical structures for these two states are combinations of elements coming from configurations of e^+He and $\mathrm{Ps^-He^{2+}}$, whereas for the higher-lying states in the Rydberg series they could be dominated by the $\mathrm{Ps^-He^{2+}}$ configurations.

Next, we comment on the results for the widths of the resonance states, especially for the higher-lying members of the Rydberg series. For the resonance states that share the same lower-lying open channels to which they autodissociate, their widths would show a monotonic decreasing manner for increasing n. For example, for the $\mathrm{Ps^-He^{2+}}(2S)$ and $\mathrm{Ps^-He^{2+}}(3S)$ states, they have the same lower-lying open channels such that they can autodissociate, for example, to the ground-state Ps plus the ground state of the $\mathrm{He^+}$ ion, with total threshold energy -2.25 a.u. Hence, the widths of these two states exhibit a monotonic decreasing behavior. However, for other higher-lying states, for example, for the $\mathrm{Ps^-He^{2+}}(4S)$ state, there is an additional open channel consisting of the ground-state Ps and the $\mathrm{He^+}$ ion in its $N = 3$ state, with the total threshold energy being -0.475 a.u. The extra open channel for this $\mathrm{Ps^-He^{2+}}(4S)$ state is attributed to a larger total width as compared to that for the $\mathrm{Ps^-He^{2+}}(3S)$ state. Similarly, for the $\mathrm{Ps^-He^{2+}}(7S)$ state, there is an extra open channel consisting of the ground-state Ps and the $\mathrm{He^+}$ ion in its $N = 6$ state with a threshold energy -0.303 a.u. As a result, the autodissociation width is not smaller than that of the $\mathrm{Ps^-He^{2+}}(6S)$ state.

Finally, we call the excited states in the Rydberg series triply excited states. First, such states are located in the doubly excited region (for the two electrons) of the target systems. Second, the $2S$ to $7S$ states reported here are the excited states of the quasi-two-body system (between the $\mathrm{He^{2+}}$ positive ion and the $\mathrm{Ps^-}$ negative ion). So, all together, we label them triply excited states in the e^+He system. As for the $e^+\mathrm{He}(2s^2)$ state, since it lies near the region where the above-mentioned triply excited states are located, one may address it as a triply excited state, or simply call it the $e^+\mathrm{He}(2s^2)$ state.

IV. SUMMARY AND CONCLUSION

In summary, we have carried out a complex-coordinate rotation calculation of high-lying S-wave resonances in positron-helium scattering using highly correlated wave functions in Hylleraas coordinates. In addition to the $e^+\mathrm{He}(2s^2)$ resonance state formed by a positron attaching to the doubly excited $2s^2\ {}^1S^e$ state in helium, we have also calculated resonance energies and widths for the $2S$–$7S$ states in the Rydberg series converging to the $\mathrm{Ps^-} + \mathrm{He^{2+}}$ threshold. The energies of $2S$–$7S$ states of the Rydberg series have been used to fit the quantum defect formula with high reliability. From the quantum defect formula, the energy levels for higher members of the Rydberg series can be estimated. It is hoped that our present findings would stimulate further investigations on the intriguing resonance phenomenon in positron physics.

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