Autoionizing $^1P^\circ$ states of He between the $N=2$ and 3 thresholds of He^+

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Doubly excited $^1P^o$ autoionizing states in He between the $N=2$ and 3 thresholds of He^+ ions are calculated by use of a method of complex-coordinate rotation. Hylleraas-type wave functions are used to calculate resonance parameters for the lowest ten resonances, and products of Slater orbitals are used for higher-lying resonances. In the $KTNn$ notation, the states reported in the present work include six members in $(113n)$ series with $(3 \le n \le 8)$, four members in the $(-113n)$ series $(3 \le n \le 6)$, four members in the $(203n)$ series $(4 \le n \le 7)$, four members in the $(003n)$ series $(4 \le n \le 7)$, and three members in the $(-203n)$ series with $(4 \le n \le 6)$. Comparisons are made with other theoretical calculations and with experimental observations.

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I. INTRODUCTION

There has been continuous experimental interest to observe the doubly excited $^1P^o$ states of helium atoms. The helium doubly excited states are located at energy regions of about 60 to 79 eV, measured from the ground state of helium atoms. They lie below each and every excitation threshold of He^+ as a result of the combination of Coulomb potential and the attractive dipole r^{-2} potential due to the *ns-np* degeneracy of the He^+ ions [1]. The doubly excited $^1P^o$ states can be accessed from the $1s^2\,^1S$ ground state by using a single-photon ultraviolet light source. Ever since the first observation of such $^1P^o$ states in the classic experiment by Madden and Codling [2–4] in 1963 using the 180-MeV synchrotron at the United States National Bureau of Standards, it has attracted continuous experimental interest to study the $^1P^o$ states as new synchrotron facilities around the globe become operational. Other facilities that were used to study the $^1P^o$ doubly excited states in He include the INS-SOR in University of Tokyo [5], the NBS 250-MeV electron synchrotron storage ring (SURF-II) [6], the Wisconsin Tantalus storage ring [7], the Stanford Synchrotron Radiation Laboratory (SSRL) [8], the Berlin electron storage ring (BESSY) [9,10], and the Daresbury Synchrotron Radiation Source (DSRS) [11]. In addition, synchrotron radiation source was also used to study photoionization of He $N=2$ state in the Orsay ACO-LURE storage ring facility [12].

Because of the recent experimental activities, accurate calculations for resonance parameters are needed to compare with the experimental measurements. On the theoretical side, studies of such highly correlated atomic systems would enhance our understanding of atomic correlation effects. In the last few years we have been able to provide some of the most accurate resonance parameters (positions and widths) for doubly excited $^1P^o$ in intrashell states (the two electrons occupy the same shell) [13]. By using a method of complex-coordinate rotation and employing Hylleraas-type wave functions, a total of eight $^1P^o$ resonances were reported in the energy region between the $N=2$ and $N=3$ He^+ threshold [13]. It was found that the convergence for the intershell resonances (the two electrons occupy different shells) was somewhat slow. As a result, we were able to report only one digit of accuracy for the widths of several narrow resonances. It is now felt that improvement of the earlier calculation is needed, especially for the intershell states. This work presents such a calculation. 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.

Various theoretical methods have also been used to study the resonance in He for the energy region between the $N=2$ and $N=3$ He^+ threshold. The earlier calculations are reviewed in Ref. [13]. Here we only mention the theoretical activities that were carried out since early 1980. Several versions of close-coupling approximations were used in the past decade to study resonances of He between the $N=2$ and $N=3$ He^+ threshold. These include the algebraic variational method by Wakid and Callaway [14], an R matrix calculation by Hayes and Scott [15], and a nine-channel many-body perturbation calculation by Solomonson, Carter, and Kelly [16]. Several modifications of the Feshbach projection formalism were used to study resonances in He. For example, the Feshbach saddle-point technique was used by Wu and Xi [17] and a saddle-point technique was used by Chung and Davis [18]. L^2 techniques have also been used recently to study resonances in He. These include the calculations by Gersbacher and Broad [19] who used Sturmian basis sets, and a K-matrix L^2 basis set calculation by Moccia and Spizzo [20]. Other theoretical methods that have been used to calculate energy levels of $^1P^o$ states include the use of adiabatic potential curves [21,22] and the

use of multiconfigurational Hartree-Fock theory [23].

