Doubly excited $^{1,3}S^e$, $^{1,3}P^o$, and $^{1,3}D^e$ resonances in He below the $n=2$ He^+ threshold

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We study doubly excited $^{1,3}S^e$, $^{1,3}P^o$, and $^{1,3}D^e$ resonances in He below the $n=2$ He^+ threshold by the saddle-point complex-rotation method with B-spline functions. We calculated 78 resonances. Recently, accurate measurements on the $^1P^o$ have been performed, which allow detailed comparisons with our *ab initio* theoretical results. For $^1P^o$, we calculate six members in the $_2(0,1)_n^+(2\leqslant n\leqslant 7)$ series, five members in the $_2(1,0)_n^-(3\leqslant n\leqslant 7)$ series, and four members in the $_2(-1,0)_n^0(3\leqslant n\leqslant 6)$ series. The resonance energies and widths are compared with accurate experimental and theoretical results. The agreement is good. For other symmetries, the energies and widths are also calculated up to $n\cong 7$, and are also in good agreement with available experimental and theoretical results. [S1050-2947(97)01912-4]

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I. INTRODUCTION

Doubly excited helium is a prototype for the study of electron-electron correlations. Since the observation [1] and interpretation [2], many experimental and theoretical efforts have been devoted to this topic to understand the strong electron-electron correlations quantitatively and qualitatively. Photoionization, electron-impact, ion-impact, beam-foil, and ejected-electron spectra techniques have been used to study the autoionizing states of helium. For many years, considerable experimental efforts (Woodruff and Samson [3], Bizau *et al.* [4], Morgan and Ederer [5], Lindle *et al.* [6], Kossman *et al.* [7], Zubek *et al.* [8], Domke *et al.* [9–11], and Schulz *et al.* [12], for examples) have been working at improving the resolution by using various synchrotron light sources. From the theoretical side, there are many different approaches. The earlier calculations have been reviewed in previous experimental works [13,3,5] and by Ho [14]. Recently, Buckman and Clark [15] reviewed both of the theoretical and experimental works. Some of the recent theoretical approaches are the algebraic variational close-coupling method [16], the close-coupling method [17,18], the complex-rotation method [19–24], the L^2 technique [25,28–33], the saddle-point complex-rotation method [26,27], the saddle-point R-matrix method [34] , the diabatic and adiabatic hyperspherical method [35,36], and the hyperspherical close-coupling method [37–39] . Herrick and Sinanoglu [40] and Lin [41] have introduced a classification scheme, which is widely used, along with a hyperspherical coordinate description of He. Very recently, because of the development of high-resolution monochromators at synchrotron-radiation facilities, accurate measurements [9–12] on the $^1P^0$ doubly excited resonances of He were performed, which allow detailed comparisons with *ab initio.* theoretical results. They have renewed the interest in studying this topic.

In the present work, the saddle-point complex-rotation method with B-spline basis functions will be used in studying the resonant helium below the $n=2$ He^+ threshold. The saddle-point method was developed by Chung [42]. Many successful results have been obtained by Chung and his coworkers [26,27,43–45] (we only refer to some of their works) by the saddle-point complex-rotation method. This method is advantageous in its simplicity, effectiveness, and stability.

II. THEORY

We have developed [46] the saddle-point complex-rotation method with B-spline functions [47]. We will briefly summarize the method here.

In a configuration interaction scheme, we constructed the wave functions in terms of B splines of order k and total number N, defined between two end points, $r_{\min}=0$ and $r_{\max}=R$, and build vacancies into the wave functions. With an exponential sequence, we have the trial wave function for a two-electron system

$$\Psi = A\{[1-P(\vec{r_1})][1-P(\vec{r_2})]\} \times \sum_{i,j,l_1,l_2} C_{i,j,l_1,l_2}\Phi_{i,j}(\vec{r_1},\vec{r_2})Y^{LM}_{l_1,l_2}\chi(1,2), \quad (1)$$

with

$$\Phi_{i,j}(\vec{r_1},\vec{r_2}) = \frac{B_{i,k}(r_1)}{r_1}\frac{B_{j,k}(r_2)}{r_2}, \quad (2)$$

