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Doubly excited $^1S^e$ resonance states of helium atoms below the N hydrogenic thresholds with $N \leq 6$

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New results for doubly excited $^1S^e$ autoionizing states of helium atoms converging on the $N=2$ to $N=6$ He^+ thresholds are calculated by use of a method of complex-coordinate rotation. Resonance parameters (both energy and width) obtained by using Hylleraas-type wave functions with 308 terms are compared with the recent close-coupling and hyperspherical-coordinate calculations.

We report new results for resonance parameters for some doubly excited $^1S^e$ states of He associated with the Nth hydrogenic thresholds, with $2 \leq N \leq 6$. The resonance parameters are calculated by using the method of complex coordinates with Hylleraas-type wave functions. We report these results so we can make an assessment on the accuracy of the recent calculations of the doubly excited He atoms.[1,2] There is, of course, continuous interest to investigate atomic resonance phenomena of two-electron systems including the recent theoretical studies of electronic motions for the doubly excited electrons,[3] and the underlying symmetries of two-electron Hamiltonians.[4] On the computational aspects to calculate resonance energy positions associated with high excitation thresholds by using the hyperspherical coordinates, Matsuzawa and coworkers[2] have calculated some doubly excited $^1S^e$ resonances for H^- and He with principal quantum numbers up to $N=6$. They have found that the accuracy of their He results below the $N=4$ threshold are within 3% of the accurate complex-coordinate calculations[5–7] (autoionization widths were not calculated in Ref. 2, however). The objectives of the present work are to report new complex-coordinate results for resonance parameters for He up to the $N=6$ He^+ threshold, and to assess the accuracy of the results in Ref. 2. The present results are also compared with those of the recent algebraic close-coupling calculations for resonances below the $N=2$ threshold.

Accurate *ab initio* calculations are also needed for investigations of the grandparent model[8] for doubly excited states. In such a model, the two electrons are treated as a single entity under the influence of the bare nucleus (the grandparent). The energy levels of the doubly excited intrashell states (the two electrons occupy the same shell) can be fitted to a Rydberg-like sequence in a screened six-dimensional Coulomb potential in hyperspherical coordinates converging to the two-electron breakup ionization limit. Due to the lack of experimental data for the highly excited states, the present accurate results associated with high excitation thresholds would help the verification of such a model.

The wave functions used in this work are of Hylleraas type,

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

where $(k+n+m)\leq\omega$, with ω a positive integer. Up to a total of $N=308$ terms ($\omega=13$) Hylleraas-type wave functions are used in this calculation.

The theoretical aspect of the complex rotation method has been discussed in previous publications[9] 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 in 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 recent review.[9] 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 positions and widths, are then deduced from conditions that a discrete complex eigenvalue was stabilized with respect to the nonlinear parameters in the wave function [Eq. (1)], and with respect to θ, the so-called rotational angle of the complex transformation $r \rightarrow r\exp(i\theta)$. The use of this method has been very successful for calculation of resonances for $L=0$ and $L=1$ states of two-electron systems below the $N=4$ hydrogenic thresholds.[5–7] We now extend this method to calculate resonances up to the region below the $N=6$ threshold.

It should also be noted that the advantage of using the method of complex-coordinate 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. Calculation of resonance positions and total width for a many-channel resonance is as straightforward as that for an elastic resonance.

Table I shows results of doubly excited resonances of He and associated with $N=2$, 3, 4, 5, and 6 He^+ thresholds. The $N=5$ and 6 doubly excited states results are reported for the first time, as well as some of the higher-lying states associated with the $N=2$, 3, and 4 thresholds. Each state in Table I is classified by a set of quantum numbers (L, S, π, K, T, N, and n), where L and S are the total angular momentum and spin, respectively, and π the parity. The quantum number N denotes the Nth threshold of the He^+ ion below which resonances lie, and n has the usual meaning for a given Rydberg series. The condition of n is $n \geq N$. Quantum numbers K and T are approximately good quantum numbers, and are the results of investigations by use of a group theoretical method.[10] They are obtained by diagonalizing the square of $|\mathbf{A}_1-\mathbf{A}_2|$, where $\mathbf{A}_1$ and $\mathbf{A}_2$ are the Runge-Lentz vectors for electrons 1 and 2, respectively. The physical meanings for K and T can be described briefly as follows, K is related to $-\langle\cos\theta_{12}\rangle$, where θ_{12} is the angle between the position vectors of the two electrons. The larger the positive K, the value of $-\langle\cos\theta_{12}\rangle$ is closer to unity. The two electrons in this situation are located near the opposite sides of the nucleus. The quantum number T describes the orientations between the orbitals of the two electrons. For example, a state with $T=0$ implies that the two electrons are moving on the same plane.