In addition to the theoretical investigations on the energy region between the $N=2$ and $N=3$ He^+ thresholds, there have also been intense theoretical studies below the $N=2$ He^+ threshold. These studies include various versions of close-coupling approximations [24–26], several modifications of the Feshbach projection formalism [17,27–29], and calculations using L^2 techniques with finite basis sets [19,30–32]. Other theoretical approaches such as a nine-channel many-body perturbation method [33] and a multichannel quantum defect theory [34] were also used to study resonances below the $N=2$ He^+ threshold.

In the present work, we now report results for the doubly excited $^1P^o$ resonant states in He below the $N=3$ threshold. The method of complex-coordinate rotation [35] is used in the present investigation. For the first ten lower-lying resonances we use Hylleraas-type wave functions to take into account of the strong electronic correlation effects. The present work is an extension of the earlier calculations [13]. We investigate the detail convergence behavior such that precise resonance parameters can be established. Our results can be used as standard nonrelativistic values for the lower-lying $^1P^o$ resonances. For the higher-lying resonances, Slater-orbital-type wave functions are used. The outer electron for these states has quantum numbers of $n \geq 5$. The use of separable wave functions enables us to have an adequate representation of the two electrons where they occupy different configurational spaces. Our results are compared with other calculations and with experimental measurements.

II. WAVE FUNCTIONS AND CALCULATIONS

The wave functions used in this work are of the Hylleraas type for the doubly excited intrashell resonances and lower-lying states (the first ten lowest-lying),

$$\Phi=\sum C_{k,m,n}\exp[-\alpha(r_1+r_2)]r_{12}^k \times[r_1^n r_2^{m+1}Y_{00}(1)Y_{10}(2) + r_2^n r_1^{m+1}Y_{00}(2)Y_{10}(1)] , \quad (1)$$

where $(k+n+m)\leq\omega$, with ω a positive integer. For $^1P^o$ resonances we use wave functions with up to $\omega=18$, which leads to $M=1330$ terms, where M denotes the total number of terms in the basis functions.

For higher-lying states we use products of Slater orbitals,

$$\Phi=A\sum_{la,lb}\sum_{i,j}C_{a_i,b_j}\eta_{a_i}(r_1)\eta_{b_j}(r_2)Y^{LM}_{la,lb}(1,2)S(\sigma_1,\sigma_2) , \quad (2)$$

where

$$\eta_{a_i}(r)=r^{na_i}\exp(-\xi_{a_i}r) .$$

In Eq. (2), A is the antisymmetrizing operator, S is a two-particle spin eigenfunction, and the η are individual Slater orbitals. Y is an eigenfunction of the total angular momentum L,

$$Y^{LM}_{la,lb}(1,2)=\sum_{m_{la}}\sum_{m_{lb}}C(la,lb,L;m_{la},m_{lb},M) \times Y_{la,m_{la}}(1)Y_{lb,m_{lb}}(2) , \quad (3)$$

with C the Clebsch-Gordan coefficients. For the intershell $3lnl'$ states with $n\geq 5$, quite extensive basis sets are used for the wave functions. We use a total of 16 s-, 15 p-, 14 d-, 13 f-, 10 g-, 9 h-, 8 i-, 5 k-, 3 l-, 2 m-, and 1 n-type orbitals. These orbitals would couple to a total of 987 terms for the $^1P^o$ states.

The Hamiltonian for the helium atom is given by

$$H=-\nabla_1^2-\nabla_2^2-\frac{2Z}{r_1}-\frac{2Z}{r_2}+\frac{2}{r_{12}}=T+V , \quad (4)$$

with $Z=2$, the charge of the nucleus, and r_1 and r_2 the coordinates of electrons with respect to the nucleus and $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$. Atomic units are used in this work with energy units in rydbergs.