$$Y^{LM}_{l_1,l_2} = \sum_{m_1,m_2}\langle l_1 l_2 m_1 m_2|LM\rangle Y_{l_1,m_1}(\hat{r_1})Y_{l_2,m_2}(\hat{r_2}), \quad (3)$$

and

$$i \geqslant j - jm, \quad (4)$$

where the numbers i and j are positive integers, which are not larger than N [48], and jm is some selected integer [49]. A is the antisymmetrization operator, $\chi(1,2)$ is the spin wave function, and $P(\vec{r})$ is a projection operator. For the present, the $1s$ orbital is the vacancy orbital. We assume it to be hydrogenic with effective nuclear charge, q. The saddle-point variation is carried out by first minimizing the energy with respect to C_{i,j,l_1,l_2} and the set of B spline basis functions, and then maximizing the energy with respect to the

TABLE I. Comparison between experimental and theoretical values for energies and widths for doubly excited $^1P^o$ below the $N=2$ threshold. 2.0(3) means 2.0 ± 0.3.

	E_2	E_3	E_4	E_5	Γ_2	Γ_3	Γ_4	Γ_5
			(eV)			(meV)		
$_2(0,1)_n^+$								
Expt.	60.150(4)	63.658(3)	64.466(2)	64.816	37.6(2)	8.3(5)	3.4(7)	2.0(3)
Theory								
Present	60.146	63.656	64.464	64.814	37.3	8.16	3.5	1.75
[19]	60.145	63.656	64.464	64.814	37.4	8.2	3.5	1.8
[25]	60.154	63.656	64.463		36.5	7.9	3.3	
[23]	60.147	63.658	64.466		37.36	8.19	3.49	
[52]	60.146	63.656	64.465		37.4	8.19	3.5	
[28]	60.156	63.661	64.467		38.3	8.39	3.58	
$_2(1,0)_n^-$								
Expt.		62.761(2)	64.136(2)	64.659(2)		0.11(2)	0.06(5)	0.03(3)
Theory								
Present		62.758	64.134	64.657		0.105	0.055	0.027
[19]		62.758	64.134	64.657		0.105	0.056	
[25]		62.756	64.132			0.098	0.047	
[23]		62.760	64.136	64.659		0.105	0.055	0.027
[52]		62.758	64.134	64.656		0.106	0.055	0.027
[28]		62.760	64.137	64.659		0.112	0.057	0.028
$_2(-1,0)_n^0$								
Expt.		64.119	64.648	64.907		<0.05		
Theory								
Present		64.118	64.648	64.906		0.00041	0.00008	
[19]		64.118	64.648	64.906		0.00044		
[25]		64.117	64.646	64.906		0.00053	0.00023	
[23]		64.118	64.648			0.00028	0.000004	
[52]		64.118				0.00037		
[28]		64.116	64.646	64.908		0.000157	0.0000376	

effective nuclear charge, q, to obtain the saddle-point energy and wave function. The B-spline basis functions with an exponential knot sequence [48,50] are employed in the present calculations. We then calculate the resonance energy and width by a complex-rotation method. We choose the open-channel components [26] to be

$$\Psi_{\text{open}} = A\psi_{1s}(\vec{r_1}) \sum_{kc=L}^{kc} C_{kc} u_{kc}(r_2)\chi(1,2), \tag{5}$$

$$u_{kc}(\vec{r_i}) = r_i^{kc} e^{-\beta r_i} Y_{L,0}(\hat{r_i}), \tag{6}$$

where ψ_{1s} is the ground-state wave function of He^+. The non-negative integer kc is chosen to be large enough to ensure the accuracy of the resonance energy and width in the calculation by the complex-rotation method. The trial wave functions are composed of the saddle-point wave functions (the closed-channel components) and the open-channel components Ψ_{open}, in which each radial coordinate r_i in $u_{kc}(\vec{r_i})$ takes the form $r_i e^{i\theta}$.

