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Systematics of energies of doubly excited states of heliumlike ions

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The dependence of the energy levels of doubly excited states of heliumlike ions on the nuclear charge Z is studied. By expressing the energy levels of doubly excited states for intrashell states in the form of a double-Rydberg formula and for intershell states using the quantum-defect method, we expand the quantum defect in each formula in powers of $1/Z$. Using known energy levels for the low- Z ions, we extract parameters of the quantum defect which allow the calculation of accurate energy levels of other ions along the helium isoelectronic sequence.

I. INTRODUCTION

In recent years, experimental studies of collisions of multiply charged ions with atoms or molecules have established that doubly excited states are formed easily in these collisions. Doubly excited states are formed either through double-electron capture or through transfer excitation where a projectile electron is excited while one of the target electrons is captured to the excited states of the projectile. Energy-gain spectroscopy was used in the earlier studies where groups of doubly excited states of the form $nl n' l'$ with fixed n and n' were observed. In recent works, high-resolution Auger electron-spectroscopy techniques have been used.¹⁻⁵ To obtain information about the collision process, individual doubly excited states associated with these electron spectra have to be identified. Since many doubly excited states are usually grouped in a narrow energy range, accurate calculations of the energy levels of these states are often not available for most atoms. Therefore a procedure for the interpolation and extrapolation along the isoelectronic sequence using existing calculated energy levels is desirable.

Doubly excited states have been investigated extensively over the last two decades.⁶ The understanding of the properties of doubly excited states has resulted in a new classification scheme⁷ where the states are classified as ${}_n(K, T)_N^A 2S+1 L^\pi$. Such a classification scheme is used to replace the $nl n l'$ notations used in the independent-electron model. In the notation above, L , S , and π have their usual meanings; n and N denote the principal quantum numbers of the outer and the inner electrons, respectively. The quantum numbers K , T , and A replace l and l' ; they are used to characterize the correlations of the two electrons. The procedure for assigning the quantum numbers; K , T , and A are given in detail in Refs. 6 and 7.

Briefly, for each N , the range of K and T are determined by⁸

$$T = 0, 1, 2, \dots, \min(L, N-1),$$

$$K = N-1-T, N-3-T, \dots, -(N-1-T),$$

and A is governed by the rule⁷

$$A = \begin{cases} \pi(-1)^{S+T} & \text{if } K > L - N \\ 0 & \text{otherwise,} \end{cases}$$

where π is the parity of the state. We just emphasize here that A can take values of $+1$, -1 , and 0 only. For the $A = +1$ states the two electrons have in-phase radial stretch, while for $A = -1$ they have out-of-phase radial stretch. For $A = 0$ states, there are little radial correlation between the two electrons and they are similar to singly excited states. The quantum number K has to do with angular correlations. For states with positive K , the two electrons tend to stay on opposite sides of the nucleus while in states with negative K the two electrons tend to be on the same side of the nucleus. The quantum number T is the projection of the total orbital angular momentum along the bielectronic axis.^{6,9}

There are a number of advantages of classifying doubly excited states using this scheme: (1) If the energy levels are ordered according to the K , T , and A quantum numbers, the energy spectra of doubly excited states exhibit rotor structure,⁶⁻⁹ meaning that states with the same K , T , and A will have higher energies for increasing L if $A = +1$ or -1 . (2) The energy level of the lowest member of each $(K, T)^+$ or $(K, T)^-$ rotor series increases with decreasing K and for a given K , with decreasing T . These systematics allow us to identify the relative positions of doubly excited states for any heliumlike ions. (3) Experimental evidence indicates that only a certain class of doubly excited states is formed in collisions. Such

quasiselection rules are quite evident for photoabsorption,¹⁰ for electron-impact excitations,^{11,12} and to a less extent for electron capture in ion-atom collisions.¹³ In general, states with $A = +1$ and positive values of K are formed in the collision, while doubly excited states with other K , T , and A quantum numbers are rarely observed in experiments. (4) There is evidence that the Auger or autoionization widths of doubly excited states behave regularly in each rotor series.¹⁴

In this article, we address the question of fitting the energy levels of doubly excited states along the isoelectronic sequence where each state is classified according to the ${}_n(K, T)_N^A$ scheme. According to this classification scheme, states in the same Rydberg series differ only in the quantum number n . We propose the double-Rydberg formula for fitting energies of intrashell states and the quantum-defect method for intershell states. These methods are summarized in Secs. II, III, and IV below, together with test results and the fitted parameters. In Sec. V a brief discussion of the extrapolation of energies along the double-Rydberg series is given; a short summary in Sec. VI concludes the paper.

II. DOUBLE-RYDBERG FORMULA

The ${}_n(K, T)_N^A$ classification scheme allows us to organize the energy levels of doubly excited states. Based on the angular correlation properties of doubly excited states for positive K , Lin and Watanabe¹⁵ generalized the double Rydberg formula^{16,17} for the energy levels of intrashell states of heliumlike ions. In this formula, the energy level of an intrashell doubly excited state is given by¹⁵

$$E = -\frac{(Z - \sigma)^2}{N^2} \quad (\text{a.u.}), \quad (1)$$

where

$$\sigma = 2\{24 + (2/N^2)[7(N + K + 1)(N + K - 1) + 7T^2 - 6L(L + 1) + 12]\}^{-1/2} \quad (2)$$