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

$$r\rightarrow r\exp(i\theta) , \quad (5)$$

and the Hamiltonian can be written as

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

Complex eigenvalues are obtained by diagonalizing the transformed Hamiltonian. The resonance parameters are determined by finding stabilized roots with respect to the variation of the nonlinear parameters α and the angle θ, with $\theta>\arg(E_{\rm res})/2$. The complex resonance energy is given by

$$E_{\rm res}=E_r-i\Gamma/2 . \quad (7)$$

The theoretical aspects of the complex rotation method have been discussed in previous publications [35] 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 [36]. 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. The final resonance parameters, both resonance position and width, are then deduced from the condition that a discrete complex eigenvalue was stabilized with respect to the changes of nonlinear parameters in the wave functions [see Eq. (1)] and the changes of θ. The optimized θ is determined 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 $3s3P\ ^1P^o$ (1) resonance, it is found that when $M=286$ terms ($\omega=10$), the resonance complex eigenvalue would exhibit the most stabilized character, i.e., $\partial|E|/\partial\theta\approx$minimum at approximately $\theta=0.35$ rad. Once the optimized value for θ is obtained, we can exam-

TABLE I. Convergence behaviors for the $3s3p\ ^1P^o(1)$ state using Hylleraas functions. In the notation of *KTNn*, this state is (1133) ($\alpha=0.66, \theta=0.35$).

ω	M	E_r (Ry)	$\frac{1}{2}\Gamma$ (Ry)
12	455	−0.671 251 928	0.007 022 46
13	560	−0.671 251 161	0.007 024 45
14	680	−0.671 251 908	0.007 023 52
15	816	−0.671 251 847	0.007 024 19
16	969	−0.671 252 156	0.007 023 55
17	1140	−0.671 251 770	0.007 023 64

ine the convergence behaviors for the resonance parameters for different expansion lengths. The lowest ten $^1P^o$ resonances are obtained by this procedure with which Hylleraas-type wave functions are used.

III. RESULTS AND DISCUSSIONS

In Table I we show the convergence behaviors for the $3s3p\ ^1P^o$ (1) state. In the notation of approximate quantum numbers *KTNn*, this state is 1133. In this work we employ quantum numbers *KTNn* to denote each resonance. The "approximately good" quantum numbers K and T were proposed by Herrick and Sinanoglu [36] and by Lin [37]. Readers are referred to the earlier references for their physical meanings [38]. For the $^1P^o$ (1) resonance (the 1133 state), we fix the nonlinear parameters $\alpha=0.66$ and the optimized θ is found at approximately 0.35 rad. We calculate the complex eigenvalue as a function of ω (and of M). Up to a total of $\omega=17$ ($M=1140$ terms) are used for this state. We determine the resonance parameters as $E_r=0.671\,251\,8\pm5\times10^{-7}$ Ry and $\Gamma/2=0.007\,023\,6\pm5\times10^{-7}$ Ry. Table II shows the convergence behaviors for the $N=3\ ^1P^o$ (2) state (the 2034 state). The optimized nonlinear parameters are found at $\alpha=0.5$ and $\theta=0.35$. We estimate this state to have parameters of $E_r=-0.571\,901\,48\pm1\times10^{-7}$ Ry and $\Gamma/2=3.409\times10^{-5}\pm1\times10^{-7}$ Ry. The results for the $^1P^o$ (3) state (the −1133 state) are shown in Table III with optimized parameters of $\alpha=0.66$ and $\theta=0.35$. From this table we determine the resonance parameters as $E_r=-0.565\,657\,94\pm1\times10^{-7}$ Ry, and $\Gamma/2=0.001\,462\,08\pm1\times10^{-7}$ Ry. Table IV shows the convergence behaviors for the $^1P^o(4)$ (1134), $^1P^o(5)$ (0034), $^1P^o(6)$ (2035), and $^1P^o(7)$ (−1134) states. We use $\alpha=0.5$ and $\theta=0.35$ for these resonances. We determine the res-

TABLE II. Convergence behaviors for the $N=3\ ^1P^o(2)$ state in He using Hylleraas functions (the quantum numbers for this state are 2034) ($\alpha=0.5$, $\theta=0.35$).