In the table we also compare with other recent theoretical results. For the resonance below the $N=2$ threshold,[11] we compare with the 14-state close-coupling calculation.[1] The agreements for the $K=+1$ states are generally good. But for the $K=-1$ states we notice that some differences[12] do exist. It is believed that the present results are quite accurate. The differences for the $K=-1$ states can be understood as follows: according to the tri-atomic-molecular-model of the doubly excited states in He,

TABLE I. Doubly excited ${}^1S^e$ resonant states in helium below the $N=6$ hydrogenic threshold. Both energy positions and widths are expressed in rydbergs.

				Present work		Other calculations[a]	
K	T	N	n	$-E_r$	$\Gamma/2$	$-E_r$	$\Gamma/2$
1	0	2	2	1.555 736	0.004 53	1.555 6	0.004 58
1	0	2	3	1.179 79	0.001 35	1.179 73	0.001 38
1	0	2	4	1.089 75	0.000 45	1.089 74	0.000 49
−1	0	2	2	1.243 855	0.000 215 6	1.241 032	0.000 231
−1	0	2	3	1.096 171	0.000 078	1.095 753	0.000 082 7
−1	0	2	4	1.055 42	0.000 05	1.055 25	0.000 052
2	0	3	3	0.707 074	0.003 004	0.705 80	
2	0	3	4	0.562 150	0.001 50	0.557 59	
2	0	3	5	0.511 90	0.000 83		
0	0	3	3	0.634 91	0.006 67	0.614 37	
0	0	3	4	0.526 77	0.002 4	0.515 02	
0	0	3	5	0.493 51	0.001 14		
−2	0	3	3	0.514 743 2	0.000 020 9	0.510 28	
3	0	4	4	0.401 99	0.001 95	0.402 43	
3	0	4	5	0.331 45	0.001 20	0.330 38	
3	0	4	6	0.301 6	0.000 8		
1	0	4	4	0.375 69	0.004 91	0.366 54	
1	0	4	5	0.313 85	0.002 75	0.306 24	
1	0	4	6	0.290 98	0.001 54		
−1	0	4	4	0.336 527	0.002 17	0.326 55	
−1	0	4	5	0.294 55	0.000 83	0.289 19	
−3	0	4	4	0.282 15	0.000 04		
4	0	5	5	0.258 83	0.001 378	0.260 55	
4	0	5	6	0.219 28	0.001 01	0.221 01	
4	0	5	7	0.200 4	0.000 68		
2	0	5	5	0.246 59	0.002 69	0.242 05	
2	0	5	6	0.210 03	0.001 82	0.205 18	
0	0	5	5	0.230 45	0.003 60	0.223 50	
0	0	5	6	0.199 28	0.001 98	0.194 12	
−2	0	5	5	0.204 75	0.001 02		
5	0	6	6	0.180 5	0.001 0	0.181 68	
5	0	6	7	0.156 1	0.000 7	0.157 23	
3	0	6	6	0.173 77	0.001 8	0.171 43	
3	0	6	7	0.150 8	0.001 3	0.147 87	
1	0	6	6	0.165 15	0.002 33		
1	0	6	7	0.143 9	0.001 8		
−1	0	6	6	0.154 44	0.001 4		

[a]The $N=2$ results are from the algebraic close-coupling calculations in Ref. 1. The $N=3$–6 results are from the hyperspherical calculations in Ref. 2.

$K=-1$ and $T=0$ states correspond to the case when the two electrons (on average) are located on the same side of the nucleus and are moving on the same plane. The use of Hylleraas-type wave functions in which the r_{12} coordinates are explicitly used, apparently, is able to incorporate effectively the correlation effects between the two electrons in the region where r_{12} is small. The differences between the complex-coordinate and close-coupling results suggests that it would be of interest to extend the 14-state close coupling for such $k=-1$ and $T=0$ states.

For the resonances associated with the $N=3$, 4, 5, and 6 thresholds, we compare resonance positions with the recent hyperspherical-coordinates calculations.[2] In Ref. 2, however, no resonance widths were calculated. It is seen that the results reported in Ref. 2 are accurate to within 4%. It is also noted that the results in Ref. 2 are less accurate for the states with negative K values. This again reflects the difficulty to incorporate the full correlation effects when the two electrons are located at the same side of the nucleus. The use of r_{12} terms explicitly is an effective way to incorporate such effects for the regions when r_{12} is small.

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[12]The differences in resonance energy are less than 0.3%.