In carrying out the complex-rotation calculation, the parameters β, kc and the coefficients C_{kc} [in Eqs. (5) and (6)] and the coefficients C_{i,j,l_1,l_2} of the saddle-point wave functions are optimized [46,51] to find stable resonant energies and widths. In practice, in using the saddle-point wave functions as the closed-channel components, we only varied these coefficients of the partial waves which make major contributions to the saddle-point energies. We found that we can combine a few terms of the saddle-point wave functions [Eq. (1)] to a single term to reduce the working space in the computer. The accuracy was deemed sufficient for our calculations. The closed-channel components for our calculation are constructed from the saddle-point wave function as follows:

$$\Psi = A\{[1-P(\vec{r_1})][1-P(\vec{r_2})]\} \times \sum_{m,n,l_1,l_2} D_{m,n,l_1,l_2} \phi_{m,n}(\vec{r_1},\vec{r_2}) Y^{LM}_{l_1,l_2} \chi(1,2), \tag{7}$$

with

$$\phi_{m,n}(\vec{r_1},\vec{r_2}) = \sum_{(i,j)_{m,n}} C_{i,j,l_1,l_2} \Phi_{i,j}. \tag{8}$$

The coefficients D_{m,n,l_1,l_2} are varied in the complex-rotation calculation. The selection of the groups $(i,j)_{m,n}$ is also optimized to obtain stable resonance energies and widths. We expect the success of grouping the saddle-point wave functions because of the flexibility of B-spline functions.

TABLE II. Energies and widths for doubly excited $^{1,3}P^0$ below the $N=2$ threshold (in a.u.). Underlined digits indicate uncertainties. Numbers is square brackets indicate powers of ten.

		$^1P^o$		$^3P^o$	
	State	E_r	Width	E_r	Width
		$_2(0,1)_n^+$		$_2(1,0)_n^+$	
Present	$n=2$	0.693069	0.1372[−2]	0.760489	0.299[−3]
[19,20]		0.69313495	0.13733[−2]	0.76049239	0.298862[−3]
[52]		0.6930920	0.137297[−2]		
[24]		0.693135	0.1373[−2]	0.760492	0.299[−3]
[16]		0.6928	0.133[−2]	0.7604512	0.301[−3]
Present	$n=3$	0.564074	0.2998[−3]	0.584671	0.824[−4]
[19,20]		0.5640850	0.301057[−3]	0.5846723	0.8225[−4]
[52]		0.5640777	0.301167[−3]		
[24]		0.56409	0.301[−3]	0.58467	0.823[−4]
[16]		0.56401	0.31[−3]	0.584652	0.77[−4]
Present	$n=4$	0.534358	0.128[−3]	0.542837	0.317[−4]
[19,20]		0.534361	0.129[−3]	0.5428373	0.316[−4]
[23]		0.534363144	0.1283[−3]		
[16]		0.534322	0.124[−3]	0.542830	0.302[−4]
Present	$n=5$	0.521501	0.644[−4]	0.525711	0.151[−4]
[19,20]		0.5214995	0.643[−4]	0.52571	0.138[−4]
[16]		0.521489	0.658[−4]	0.5257083	0.144[−4]
Present	$n=6$	0.514732	0.371[−4]	0.517107	0.86[−5]
[19,20]		0.51473265	0.361[−4]	0.51711	0.76[−5]
[16]		0.514720	0.38[−4]		
Present	$n=7$	0.510725	0.225[−4]	0.512206	0.54[−5]
[19,20]		0.510750		0.51219	
[16]		0.510670			
		$_2(1,0)_n^-$		$_2(0,1)_n^-$	
Present	$n=3$	0.597074	0.384[−5]	0.579030	0.185[−5]
[19,20]		0.5970738	0.385[−5]	0.57903099	0.1894[−5]
[52]		0.59707496	0.38999[−5]		
[24]		0.59707	0.384[−5]	0.57903	0.188[−5]
[16]		0.5970725	0.389[−5]	0.5790245	0.178[−5]
Present	$n=4$	0.546490	0.202[−5]	0.539558	0.790[−6]
[19,20]		0.5464933	0.205[−5]	0.53955879	0.771[−6]
[52]		0.54649029	0.20220[−5]		
[16,34]		0.546457	0.208[−5]	0.539501	0.445[−5]
Present	$n=5$	0.527295	0.988[−6]	0.523946	0.410[−6]
[19,20]		0.5272950		0.523945	
[23]		0.527297769	0.9821[−6]		
[16,34]		0.527289	0.102[−5]	0.522106	0.348[−6]
Present	$n=6$	0.5179395	0.54[−6]	0.516079	0.23[−6]
[19,20]		0.5179355		0.516077	
[16]		0.517930	0.39[−6]		
Present	$n=7$	0.5126789	0.32[−6]	0.511547	0.15[−6]
[19,20]		0.5126675		0.511551	
		$_2(-1,0)_n^0$		$_2(-1,0)_n^-$	
Present	$n=3$	0.547087	0.15[−7]	0.548841	0.130[−7]
[19,20]		0.5470927	0.16[−7]	0.54884435	0.127[−7]
[23]		0.547092709	0.105[−7]		
[52]		0.5470880	0.1375[−7]		
[24]		0.5471	<0.1[−6]	0.54884	0.16[−7]
[16]				0.54879738	0.109[−7]