ω	M	E_r (Ry)	$\frac{1}{2}\Gamma$ (Ry)
14	680	−0.571 901 539	0.000 034 159 4
15	816	−0.571 901 483	0.000 034 071 6
16	969	−0.571 901 489	0.000 034 097 3
17	1140	−0.571 901 485	0.000 034 091 8

TABLE III. Convergence behaviors for the $N=3\ ^1P^o(3)$ state in He using Hylleraas functions (the quantum numbers for this state are −1133) ($\alpha=0.66$, $\theta=0.35$).

ω	M	E_r (Ry)	$\frac{1}{2}\Gamma$ (Ry)
12	455	−0.565 657 351	0.001 461 32
13	560	−0.565 657 804	0.001 462 05
14	680	−0.565 657 916	0.001 462 03
15	816	−0.565 657 964	0.001 462 09
16	969	−0.565 657 930	0.001 462 08
17	1140	−0.565 657 942	0.001 462 08

TABLE IV. Convergence behaviors for the $N=3\ ^1P^o(4)$, $^1P^o(5)$, $^1P^o(6)$, and $^1P^o(7)$ states in He. The quantum numbers for these states are 1134, 0034, 2035, and −1134, respectively ($\alpha=0.5$, $\theta=0.35$).

ω	M	E_r (Ry)	$\frac{1}{2}\Gamma$ (Ry)
		$^1P^o(4)$	
14	680	−0.542 390 657	0.002 895 68
15	816	−0.542 387 720	0.002 895 43
16	969	−0.542 386 832	0.002 895 86
17	1140	−0.542 386 525	0.002 895 91
		$^1P^o(5)$	
14	680	−0.535 287 988	0.000 022 642 7
15	816	−0.535 288 001	0.000 022 687 2
16	969	−0.535 288 000	0.000 022 678 4
17	1140	−0.535 288 001	0.000 022 679 2
		$^1P^o(6)$	
14	680	−0.514 891 10	0.000 037 376 8
15	816	−0.514 861 318	0.000 017 856 9
16	969	−0.514 864 805	0.000 022 678 4
17	1140	−0.514 864 500	0.000 021 733 5
		$^1P^o(7)$	
14	680	−0.503 166 838	0.000 523 694
15	816	−0.503 154 426	0.000 519 273
16	969	−0.503 156 393	0.000 519 332
17	1140	−0.503 157 419	0.000 520 003

TABLE V. Convergence behaviors for the $N=3\ ^1P^o(8)$, $^1P^o(9)$, and $^1P^o(10)$ states in He using Hylleraas functions ($\alpha=0.4$, $\theta=0.3$).

ω	M	E_r (Ry)	$\frac{1}{2}\Gamma$ (Ry)
		$^1P^o(8)$	
16	969	−0.501 548	0.001 303
17	1140	−0.501 551	0.001 300
18	1330	−0.501 547	0.001 298
		$^1P^o(9)$	
16	969	−0.496 448 93	0.000 010 73
17	1140	−0.496 448 76	0.000 010 72
18	1330	−0.496 448 80	0.000 010 73
		$^1P^o(10)$	
16	969	−0.491 035 302	1.41×10^{-7}
17	1140	−0.491 035 304	1.37×10^{-7}
18	1330	−0.491 035 305	1.36×10^{-7}

TABLE VI. The lowest ten $^1P^o$ resonance states below the $N=3$ He^+ threshold. For each resonance, the first row entry is the resonance position, the second row is half the width.

