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Resonance positions and widths of doubly excited N^{5+} ions associated with $N=3$, 4, and 5 N^{6+} thresholds

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Some doubly excited autoionizing states of heliumlike nitrogen ions converging on the $N=3$, $N=4$, and $N=5$ hydrogenic thresholds are calculated by a method of complex-coordinate rotation. Hylleraas-type wave functions are used for $L=0$ and $L=1$ resonances, and products of Slater-orbital-type wave functions with expansion lengths up to 323 terms for $L \geq 2$. Results can be used for experimental references in the recently identified doubly excited autoionization states of N^{5+} ions in double-electron charge-transfer collision experiments between N^{7+} ions and helium atoms.

I. INTRODUCTION

Recently, there has been considerable interest in experimental investigations of electron-transfer collisions between a highly stripped ion and a two-electron helium atom. In such processes, although one-electron captures would dominate the electron-transfer collisions, it was found that two-electron capture processes are also important. For example, the two-electron capture into doubly excited autoionization states of N^{5+} ions were observed in collisions of N^{7+} ions with He atoms[1-3] and with H_2 molecules.[2] In the scattering experiments between He and N^{7+} ions,[1,3] the doubly excited states were observed in energy gain spectra of N^{6+} ions. In the collision experiment between H_2 and N^{7+} ions, some states were identified in ejected electron spectra. Similarly, there is also interest in production of doubly excited autoionization states of O^{6+} ions below the $N=3$ and $N=4$ thresholds in collisions of O^{8+} ions with He atoms.[4] To interpret and identify satellite lines of such highly stripped ions, which in turn would play an important role in spectroscopic diagnostics of high-temperature astrophysical and laboratory plasmas, knowledge of the doubly excited autoionizing states are needed.

This work presents a theoretical study of doubly excited resonances of N^{5+} ions. The method of complex-coordinate rotation (for example, see Ref. 5 and references therein) is used for the present investigation. The advantage of using this method is that resonance parameters (both resonance positions and total widths) 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 opened. Calculation of resonance position and total width for a many-channel resonance is as straightforward as that for an elastic resonance. The use of this method has been very successful for calculations of resonances for $L=0$ and $L=1$ resonant states of two-electron atoms. In a series of extensive papers, resonance parameters have been published for $N=2$ (Ref. 6), $N=3$ (Ref. 7), and $N=4$ (Ref. 8) resonances for two-electron systems with $Z=2$–10. In these papers several lower-lying doubly excited $^1S^e$, $^1P^o$, and $^3P^o$ resonances were calculated. Some of the theoretical resonances have been identified and were found to have good agreements with experimental observations.[1,2] We now extend calculations to $L \geq 2$ states. This work concentrates on doubly excited states of N^{5+} ions because of the recent experimental interest.

Doubly excited resonances may also have strong effects on collision strengths (related to excitation cross sections) in electron-ion scattering. Collision strengths in electron-ion scattering are important for investigations of collisional equilibrium problems in diagnostics of laboratory and astrophysics plasmas. Hayes and Seaton[9] examined resonance effects on collision strengths in e-O^{7+} scattering in a close-coupling calculation. Some so-called $3l3l'$ resonances were shown graphically (numerical values of the doubly excited $N=3$ resonances were not published). The algebraic variational close-coupling method has been used to calculate some doubly excited resonances below the $N=3$ hydrogenic thresholds for C^{4+} and O^{6+} by Abu-Salbi and Callaway,[10] and for N^{7+} by Oza.[11] Here we report results for some lower-lying resonances associated with $N=3$, 4, and 5 hydrogenic N^{6+} thresholds.

II. WAVE FUNCTIONS

The wave functions used in this work are of Hylleraas type for $L=0$ and $L=1$ resonances,

$$\psi = \sum C_{klm} \exp[-\alpha(r_1+r_2)] r_{12}^k \times [r_1^l r_2^{m+L} Y_{00}(1) Y_{L0}(2) + r_2^l r_1^{m+L} Y_{00}(2) Y_{L0}(1)] , \tag{1}$$

where $(k+l+m) \leq \omega$, with ω a positive integer, and products of Slater orbitals for resonances with $L \geq 2$:

$$\psi = A \sum_{la,lb} \sum_{i,j} C_{a_i,b_j} \eta_{a_i}(r_1) \eta_{b_j}(r_2) \times Y_{la,lb}^{LM}(1,2) S(\sigma_1,\sigma_2) , \tag{2}$$

where

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

TABLE I. Individual Slater-orbital-type wave functions used.