TABLE II. (continued).

		$^1P^o$		$^3P^o$	
	State	E_r	Width	E_r	Width
Present	$n=4$	0.527613	0.3[−8]	0.528637	0.66[−8]
[19,20]		0.5276103		0.52863841	
[23]		0.527616338	0.14[−9]		
[34]				.528009	0.240[−6]
Present	$n=5$	0.518115		0.518708	0.32[−8]
[19,20]		0.5181148		0.51869300	
[34]				0.516530	0.713[−6]
Present	$n=6$	0.512789		0.513155	0.16[−8]
[19,20]		0.5127880		0.51314450	

III. RESULTS AND DISCUSSIONS

We calculated 78 resonances ($^{1,3}S^e$, $^{1,3}P^o$, and $^{1,3}D^e$). The saddle-point and resonance energies are converged to be accurate to the first six digits except $_2(-1,0)^+_{2,3}$ $^1S^e$, $_2(0,1)^+_{2,3}$, $_2(1,0)^-_4$, $_2(-1,0)^0_3$ $^1P^o$ and $_2(1,0)^+_{2-4}$, $_2(0,1)^0_{3,4}$ $^1D^e$. In carrying out the saddle-point variation, we calculated $^1S^e$ by including partial waves, $(l_1,l_2)=(0,0)$, (1,1), (2,2), (3,3), (4,4), (5,5), (6,6), (7,7), with $R=250$ a.u. or 550 a.u. and $^3S^e$ by including partial waves up to $l_1,l_2\leqslant 6$. For $^{1,3}P^o$, we included six partial waves, $(l_1,l_2)\leqslant(5,6)$, with $R=300$ a.u. or 600 a.u. Seven partial waves, $(l_1,l_2)=(0,2)$, (1,1), (1,3), (2,2), (2,4), (3,3), and (3,5) are used to calculate $^{1,3}D^e$ with $R=300$ a.u. or 640 a.u. We truncated the partial waves because of the limited space in the computer, and the accuracy of the calculations. In the calculation of the complex-rotation method, the resonance energies and widths are stable for kc [Eq. (5)] about 16. The range of β and θ, in which we obtained stable resonance energies and widths, vary for different states. $\Delta\beta$ and $\Delta\theta$ are not less than 0.1 in the worst case.

In Table I, we compare our results of $^1P^o$ with the recent experimental results [11,12] and other theoretical results [19,25,23,52,28]. The theoretical results are converted to eV by using Ry=13.603 83 eV and I_∞ (the double-ionization threshold) = 79.003 eV. A more complete list of theoretical works can be found in the article of Domke *et al.* [11]. Our results agree well with experiment [11,12]. The widths of $_2(-1,0)^0_n$ are so small that no experimental results are available to compare with the theoretical results. The theoretical results listed in Table I generally agree well with each other and with experiment [11,12]. The various theoretical widths of $_2(-1,0)^0_n$ show a spread, but our width of $_2(-1,0)^0_3$ agrees very well with Ho's result [19].