State	*KTNn*	Present	Ref. [13]
$^1P^o(1)$	1133	$-0.671\,251\,8\pm5\times10^{-7}$	−0.671 25
		$0.007\,023\,6\pm5\times10^{-7}$	0.007 0
$^1P^o(2)$	2034	$-0.571\,901\,48\pm1\times10^{-7}$	−0.571 90
		$3.409\times10^{-5}\pm1\times10^{-7}$	0.000 028
$^1P^o(3)$	−1133	$-0.565\,657\,94\pm1\times10^{-7}$	−0.565 65
		$0.001\,462\,08\pm1\times10^{-7}$	0.001 45
$^1P^o(4)$	1134	$-0.542\,386\,5\pm1\times10^{-6}$	−0.542 45
		$0.002\,895\,9\pm1\times10^{-6}$	0.003 1
$^1P^o(5)$	0034	$-0.535\,288\,00\pm1\times10^{-8}$	−0.535 285
		$2.2679\times10^{-5}\pm1\times10^{-8}$	0.000 01
$^1P^o(6)$	2035	$-0.514\,864\,5\pm1\times10^{-6}$	−0.514 86
		$2.17\times10^{-5}\pm1\times10^{-6}$	0.000 015
$^1P^o(7)$	−1134	$-0.503\,157\pm2\times10^{-6}$	−0.503 2
		$5.20\times10^{-4}\pm2\times10^{-6}$	0.000 5
$^1P^o(8)$	1135	$-0.501\,55\pm1\times10^{-5}$	0.501 8
		$0.001\,30\pm1\times10^{-5}$	0.001 2
$^1P^o(9)$	0035	$-0.496\,448\,8\pm5\times10^{-7}$	
		$1.07\times10^{-5}\pm5\times10^{-7}$	
$^1P^o(10)$	−2034	$-0.491\,035\,30\pm1\times10^{-8}$	
		$1.36\times10^{-7}\pm1\times10^{-8}$	

onance parameters for the $^1P^o(4)$ state as $E_r=-0.542\,386\,5\pm1\times10^{-6}$ Ry, and $\Gamma/2=0.002\,895\,9\pm1\times10^{-6}$ Ry. The $^1P^o(5)$ would lie at $E_r=-0.535\,288\,00\pm1\times10^{-8}$ Ry with $\Gamma/2=2.2679\times10^{-5}\pm1\times10^{-8}$ Ry. The $^1P^o(6)$ state is determined as $E_r=-0.514\,864\,5\pm1\times10^{-6}$ Ry and $\Gamma/2=2.17\times10^{-5}\pm1\times10^{-6}$ Ry, and the $^1P^o(7)$ state as $E_r=-0.503\,157\pm2\times10^{-6}$ Ry and $\Gamma/2=5.20\times10^{-4}\pm2\times10^{-6}$ Ry. In Table V we show results for the $^1P^o(8)$, $^1P^o(9)$, and $^1P^o(10)$ resonances. The quantum numbers of these states are 1135, 0035, and −2034, respectively. For all three resonances we use the optimized nonlinear parameters $\alpha=0.4$ and $\theta=0.30$. In order to have a better estimate on the errors for the resonance parameters, we extend the calculation to $\omega=18$ and $M=1330$ terms. Resonance parameters are determined for $^1P^o(8)$ as $E_r=-0.501\,55\pm1\times10^{-5}$ Ry and $\Gamma/2=0.001\,30\pm1\times10^{-5}$ Ry for $^1P^o(9)$ as E_r

TABLE VII. Comparison of $3s3p\ ^1P^o$ resonance with other theoretical calculations.

E_r (Ry)	$\frac{\Gamma}{2}$ (Ry)	Reference
−0.671 251 8	0.007 023 6	Ho (1991)[a]
−0.670	0.006 95	Wakid and Callaway (1980)[b]
−0.668 5	0.005 48	Senashenko and Wague (1979)[c]
−0.671 388		Nicolaides and Komninos (1987)[d]
−0.670 7	0.006 6	Hayes and Scott (1988)[e]
−0.675 8		Koyoma, Takafuji, and Matsuzawa (1989)[f]
−0.675 58		Sadeghpour (1990)[g]
−0.671 14	0.007 04	Gershacher and Broad (1990)[h]
−0.669 27	0.004 20	Wu and Xi (1990)[i]
−0.670 766	0.006 763	Moccia and Spizzo (1991)[j]

[a]Complex-rotation, 1140-term Hylleraas, present calculation.
[b]Algebraic close coupling [14].
[c] Reference [39].
[d]Multicontigurational Hartree-Fock calculation [23].
[e]*R*-matrix calculation [15].
[f]Adiabatic potential curves [21].
[g]Adiabatic potential curves [22].
[h]L^2 technique with Sturmian functions [19].
[i]Feshbach saddle-point technique [17].
[j]*K*-matrix L^2 basis-set calculation [20].