	$^1D^e$	$^3D^e$	$^1F^o$	$^3F^o$	$^1G^e$	$^3G^e$	
s	9	9	9	9	9	10	
p	8	8	8	8	8	9	
d	7	7	7	7	7	7	
f	6	6	6	6	6	6	
g	4	5	5	5	5	5	
h	3	4	3	3	4	4	
i	2	3	2	2	3	3	
k	2	2	1	1	1	2	
l	1				1	1	
m							
Total	281	277	283	283	320	319	
	$^1H^o$	$^3H^o$	$^1I^e$	$^3I^e$	$^1K^o$	$^3K^o$	$^1L^e$
s	9	9	10	10	10	10	10
p	8	8	9	9	9	9	9
d	7	7	8	8	8	8	8
f	6	6	7	7	7	7	7
g	5	5	6	6	6	6	6
h	4	4	4	5	5	5	5
i	3	3	3	3	3	3	4
k	2	2	2	1	2	2	
l	1	1	1		1	1	
m	1	1			1	1	
Total	301	301	310	270	270	270	290
	$^3P^e$	$^1D^o$	$^3D^o$	$^1F^e$	$^3F^e$	$^1G^o$	$^3G^o$
p	10	10	10	9	9	9	9
d	9	9	9	8	8	8	8
f	8	8	8	7	7	7	7
g	7	7	6	6	6	6	6
h	6	6	5	5	5	5	5
i	5	4	4	4	3	3	3
k	4		3	3	2	2	2
l	3		2	2	1	1	1
m	2		1	1			
n	1						
Total	220	284	280	280	287	283	283
	$^1H^e$	$^3H^e$	$^1I^o$	$^3I^o$	$^3K^e$		
p	9	9	9	9	9		
d	8	8	8	8	8		
f	7	7	7	7	7		
g	6	6	6	6	6		
h	5	5	5	5	5		
i	4	4	4	4	4		
k	3	3	3	3	3		
l	2	2	2	2	2		
m					1		
Total	296	323	280	280	261		

In Eq. (2), A is the antisymmetrizing operator, S is a two-particle spin eigenfunction, Y is a two-particle spherical harmonic, and the η are individual Slater orbitals. It has been suggested that use of Slater orbitals to calculate resonances of high angular momenta and associated with high excitation thresholds can produce accurate results. This is supported by the hydrogen negative ion results that the resonance parameters for some $L \geq 2$ states agree well with an extensive 18-state close-coupling calculation.[12] Also, good agreements have been found between a

TABLE II. Doubly excited resonances of N^{5+} ions associated with $N=3$ N^{6+} threshold. Resonance energies and widths are expressed in Rydbergs.

$^{2s+1}L^{\pi}$	$-E_r$	Γ	K	T	N	n
		$\pi=(-1)^L$				
$^1S^e$	10.2159	0.009 98	2	0	3	3
$^1S^e$	9.8560	0.0436	0	0	3	3
$^1S^e$	9.208 40	0.000 536	−2	0	3	3
$^1P^o$	10.042 85	0.0295	1	1	3	3
$^1P^o$	9.4735	0.0074	−1	1	3	3
$^3P^o$	10.1917	0.007 78	2	0	3	3
$^3P^o$	9.826 48	0.002 74	0	0	3	3
$^1D^e$	10.1220	0.0129	2	0	3	3
$^1D^e$	9.8773	0.0234	0	2	3	3
$^1D^e$	9.5583	0.0070	0	0	3	3
$^3D^e$	9.9683	0.0016	1	1	3	3
$^1F^o$	9.7025	0.0250	1	1	3	3
$^3F^o$[a]	10.0165		2	0	3	3
$^1G^e$	9.7275	0.050	2	0	3	3
		$\pi=(-1)^{L+1}$				
$^3P^e$	10.066	0.005	1	1	3	3
$^3P^e$[a]	9.6717		−1	1	3	3
$^1D^o$	10.0080	0.0006	1	1	3	3
$^3D^o$	9.889 12	0.0082	0	2	3	3
$^3F^e$	9.8411	0.0083	1	1	3	3

[a] The widths of these states are extremely narrow.