In Table II, our results of resonance energies and widths for $^1P^o$ ($^3P^o$) are shown for $_2(0,1)^+_n$, $_2(1,0)^-_n$, and $_2(-1,0)^0_m$($_2(1,0)^+_n$, $_2(0,1)^-_n$, and $_2(-1,0)^-_m$) series ($n\leqslant 7$, $m\leqslant 6$) and compared with other theoretical results [19,23,52,20,24,16,34]. Our results of the widths generally agree well with other theoretical results except those of Wu and Xi [34] as shown in Table II. The agreement is better for the larger widths. Few works of the widths on the higher members of $2(1,0)^-_n$, and $_2(-1,0)^0_n$ $^1P^o$ and $_2(0,1)^-_n$, and $_2(-1,0)^-_n$ $^3P^o$ are available to the author's knowledge. Oza [16] did not calculate the $_2(0,1)^-_n$ and $_2(-1,0)^-_n$ series ($n\geqslant 4$) of $^3P^o$, and therefore we list those of Wu and Xi [34] in Table II. The widths of Wu and Xi [34] for $_2(0,1)^-_4$ and $_2(-1,0)^-_{4,5}$ of $^3P^o$ are much larger than ours. Their resonance energies are larger than ours and those of Ho [20]. According to Fano and Cooper [53], the widths of a given Rydberg series decrease according to the third power of the reduced quantum number, $n^*=n-\mu$ (μ is the quantum defect). We estimated the quantum defects to be 0.17, 0.72, and −0.17, respectively, for $_2(0,1)^+_n$, $_2(1,0)^-_n$, and $_2(-1,0)^0_n$ series of $^1P^o$. They agree very well with the results of Domke *et al.* [11]. The quantum defects are also estimated to be 0.60, 0.42, and −0.17, respectively, for $_2(1,0)^+_n$, $_2(0,1)^-_n$, and $_2(-1,0)^-_n$ series of $^3P^o$ from the present results. Except for $_2(-1,0)^0_n$ series of $^1P^o$, the reduced widths ($n^{*3}\Gamma$) are nearly constant for higher members of $^{1,3}P^o$. Our width and that of Wintgen and Delande [23] are too small for $_2(-1,0)^0_4$ of $^1P^o$. We think that our width of $_2(1,0)^-_6$ of $^1P^o$ is more reliable than that of Oza [16] by examining the constancy of the reduced widths. And so are our widths of $_2(-1,0)^-_n$ series of $^3P^o$ more reliable than those of Wu and Xi [34]. Our resonance energies for higher members of $^3P^o$ states agree with the results [19,20], which were calculated with Hylleraas functions, better than for the lower members or $^1P^o$ states. It is similar to what we found for the energies of lower states of singly excited He [48,54,55]. However, our resonance energies of the lower members of $^1P^o$ are shown to be in good agreement with the accurate experimental results [11,12] as well as Ho's results [19].

In Tables III and IV, the present results of the resonance energies and widths for $^{1,3}S^e$ and $^{1,3}D^e$ are shown and compared with those of Ho [21], Ho and Bhatia [22], Lindroth [24], Oza [16], Wu and Xi [34], and Macías *et al.* [57]. The agreement amongst the present results and those of Ho [21], Ho and Bhatia [22], Lindroth [24], and Oza [16] is good. Ho [21], Ho and Bhatia [22], and Lindroth [24] only calculated lower members of the $^{1,3}S^e$ and $^{1,3}D^e$ series. Our results agree with theirs very well except for the resonance energies for $_2(-1,0)^+_{2,3}$ of $^1S^e$ and $_2(1,0)^+_{2,3}$ of $^1D^e$. The agreement also tends to be better for higher members or triplet states as we found in Table II. The resonance energies of $^1S^e$, calculated by Wu and Xi [34] and Macías and Riera [56], are close to those of Ho [21], Lindroth [24], Oza [16], and ours. However, the widths of Wu and Xi [34] are too small, especially for higher members of the $_2(1,0)^+_n$ series of $^1S^e$, and

TABLE III. Energies and widths for doubly excited $^{1,3}S^e$ below the $N=2$ threshold (in a.u.). Underlined digits indicate uncertainties. $_2(K,T)_n^{+,-}$ means $A=1$ for $^1S^e$ and $A=-1$ for $^3S^e$. Numbers in square brackets indicate powers of ten.