$=-0.496\,448\,8\pm5\times10^{-7}$ Ry and $\Gamma/2=1.07\times10^{-5}\pm5\times10^{-7}$ Ry, and for $1P^o(10)$, $E_r=-0.491\,035\,30\pm1\times10^{-8}$ Ry and $\Gamma/2=1.36\times10^{-7}\pm1\times10^{-8}$ Ry.

In Table VI we summarize the lowest ten $^1P^\circ$ resonances in the present calculation and compare them with those obtained in the earlier complex-rotation calculation. It is seen that the resonance positions reported in Ref. [13] are very good. The present calculation does provide an improvement for the widths for the $^1P^o(2)$, $^1P^o(4)$, $^1P^o(5)$, $^1P^o(6)$ resonances. Furthermore, with the small errors estimated in the present work, our results can be considered as standard nonrelativistic resonance parameters. It is noted that for the $2s2p\ ^1P^o$ state, the relativistic effects would lower the nonrelativistic resonance position by 5.2×10^{-5} Ry [27]. In Table VII we compare our $3s3p\ ^1P^o$ state with other recent calculations. It is seen that the results obtained by Gershacher and Broad [19], who used an L^2 technique with Sturmian functions, agree best with out values.

For higher-lying states [for $^1P^o(11)$ to $^1P^o(21)$] we use separable wave functions such as products of Slater orbitals. Table VIII shows the parameters used to construct the two-electron wave functions. All the nonlinear parameters are then multiplied by a constant scaling factor α'. Resonance parameters are deduced by the stabilization conditions with respect to the changes of α' and of θ. For example, for the $^1P^o(11)$ state, the resonance energy exhibits the most stabilized behavior when $\alpha'=0.5$ and $\theta=0.2$. No error estimates are however made for the higher-lying resonances.

In Table IX we compare our results with experimental observations. In converting our results into eV, the reduced rydberg 1 Ry = 13.603 876 eV, and the ground-state energy of $E=-5.807\,448\,75$ Ry are used. It is seen that the recent measurements [7–10] for the widths of the 1133 state (ranging from 0.178 to 0.2 eV) are much closer to the present theoretical value of 0.1911 eV than the earlier experimental [4] value of 0.132 ± 0.014 eV. It

TABLE VIII. Parameters used in the Slater-orbital basis.

$l=0$		$l=1$		$l=2$		$l=3$	
n_j	ξ_j	n_j	ξ_j	n_j	ξ_j	n_j	ξ_j
0	1.0	1	1.0	2	1.0	3	1.0
1	1.0	2	1.0	3	1.0	4	1.0
2	1.0	3	1.0	4	1.0	5	1.0
3	1.0	4	1.0	5	1.0	6	1.0
4	1.0	5	1.0	6	1.0	7	1.0
5	1.0	6	1.0	7	1.0	3	0.5
6	1.0	7	1.0	2	0.5	4	0.5
7	1.0	1	0.5	3	0.5	5	0.5
0	0.5	2	0.5	4	0.5	6	0.5
1	0.5	3	0.5	5	0.5	3	0.25
2	0.5	4	0.5	2	0.25	4	0.25
3	0.5	1	0.25	3	0.25	5	0.25
0	0.25	2	0.25	4	0.25	6	0.25
1	0.25	3	0.25				
2	0.25	4	0.25				
3	0.25						

$l=4$		$l=5$		$l=6$		$l=7$	
n_j	ξ_j	n_j	ξ_j	n_j	ξ_j	n_j	ξ_j
4	1.0	5	1.0	6	1.0	7	1.0
5	1.0	6	1.0	7	1.0	8	1.0
6	1.0	7	1.0	8	1.0	7	0.5
7	1.0	8	1.0	9	1.0	8	0.5
8	1.0	9	1.0	6	0.5	7	0.25
9	1.0	5	0.5	7	0.5	8	0.25
4	0.5	6	0.5	6	0.25		
5	0.5	5	0.25	7	0.25		
4	0.25	6	0.25				
5	0.25						