TABLE III. Doubly excited resonances of N^{5+} ions associated with $N=4$ N^{6+} threshold. Resonance energies and widths are expressed in Rydbergs.

$^{2s+1}L^{\pi}$	$-E_r$	Γ	K	T	N	n
		$\pi=(-1)^L$				
$^1S^e$	5.765	0.006	3	0	4	4
$^1S^e$	5.6335	0.029	1	0	4	4
$^1S^e$	5.432	0.044	−1	0	4	4
$^1S^e$	5.082 68	0.0003	−3	0	4	4
$^1P^o$	5.7021	0.0162	2	1	4	4
$^1P^o$	5.531	0.0480	0	1	4	4
$^1P^o$	5.2162	0.0056	−2	1	4	4
$^3P^o$	5.7570	0.0052	3	0	4	4
$^3P^o$	5.6251	0.0158	1	0	4	4
$^3P^o$	5.422 45	0.0036	−1	0	4	4
$^1D^e$	5.7388	0.0078	3	0	4	4
$^1D^e$	5.6380	0.0200	1	2	4	4
$^1D^e$	5.5865	0.0236	1	0	4	4
$^1D^e$	5.4547	0.0250	−1	2	4	4
$^1D^e$	5.2732	0.0060	−1	0	4	4
$^3D^e$	5.6815	0.0108	2	1	4	4
$^3D^e$	5.494 25	0.0040	0	1	4	4
$^1F^o$	5.6362	0.0175	2	1	4	4
$^1F^o$	5.5683	0.0240	0	3	4	4
$^1F^o$	5.3435	0.0190	0	1	4	4
$^3F^o$	5.7105	0.0066	3	0	4	4
$^3F^o$	5.6099	0.0029	1	2	4	4
$^3F^o$	5.5333	0.0002	1	0	4	4
$^1G^e$	5.6597	0.0115	3	0	4	4
$^1G^e$	5.5225	0.034	1	2	4	4
$^1G^e$	5.3807	0.030	1	0	4	4
$^3G^e$	5.5788	0.0008	2	1	4	4
$^1H^o$	5.4313	0.049	2	1	4	4
$^3H^o$	5.600 05	0.002	3	0	4	4
$^1I^e$	5.442	0.075	3	0	4	4

TABLE III. (*Continued*).

$^{2s+1}L^{\pi}$	$-E_r$	Γ	K	T	N	n
		$\pi=(-1)^{L+1}$				
$^3P^e$	5.7050	0.008	2	1	4	4
$^3P^e$	5.5556	0.015	0	1	4	4
$^3P^e$[a]	5.3491		−2	1	4	4
$^1D^o$	5.6897	0.0070	2	1	4	4
$^1D^o$	5.5344	0.0011	0	1	4	4
$^3D^o$	5.6391	0.0154	1	2	4	4
$^3D^o$	5.4584	0.0065	−1	2	4	4
$^1F^e$	5.6082	0.0020	1	2	4	4
$^3F^e$	5.6569	0.0054	2	1	4	4
$^3F^e$	5.5725	0.0136	0	3	4	4
$^3F^e$	5.453 95	0.0058	0	1	4	4
$^1G^o$	5.608 04	0.000 42	2	1	4	4
$^3G^o$	5.524 74	0.0149	1	2	4	4
$^3H^e$	5.5068	0.021	2	1	4	4

[a] The widths of these states are extremely narrow.

TABLE IV. Doubly excited resonances of N^{5+} ions associated with $N=5$ N^{6+} threshold. Resonance energies and widths are expressed in Rydbergs.