		$^1S^e$		$^3S^e$	
	State	E_r	Width	E_r	Width
Present	$_2(1,0)_2^{+,-}$	0.77787	0.453[−2]		
[21]		0.777868	0.453[−2]		
[24]		0.777868	0.4541[−2]		
[16]		0.7778	0.458[−2]		
[34]		0.777879	0.333[−2]		
[56]		0.778405	0.542[−2]		
Present	$_2(1,0)_3^{+,-}$	0.589896	0.137[−2]	0.602577	0.665[−5]
[21]		0.589895	0.135[−2]		
[24]		0.58989	0.136[−2]	0.60258	0.664[−5]
[16]		0.589865	0.138[−2]	0.602576765	0.642[−5]
[34]		0.589957	0.926[−3]		
[56]		0.589925	0.134[−2]	0.602589	0.665[−5]
Present	$_2(1,0)_4^{+,-}$	0.544882	0.50[−3]	0.548841	0.310[−5]
[21]		0.544875	0.45[−3]		
[16]		0.54487	0.49[−3]	.54884039	0.307[−5]
[34]		0.544892	0.401[−3]		
[56]		0.544878	0.471[−3]	0.548844	0.310[−5]
Present	$_2(1,0)_5^{+,-}$	0.526687	0.23[−3]	0.528414	0.154[−5]
[16]		0.52679	0.21[−3]	0.5284136	0.150[−5]
[34]		0.526619	0.194[−3]		
[56]		0.526674	0.201[−3]	0.518336	0.801[−6]
Present	$_2(1,0)_6^{+,-}$	0.517641	0.12[−3]	0.518546	0.86[−6]
[16]		0.517632	0.110[−3]		
[34]		0.517417	0.197[−4]		
[56]		0.517260	0.131[−3]	0.518336	0.801[−6]
Present	$_2(1,0)_7^{+,-}$	0.512514	0.69[−4]	0.513046	0.52[−6]
[16]		0.512455			
[56]				0.507694	0.340[−5]
Present	$_2(-1,0)_2^{+,-}$	0.62181	0.2178[−3]		
[21]		0.621928	0.2156[−3]		
[24]		0.621926	0.216[−3]		
[16]		0.620516	0.231[−3]		
[34]		0.622255	0.647[−3]		
[56]		0.619277	0.286[−3]		
Present	$_2(-1,0)_3^{+,-}$	0.548070	0.775[−4]	0.559745	0.261[−6]
[21]		0.5480855	0.78[−4]		
[24]		0.54809	0.762[−4]	0.55975	0.256[−6]
[16]		0.5478765	0.827[−4]	0.5597187	0.23[−6]
[34]		0.547908	0.255[−3]		
[56]		0.547759	0.106[−3]	0.559670	0.277[−6]
Present	$_2(-1,0)_4^{+,-}$	0.527707	0.49[−4]	0.532505	0.143[−6]
[21]		0.527710	0.5[−4]		
[16]		0.527625	0.52[−4]	0.5324929	0.15[−6]
[34]		0.527697	0.959[−4]		
[56]		0.527586	0.676[−4]	0.532476	0.153[−6]
Present	$_2(-1,0)_5^{+,-}$	0.518100	0.32[−4]	0.520549	0.82[−7]
[16]		0.518056	0.35[−4]		
[34]		0.517786	0.155[−3]		
[56]		0.517865	0.445[−4]	0.520510	0.120[−6]
Present	$_2(-1,0)_6^{+,-}$	0.512762	0.22[−4]	0.514180	0.48[−7]
[34]		0.512554	0.908[−4]		
[56]		0.508513	0.283[−4]	0.512268	0.198[−8]
Present	$_2(-1,0)_7^{+,-}$			0.510378	0.30[−7]

TABLE IV. Energies and widths for doubly excited $^{1,3}D^e$ below the $N=2$ threshold (in a.u.). Underlined digits indicate uncertainties. $_2(K,T)_n^{+,-}$ means $A=1$ for $^1D^e$ and $A=-1$ for $^3D^e$. Numbers in square brackets indicate powers of ten.