$l=8$		$l=9$		$l=10$	
n_j	ξ_j	n_j	ξ_j	n_j	ξ_j
8	1.0	9	1.0	10	1.0
8	0.5	9	0.5		
8	0.25				

is also noted that the experimental widths for the -1133 state are substantially larger than those of the theoretical values. For example, the results from the Wisconsin experiment [7] (0.07 eV) and the DSRS experiment [11] (0.073±0.015 eV) are much larger than the results from the present calculation (0.039 eV), the nine-state algebraic close-coupling calculation [14] (0.030 eV), and the recent L^2 basis set calculation [20] (0.0374 eV). Such a discrepancy between theory and experiment has yet to be resolved.

Table X summarizes our results for all the resonances we have calculated between the $N=2$ and $N=3$ thresholds of He^+. We are able to locate six members for the $113n$ series, with $3\leq n\leq 8$, four members for the $-113n$ series with $3\leq n\leq 6$. We have also determined parameters for four members in the $203n$ series, $4\leq n\leq 7$, four members in the $003n$ series, $4\leq n\leq 7$, and three members in the $-203n$ series, with $4\leq n\leq 6$. In Table X we also compare the recent results by Moccia and Spizzo [20] who carried out a K-matrix L^2 basis set calculation. In general their results agree reasonably well with ours. Their widths for the $113n$ series differ from our results ranging from 4% for the 1133 state to 25% for the 1135 state. The agreements for the $-113n$, $203n$, and the $003n$ series are very good. Their widths for the $-203n$ series, however, differ substantially with ours. Furthermore, as they have mentioned in Ref. [20], their width for the -2035 state has a larger value than that of -2034, in contrast to what might expect of that for a Rydberg series.

In Table X we also compare results obtained by Solomonson, Carter, and Kelly [16], who carried out a nine-channel many-body perturbation calculation. They have obtained widths for the $203n$, $003n$, and $-203n$ series. While their results for the $203n$ series are reasonably accurate, the $003n$ results are almost double our values and

TABLE IX. Comparison of the present calculations with experimental observations for the $^1P^o$ resonance states in He.

KTNn	E_r (eV)	Γ (eV)	Reference
1133	69.8722	0.1911	a
	69.919±0.007	0.132±0.014	b
	69.917±0.012	0.178±0.012	c
	69.917±0.012	0.178±0.012	d
	69.914±0.015	0.200±0.020	e
	69.880±0.022	0.180±0.015	f
1134	71.625	0.0788	a
	71.66±0.01		b
	71.601±0.018	0.096±0.015	c
	71.625		f
1135	72.181	0.0354	a
	72.20±0.01		b
	72.181±0.015	0.067±0.015	c
	72.174		f
1136	72.448	0.0207	a
	72.47±0.011		b
	72.453±0.011	0.038±0.015	c
	72.423		f
1137	72.600	0.0133	a
	72.61		b
	72.59±0.01		c
	72.561		f
1138	72.696	0.007 78	a
	72.70		b
	72.67±0.01		c
	72.640		f
-1113	71.3086	0.0398	a
	71.30±0.04	0.07	c
	71.261±0.030	0.073±0.015	f

[a]Present calculation.
[b]NBS-I (1973) [4].
[c]Wisconsin (1982) [7].
[d]SSRL (1987) [8].
[e]BESSY (1988) [9].
[f]DSRS (1989) [11].

those of Ref. [20]. Their widths for the $-203n$ series are almost 20 times larger than the present calculation. Wu and Xi [17] also calculated resonances in this energy region by using a saddle-point complex-rotation method. However, except for the lowest $3s3p\ ^1P^o$ state, these authors did not calculate the widths for the $N=3$ resonances.