$^{2s+1}L^{\pi}$	$-E_r$	Γ	K	T	N	n
		$\pi=(-1)^{L}$				
$^1S^e$	3.696	0.008	4	0	5	5
$^1S^e$	3.6355	0.017	2	0	5	5
$^1S^e$	3.550	0.040	0	0	5	5
$^1S^e$	3.425	0.040	−2	0	5	5
$^1S^e$	3.208 86	0.000 21	−4	0	5	5
$^1P^o$	3.666 9	0.0100	3	1	5	5
$^1P^o$	3.594	0.029	1	1	5	5
$^1P^o$	3.487	0.0500	−1	1	5	5
$^1P^o$	3.288	0.0050	−3	1	5	5
$^3P^o$	3.692 75	0.004 20	4	0	5	5
$^3P^o$	3.6315	0.0130	2	0	5	5
$^3P^o$	3.5453	0.020	0	0	5	5
$^3P^o$	3.4194	0.0038	−2	0	5	5
$^1D^e$	3.6860	0.0052	4	0	5	5
$^1D^e$	3.6363	0.0146	2	2	5	5
$^1D^e$	3.6205	0.0160	2	0	5	5
$^1D^e$	3.554	0.024	0	2	5	5
$^1D^e$	3.522	0.034	0	0	5	5
$^1D^e$	3.4437	0.023	−2	2	5	5
$^1D^e$	3.325	0.0040	−2	0	5	5
$^3D^e$	3.6590	0.0084	3	1	5	5
$^3D^e$	3.5800	0.0168	1	1	5	5
$^3D^e$	3.4609	0.0044	−1	1	5	5
$^1F^o$	3.6443	0.0124	3	1	5	5
$^1F^o$	3.6028	0.0190	1	3	5	5
$^1F^o$	3.5498	0.0250	1	1	5	5
$^1F^o$	3.5115	0.0260	−1	3	5	5
$^1F^o$	3.366	0.0150	−1	1	5	5
$^3F^o$	3.6755	0.0056	4	0	5	5
$^3F^o$	3.6248	0.0078	2	2	5	5
$^3F^o$	3.6023	0.011	2	0	5	5
$^3F^o$	3.5417	0.0034	0	2	5	5
$^3F^o$	3.4876	0.0013	0	0	5	5
$^1G^e$	3.6587	0.0074	4	0	5	5
$^1G^e$	3.6040	0.0096	2	2	5	5

TABLE IV. (*Continued.*)

$^{2s+1}L^{\pi}$	$-E_r$	Γ	K	T	N	n
$\pi=(-1)^L$						
$^1G^e$	3.5749	0.0066	2	0	5	5
$^1G^e$	3.5668	0.0272	0	4	5	5
$^1G^e$	3.492	0.030	0	2	5	5
$^1G^e$	3.393	0.022	0	0	5	5
$^3G^e$	3.6245	0.0080	3	1	5	5
$^3G^e$	3.5875	0.0038	1	3	5	5
$^3G^e$	3.5148	0.0012	1	1	5	5
$^1H^o$	3.591	0.0150	3	1	5	5
$^1H^o$	3.543	0.0290	1	3	5	5
$^1H^o$	3.4225	0.037	1	1	5	5
$^3H^o$	3.6374	0.0055	4	0	5	5
$^3H^o$	3.5775	0.0030	2	2	5	5
$^3H^o$	3.5348	0.0009	2	0	5	5
$^1I^e$	3.6032	0.0114	4	0	5	5
$^1I^e$	3.521	0.038	2	2	5	5
$^1I^e$	3.442	0.050	2	0	5	5
$^3I^e$	3.5552	0.0028	3	1	5	5
$^1K^o$	3.466	0.060	3	1	5	5
$^3K^o$	3.5669	0.0062	4	0	5	5
$^1L^e$	3.466	0.09	4	0	5	5
$\pi=(-1)^{L+1}$						
$^3P^e$	3.666	0.016	3	1	5	5
$^3P^e$	3.5965	0.018	1	1	5	5
$^3P^e$	3.5015	0.015	−1	1	5	5
$^3P^e$[a]	3.379		−3	1	5	5
$^1D^o$	3.6615	0.0070	3	1	5	5
$^1D^o$	3.590	0.0096	1	1	5	5
$^1D^o$	3.4944	0.0014	−1	1	5	5
$^3D^o$	3.6365	0.0114	2	2	5	5
$^3D^o$	3.5545	0.0192	0	2	5	5
$^3D^o$	3.4425	0.0058	−2	2	5	5
$^1F^e$	3.6242	0.0076	2	2	5	5
$^1F^e$	3.5378	0.0025	0	2	5	5
$^3F^e$	3.6497	0.0059	3	1	5	5
$^3F^e$	3.6035	0.0150	1	3	5	5
$^3F^e$	3.5725	0.0059	1	1	5	5
$^3F^e$	3.5145	0.0134	−1	3	5	5
$^3F^e$	3.4486	0.0040	−1	1	5	5
$^1G^o$	3.6328	0.0044	3	1	5	5
$^1G^o$	3.5880	0.0032	1	3	5	5
$^1G^o$	3.545 97	0.0003	1	1	5	5
$^3G^o$	3.6035	0.0060	2	2	5	5
$^3G^o$	3.571	0.0156	0	4	5	5
$^3G^o$	3.4870	0.011	0	2	5	5
$^1H^e$	3.5748	0.0020	2	2	5	5
$^3H^e$	3.6081	0.0034	3	1	5	5
$^3H^e$	3.5450	0.0200	1	3	5	5
$^3H^e$	3.488	0.0150	1	1	5	5
$^1I^o$	3.5756	0.0024	3	1	5	5
$^3I^o$	3.518	0.024	2	2	5	5
$^3K^e$	3.508	0.035	3	1	5	5