		$^1D^e$		$^3D^e$	
	State	E_r	Width	E_r	Width
Present	$_2(1,0)_2^{+,-}$	0.70183	0.236[−2]		
[22]		0.7019457	0.23622[−2]		
[24]		0.701946	0.2362[−2]		
[16]		0.701655	0.241[−2]		
[57]		0.69865	0.261[−2]		
Present	$_2(1,0)_3^{+,-}$	0.569193	0.560[−3]	0.583784	0.312[−7]
[22]		0.569221	0.555[−3]	0.58378427	0.286[−7]
[24]		0.56922	0.556[−3]	0.58378	0.30[−7]
[16]		0.569115	0.57[−3]	0.58378017	0.321[−7]
[57]		0.56826	0.625[−3]	0.58321	0.404[−8]
Present	$_2(1,0)_4^{+,-}$	0.536715	0.234[−3]	0.541679	0.10[−7]
[22]		0.536727	0.233[−3]		
[16]		0.53669	0.237[−3]	0.54167657	0.115[−7]
[57]		0.53616	0.268[−3]	0.54124	0.150[−7]
Present	$_2(1,0)_5^{+,-}$	0.522737	0.118[−3]	0.525018	0.48[−8]
[16]		0.52272	0.119[−3]	0.52501735	0.51[−8]
[57]		0.52210	0.135[−3]	0.52451	0.930[−7]
Present	$_2(1,0)_6^{+,-}$	0.515451	0.676[−4]	0.516687	0.25[−8]
[16]		0.51544	0.68[−4]		
[57]		0.51480	0.893[−4]	0.51313	0.122[−5]
Present	$_2(1,0)_7^{+,-}$	0.511178	0.418[−4]		
[16]		0.51112150	0.433[−4]		
Present	$_2(1,0)_8^{+,-}$	0.508499	0.26[−4]		
[16]		0.508272	0.318[−4]		
Present	$_2(0,1)_3^0$	0.556417	0.201[−4]	0.560684	0.756[−5]
[22]		0.5564303	0.201[−4]	0.560687	0.75[−5]
[24]		0.55643	0.200[−4]	0.56069	0.751[−5]
[16]		0.5563903	0.199[−4]	0.5606695	0.74[−5]
[57]		0.55552	0.108[−4]	0.55969	0.408[−5]
Present	$_2(0,1)_4^0$	0.531506	0.112[−4]	0.533462	0.382[−5]
[22]		0.5315012	0.11[−4]	0.533462	0.382[−5]
[16]		0.53150	0.111[−4]	0.53345656	0.382[−5]
[57]		0.53080	0.393[−5]	0.53238	0.348[−5]
Present	$_2(0,1)_5^0$	0.520114	0.640[−5]	0.521130	0.208[−5]
[16]		0.52011	0.629[−5]	0.5211277	0.205[−5]
[57]		0.51901	0.739[−6]	0.51985	0.161[−5]
Present	$_2(0,1)_6^0$	0.513950	0.382[−5]	0.514540	0.12[−5]
[16]		0.513944	0.381[−5]		
Present	$_2(0,1)_7^0$	0.510242	0.26[−5]		
Present	$_2(0,1)_8^0$	0.507836	0.17[−5]		
Present	$_2(-1,0)_4^0$	0.529292	0.121[−7]	0.529312	0.7[−10]
[22]		0.529292995	0.13[−7]		
[16]		0.52928885	0.125[−7]	0.52930856	0.732[−10]
[57]		0.52900	0.302[−7]	0.52793	0.127[−7]
Present	$_2(-1,0)_5^0$	0.519000		0.519016	
[57]		0.51251		0.51313	
Present	$_2(-1,0)_6^0$	0.513310		0.513322	

too large for higher members of the $_2(-1,0)_n^+$ series of $^1S^e$ in comparison with other theoretical results. The widths of Macías and Riera [56] for $^{1,3}S^e$ agree with ours except for $_2(1,0)_7^-$ and $_2(-1,0)_{6,7}^-$ $^3S^e$. We also find the resonance energies and widths of Macías *et al.* [57] are less in agreement with ours for higher members of the $^{1,3}D^e$ series. Examining the reduced widths, we think our results are reliable for these states. The quantum defects are estimated to be 0.67 and 0.26