Finally, we mention that although we use the notations of $KTNn$ to classify the $^1P^o$ resonances, there also exist other classification schemes to describe such states in the

TABLE X. Doubly excited $^1P^o$ resonances between the $N=2$ and $N=3$ thresholds of He^+.

$KTNn$	Present	Wave functions used	Ref. [20]	Ref. [16]
		E (Ry)		
1133	−0.671251 8	Hylleraas	−0.670 766	
1134	−0.542386 5	Hylleraas	−0.541 547	
1135	−0.501 552	Hylleraas	−0.501 117	
1136	−0.481 89	Slater	−0.481 535	
1137	−0.470 75	Slater	−0.470 582	
1138	−0.463 705	Slater	−0.463 805	
−1133	−0.565 657 94	Hylleraas	−0.564 834	
−1134	−0.503 157	Hylleraas	−0.502 293	
−1135	−0.481 69	Slater	−0.481 211	
−1136	−0.470 48	Slater		
2034	−0.571 901 48	Hylleraas	−0.571 744	−0.571 479
2035	−0.514 864 5	Hylleraas	−0.417 604	−0.514 878
2036	−0.488 82	Slater	−0.488 790	−0.488 790
2037	−0.474 87	Slater	−0.474 860	−0.474 882
0034	−0.535 288 00	Hylleraas	−0.534 637	−0.533 623
0035	−0.496 448 8	Hylleraas	−0.496 214	−0.495 839
0036	−0.478 58	Slater	−0.478 484	−0.478 271 1
0037	−0.468 866	Slater		
−2034	−0.491 035 30	Hylleraas	−0.490 282	−0.488 893
−2035	−0.476 12	Slater	−0.475 853	−0.474 735
−2036	−0.467 32	Slater		
		$\frac{\Gamma}{2}$ (Ry)		
1133	0.007 023 6		0.006 763	
1134	0.002 895 9		0.003 006 5	
1135	0.001 30		0.001 069	
1136	0.000 76		0.000 742	
1137	0.000 49			
1138	0.000 286			
−1133	0.001 462 08		0.001 375	
−1134	0.000 520		0.000 668 9	
−1135	0.000 219		0.000 218 7	
−1136	0.000 097			
2034	3.049×10^{-5}		3.216×10^{-5}	3.326×10^{-5}
2035	2.17×10^{-5}		2.187×10^{-5}	2.176×10^{-5}
2036	1.3×10^{-5}		1.3195×10^{-5}	1.323×10^{-5}
2037	8×10^{-6}		8.306×10^{-6}	8.085×10^{-6}
0034	2.2679×10^{-5}		2.146×10^{-5}	4.263×10^{-5}
0035	1.07×10^{-5}		1.011×10^{-5}	2.025×10^{-5}
0036	5.8×10^{-6}		6.8×10^{-6}	1.099×10^{-5}
0037	2.6×10^{-6}			
−2034	1.36×10^{-7}		5.55×10^{-8}	3.271×10^{-6}
−2035	$<1.0\times10^{-7}$		1.85×10^{-7}	2.286×10^{-6}
−2036	$<1.0\times10^{-7}$			

TABLE XI. Different classifications for $^1P^o$ states below the $N=3$ He^+ threshold.

$KTNn$	Ref. [40]	Approximate mixings	Lowest n
$113n$	$(3,na)$	$(3snp+ns3p)+(3pnd+np3d)$	3
$-113n$	$(3,nb)$	$(3snp+ns3p)-(3dnf+np3d)$	3
$203n$	$(3,nc)$	$(3snp-ns3p)+(3pnd-np3d)$	4
$003n$	$(3,nd)$	$(3pnd-np3d)+(3snp-ns3p)+3dnf$	4
$-203n$	$(3,ne)$	$(3pnd-3dnf)$	4

literature. In Table XI, we list these schemes as well as the dominate configurations for these resonances.

In summary, we have carried out an elaborate calculation for doubly excited $^1P^o$ resonant states in He between the $N=2$ and $N=3$ He^+ thresholds. Using a method of complex-coordinate rotation, a total of 21 resonances are reported. Our accurate results are useful references for experimental investigations and can also provide accessment of merits for other theoretical calculations.

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