[a] The widths of these states are extremely narrow.

14-state close-coupling calculation[10] and unpublished complex-coordinate results for $Z=6$ resonances below the $N=3$ threshold.

In this work, quite extensive basis sets are used in the wave functions. The detailed information about various orbitals used in the wave functions are listed in Table I. For example, for the $^1D^e$ resonances we use orbitals of 9 *s* types, 8 *p* types, 7 *d*, 6 *f*, 4 *g*, 3 *h*, 2 *i*, 2 *k*, and 1 *l* type. These orbitals would couple to a total of 281 terms for the $^1D^e$ states. The actual numbers of terms for other

TABLE V. Comparisons between complex-coordinate and close-coupling results for resonances below the $N=3$ N^{6+} threshold.

Complex coordinates			Close-coupling (Ref. 11)	
$-E_r$ (Ry)	Γ (Ry)		$-E_r$ (Ry)	Γ (Ry)
		$^1S^e$		
10.2159	0.009 94		10.2159	0.0102
9.8560	0.040 36		9.855	0.0406
9.208 40	0.000 536			
8.003 87	0.006 44		8.004	0.0064
7.775 92	0.0214		7.770	0.0218
7.481 36	0.000 19			
7.0503	0.0036		7.050	0.0030
6.9280	0.0102		6.924	0.0106
6.7802	0.000 082			
		$^3S^e$		
8.067 81	0.000 098		8.0678	0.000 106
7.915 78	0.000 34		7.9152	0.000 36
7.6597				
7.073 77	0.000 16			
6.9822				
6.8531				
		$^1P^o$		
10.042 85	0.0295		10.0427	0.0296
9.4735	0.0074		9.462	0.0084
8.0560	0.0002		8.0560	0.000 116
7.8915	0.0156		7.890	0.0156
7.8876	0.0013		7.887	0.001 02
7.5908			7.582	0.0040
7.547				
7.069				
6.991	0.010		6.989	0.0082
6.970				
6.837				
6.815			6.805	0.000 15
		$^3P^o$		
10.1917	0.007 78		10.1918	0.0076
9.826 48	0.002 74		9.825	0.0032
7.995 07	0.000 266			
7.990 62	0.0042		7.9906	0.0043
7.7868	0.000 192		7.7845	0.000 52
7.776 38	0.000 84			
7.6071	0.000 02			
7.046				
7.0303			7.0287	0.000 22
6.9318				
6.9136				
6.8420				
		$^1D^e$		
10.1220	0.0129		10.1219	0.0131
9.8773	0.0234		9.8765	0.0240
9.5583	0.0070		9.551	0.0086
7.954 15	0.0001		7.953 97	0.000 11
7.9515	0.0070		7.951	0.0074
7.7998	0.0130		7.798	0.0132
7.6795	0.0010			
7.5862	0.0006			
7.0244	0.003		7.0234	0.0033
7.0075			7.0066	0.000 11

TABLE V. (*Continued.*)