TABLE V. Comparison of the present results ($^1S^e$, $^3P^o$, and $^{1,3}D^e$) with the experiments observing the electrons ejected in the process of autoinization. [57.84(4) means 57.84 ± 0.04, etc.]

State	Hicks and Comer [58]	Gelebart *et al.* [59]	Present
		E_r (in eV)	
$_2(1,0)_2^+$ $^1S^e$	57.84(4)	57.80(3)	57.839
$_2(1,0)_3^+$ $^1S^e$	62.96(3)		62.953
$_2(1,0)_4^+$ $^1S^e$	64.20(3)		64.178
$_2(1,0)_5^+$ $^1S^e$	64.69(4)		64.673
$_2(-1,0)_2^+$ $^1S^e$	62.08(4)	62.12(3)	62.095
$_2(1,0)_3^+$ $^3P^o$	63.09(3)	63.08(3)	63.095
$_2(1,0)_4^+$ $^3P^o$	64.25(3)		64.234
$_2(1,0)_5^+$ $^3P^o$	64.71(4)		64.700
$_2(1,0)_2^+$ $^1D^e$	59.91(3)	59.89(3)	59.908
$_2(1,0)_3^+$ $^1D^e$	63.52(3)		63.517
$_2(1,0)_4^+$ $^1D^e$	64.41(3)		64.400
		Γ (in eV)	
$_2(1,0)_2^+$ $^1S^e$	0.138(15)	0.138(15)	0.123
$_2(1,0)_3^+$ $^1S^e$	0.041(10)		0.0373
$_2(1,0)_3^+$ $^3P^o$	< 0.015	$\simeq 0.01$	0.00814
$_2(1,0)_2^+$ $^1D^e$	0.072(18)		0.064

(0.81 and 0.06), respectively, for $_2(1,0)_n^+$ and $_2(-1,0)_n^+$ series of $^1S^e$ [$_2(1,0)_n^-$ and $_2(-1,0)_n^-$ series of $^3S^e$] and 0.31, 0.013, and -0.13 (0.53, 0.136, -0.13), respectively, for $_2(1,0)_n^+$, $_2(0,1)_n^0$, and $_2(-1,0)_n^0$ series of $^1D^e$ [$_2(1,0)_n^-$, $_2(0,1)_n^0$, and $_2(-1,0)_n^0$ series of $^3D^e$].

In Table V, our results of the resonance energies and widths for $^1S^e$, $^3P^o$, and $^1D^e$ are compared with experimental results [58,59]. The experimental resonance positions are renormalized with respect to the lowest $^1P^o$ resonance (60.15 eV). Our present results are converted to eV by using Ry=13.603 83 eV and I_∞ (the double-ionization threshold) =79.003 eV. Our results are in very good agreement with the experimental results. It shows that our results for $_2(-1,0)_{2,3}^+$ of $^1S^e$ and $_2(1,0)_{2,3}^+$ of $^1D^e$ are not necessarily worse than those of Ho [21], Ho and Bhatia [22], and Lindroth [24]. In conclusion, the saddle-point complex-rotation method with B-spline functions has been used successfully to calculate the doubly excited resonant states ($^{1,3}S^e$, $^{1,3}P^o$, and $^{1,3}D^e$) of He below the $n=2$ threshold. We obtain accurate results not only for the lower states but also for the higher states, in comparing with the experimental and other theoretical results and judging from the constancy of reduced widths. It is also impressive that our results agree very well with the most accurate previous results given by Hylleraas wave functions. In our calculations, the ranges of β and θ are generally so large that we can obtain stable resonance energies and widths easily. It is advantageous for us to calculate the small widths.

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