Complex coordinates		Close-coupling (Ref. 11)	
$-E_r$ (Ry)	Γ (Ry)	$-E_r$ (Ry)	Γ (Ry)
$^1D^e$			
6.940 15	0.0072	6.939	0.0063
6.885			
6.852 37			
6.832 48			
$^3D^e$			
9.9683	0.0016	9.9681	0.001 94
8.0292	0.000 26		
7.914 15	0.000 30		
7.8618	0.0010	7.8616	0.001 06
7.8101			
7.677 75			
7.0512	0.0002	7.0511	0.000 14
6.983 30			
6.9735	0.000 24		
6.9315			
6.874			
6.8525			
$^1F^o$			
9.7025	0.025	9.7013	0.0261
7.978 23	0.000 30		
7.8134	0.0026	7.813	0.0028
7.7075	0.0112	7.705	0.0125
7.5963			
7.0225			
6.9468	0.0012		
6.8954	0.0054	6.894	0.0060
6.8620			
6.840			
$^3F^o$			
10.0165		10.0162	0.000 08
7.902 58			
7.871 05	0.000 10		
7.8300	0.000 70	7.828	0.000 63
7.7292	0.000 20	7.726	0.000 33
6.9985			
6.9620			
6.9468	0.0004		
6.8995		6.8986	0.000 16
6.8633			
$^1G^e$			
9.7275	0.050	9.720	0.04
7.793	0.020		
7.6396	0.0052		
6.9495	0.0080		
6.9165			
6.8695			
6.8585			
$^3G^e$			
7.879 35			
7.795			
6.9712			
6.9324			
6.9153			
6.8701			

TABLE V. (*Continued*).

Complex coordinates		Close-coupling (Ref. 11)	
$-E_r$ (Ry)	Γ (Ry)	$-E_r$ (Ry)	Γ (Ry)
	$^1H^o$		
7.6350	0.0040		
6.8845			
6.8605	0.0020		
	$^3H^o$		
7.8358	0.0020		
6.9508	0.0008		
6.8875			

resonant states differ slightly depending on different angular momenta and parities. But in any case, no less than 220 terms are used in the present calculation. The total numbers of terms for different angular momenta and parities are also shown in Table I. By using such extensive basis sets, components of open channels below various thresholds are included in the wave functions either explicitly or implicitly. This is the reason why we are able to calculate the total widths for such resonances.

III. CALCULATIONS AND RESULTS

The theoretical aspect of the complex rotation method is discussed in previous publications (see Ref. 5, for example) 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 rotation calculations will then be carried out. The use of the stabilization method as a first step for the complex rotation method has been demonstrated in previous calculations.[5] Once the stabilized wave functions for a particular resonance are obtained, a straightforward complex-rotation method is then applied, and the so-called "rotational paths" are examined. The final resonance parameters, both resonance positions and total widths, are deduced from conditions that the discrete complex eigenvalue is stabilized with respect to the nonlinear parameters in the wave functions [Eqs. (1) and (2)] and with respect to θ, the so-called rotational angle of the complex transformation $r \rightarrow r\exp(i\theta)$.

Results for doubly excited resonances associated with the $N=3$, $N=4$, and $N=5$ hydrogenic thresholds are reported in Tables II, III, and IV, respectively. Both states with parities $(-1)^L$ and $(-1)^{L+1}$ are calculated. Each state in Tables II–IV is classified by a set of quantum numbers (L,S,π,K,T,N,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 N^{6+} ions below which resonances lie, and n has the usual meaning for a given Rydberg series. The condition of n is $n \geq N$. In Tables II–IV, we only show the lowest member for a given Rydberg series. In other words all the resonant states reported in Tables II–IV have values of $n=N$. States in which both electrons occupy the same shell are called the intrashell resonant states. The quantum numbers K and T are approximately good quantum numbers, and are the results of investigations by Herrick and Sinanoglu[13] using a group-theoretical method. The quantum numbers are obtained by diagonalizing the square of $|\mathbf{A}_1-\mathbf{A}_2|$, where $\mathbf{A}_1$ and $\mathbf{A}_2$ are the Runge-Lenz vectors for electron 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 closer the value of $\langle\cos\theta_{12}\rangle$ is 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. The quantum numbers K and T hence describe the angular correlations between the two doubly excited electrons.

Hyperspherical coordinates have also been used to investigate classifications of doubly excited resonances in two-electron systems.[14] The angular correlation quantum numbers K and T discussed in Ref. 14 are similar to those of Ref. 13. In addition, a parameter "A" is used to describe radial correlations in Ref. 14, and A is related to other quantum numbers by[15]

$$A=\begin{cases}\pi(-1)^{S+N-K-1} & \text{for all } K>L-N\,,\\ 0 & \text{otherwise}\,.\end{cases} \tag{3}$$

There are very limited theoretical calculations for doubly excited states of N^{5+} ions in the literature. These include the calculation carried out by Bachau,[16] who use a truncated diagonalization method to calculate some $N=3$ and $N=4$ resonances, and recently by Oza,[11] who used a 14-state close-coupling approximation to calculate resonances below the $N=3$ threshold. The calculation by Bachau,[16] however, is not as accurate as those reported here because of the extremely limited basis sets used (no more than 30) to represent the closed space part of the wave function. Also, the omission of Feshbach shifts between closed channels and open channels in his calculations is another source of error. The close-coupling calculation would provide results with accuracy close to the present complex-coordinate calculations. Comparison between the complex-coordinate and close-coupling results for states with parities of $(-1)^L$ is given in Table V. Agreements are, in general, quite good. For collision experiments[2] between the N^{7+} ions and He atoms, and between the N^{7+} ions and H_2 molecules, higher resonances for some series are of interest. Table V also shows higher

TABLE VI. Possible identification of experimental peaks (given in eV under the entry ΔE) for doubly excited $3ln'l$ states of N^{5+} ions autoionizing to the $N=2$ threshold of N^{6+} ions. Only states of parity $(-1)^L$ and of large widths are given.

										Experiment (Ref. 2)	
N	n'		$^1S^e(2,0)$	$^1S^e(0,0)$	$^1P^o(1,1)$	$^1D^e(2,0)$	$^1D^e(0,2)$	$^1F^o(1,0)$	$^1G^e(2,0)$	N^{7+}-He	N^{7+}-H_2
3	3	$-E$ (Ry)	10.2159	9.8560	10.042 85	10.122	9.8773	9.7025	9.7275		
		ΔE (eV)	27.68	32.45	30.03	28.95	32.28	34.66	34.32		
3	4	$-E$ (Ry)	8.003 87	7.775 92	7.8905	7.9515	7.7998	7.7075	7.793		
		ΔE (eV)	57.77	60.87	59.32	58.49	60.55	61.80	60.64	57.1,58.6,60.9	56.9,58.7,61.1
3	5	$-E$ (Ry)	7.050 30	6.9280	6.991	7.0244	6.940 15	6.8954	6.9495		
		ΔE (eV)	70.75	72.41	71.553	71.10	72.25	72.85	72.12	70.3–71.4	71.1

members of resonances below the $N=3$ threshold. Table VI shows some of the higher-lying resonances as compared with possible identifications in the two-electron capture experiments. These states are expressed in eV as they autoionize to the $N=2$ threshold of the N^{6+} ions. Here, we only show states of parity $(-1)^L$ and with large autoionization widths. Agreements between the present theoretical values and experimental peaks are quite good.

IV. SUMMARY AND DISCUSSIONS

In summary, we have carried out an extensive complex-coordinate calculation for the doubly excited resonances of N^{5+} ions associated with $N=3$, $N=4$, and $N=5$ N^{6+} thresholds. The resonance parameters as calculated by using the method of complex-coordinate rotation are quite accurate. The resonance positions and widths are useful for experimental investigations of double-electron capture processes in ion-atom scattering. On the theoretical side, the resonance parameters reported here are useful references for studies of electron correlation effects by use of the group-theoretical method and by use of hyperspherical coordinates. For example, the present results can be used to test the triatomic molecular model of the doubly excited states as proposed by Kellman and Herrick.[17] These authors observed that the model is less applicable for high-Z ions than for low-Z systems such as H^- and He. The present numerical results for $Z=7$ are therefore useful in studies of atomic correlations. Also, accurate results are needed for investigations of the grandparent model[18] 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 can be fitted to a Rydberg-like sequence in a screened six-dimensional Coulomb potential in hyperspherical coordinates, converging to the two-electron break-up ionization limit. Again, 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 a such a model. In addition, since we are able to provide values of widths for resonances, and the widths are inversely proportional to lifetimes of such doubly excited states, the present results may help in future studies to gain some insight of the symmetry of these two electron systems, and the underlying mechanism of atomic autoionization.

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