is related to the expectation value of $\langle \cos\theta_{12} \rangle$, where θ_{12} is the angle of the two electrons with respect to the nucleus. This expectation value can be expressed in terms of quantum numbers K , T , and L if the doubly excited states are approximated by wave functions derived using the SO(4) theory.⁸ In deriving (1), the two electrons are assumed to stay at equal distances from the nucleus. This simple expression gives energy levels of intrashell doubly excited states (for positive K) accurate to the order of about 1%.¹⁵ To achieve higher accuracy, we generalize (1) to

$$E = -\frac{(Z - \sigma)^2}{(N - \delta)^2} \quad (\text{a.u.}), \quad (3)$$

where δ is the quantum defect. For each state, σ is given by Eq. (2) and δ is to be treated as a fitting parameter. To account for the variation of δ with respect to the nuclear charge Z , we expand

$$\delta = a/Z + b/Z^2 + c/Z^3. \quad (4)$$

In this way, each intrashell doubly excited states along

TABLE I. Comparison of fitted energy levels with calculations of Bachau for “3s²” or ${}_3(2,0)_3^+ {}^1S^e$ state for $Z = 5-10$. Two- and three-term $1/Z$ expansion of the quantum defect are used to fit the double-Rydberg formula. Entries are the binding energies in eV’s measured from the double-ionization threshold.

Z	Two term	Three term	Bachau ^a
5	69.11	69.11	69.09
6	101.03	101.03	101.00
7	138.99	139.00	138.99
8	183.00	183.00	182.99
9	233.06	233.06	233.05
10	289.16	289.17	289.16

^aFrom Ref. 21.

the isoelectronic sequence is parametrized by the constants a , b , and c . We note that σ is independent of Z .

Systematics of the energy levels of doubly excited states are not available. The more accurate variational calculations are usually limited to a few lower states and to low- Z ions.¹⁸⁻²¹ One of the more extensive energy-level tabulations is the large-scale configuration-interaction calculations done by Lipsky *et al.*¹⁸ where the energies of $2lnl'$ and $3lnl'$ states for $n < 7$ and $L < 4$ for $Z = 1-5$ have been calculated. We use their data for $Z = 2, 3$, and 4 to solve for the parameters a , b , and c . From these values of a , b , and c , the energies for other Z 's are easily calculated from Eq. (3).

In this paper, we use three parameters for fitting the quantum defects. In fact, for states with large K where the double-Rydberg formula is expected to work better, a two-parameter fitting is quite adequate. In Table I we show that the energies of the “3s²” or the ${}_3(2,0)_3^+ {}^1S^e$ state for $Z = 5-10$ calculated using a two- (with the $Z = 2$ and 3 data) or a three-parameter fitting of the quantum defect give practically the same results. The energy levels in this article are given in eV to the second decimal point. This is more accurate than the highest resolution one can achieve in Auger-electron spectroscopy to date. To the second digit, we note that the two-parameter results are identical to the more limited configuration-interaction (CI) calculations for the $Z = 5-10$ ions of Bachau.²¹ Similarly, in Table II we show the energy levels obtained from such a procedure for the “3s3p” or the ${}_3(1,1)_3^+ {}^1P^o$ state for $Z = 5-10$ and the comparison with the results of Bachau. The discrepancy is again quite small.

TABLE II. Comparison of energy levels for “3s3p” or ${}_3(1,1)_3^+ {}^1P^o$ state using a three-term fitting and the results of Bachau.

Z	Three term	Bachau ^a
5	67.50	67.48
6	99.04	99.02
7	136.64	136.62
8	180.27	180.24
9	229.96	229.92
10	285.68	285.65

^aFrom Ref. 21.

TABLE III. Energy levels of $2l/2l'$ states for $Z=5$ calculated using the fitting procedure as compared with the calculations of Lipsky *et al.* (Ref. 18).

State	Two term		Three term		Ref. 18
	Double-Rydberg formula	Quantum-defect theory	Double-Rydberg formula	Quantum-defect theory	
$(1,0)^+ 1S^e$	153.87	153.63	153.90	153.90	153.90
$3P^o$	152.55	152.30	152.60	152.61	152.60
$1D^e$	146.41	146.20	146.57	146.58	146.58
$(0,1)^+ 1P^o$	145.81	145.66	145.91	145.92	145.92
$3P^e$	148.46	148.32	148.58	148.59	148.58
$(-1,0)^+ 1S^e$	138.68	139.56	139.21	139.16	139.22

III. QUANTUM-DEFECT METHOD

For intershell states where the two electrons have different radii, the concept of the double-Rydberg formula does not apply. In this case, one may apply the conventional single-channel quantum-defect theory where the energies are expressed as

$$E(n, N) = -\frac{Z^2}{2N^2} - \frac{(Z-1)^2}{2(n-\delta)^2} \quad (\text{a. u.}), \quad (5)$$

where we can also expand the quantum defect δ in the form of Eq. (4) for each state. This method was used often in the analysis of the spectra of singly excited states along the isoelectronic sequence. The question may arise as to whether one should also use (5) for intrashell doubly excited states, particularly for those intrashell states which have negative values of K . These latter states are often not "pure" intrashell states, meaning that in a CI-

type calculation the coefficients of intershell configurations are often not small. This can be easily understood since for negative K states, the two electrons tend to stay on the same side of the nucleus. To maintain such a strong angular correlation, one of the electrons has to move farther out from the other electron to achieve a weaker electron-electron repulsion. Such a geometry is described by configurations where n and N are different. In this respect, a quantum-defect-type fitting of the energy levels is also possible. Thus the question arises as to which formula is more appropriate.

To answer this question, we use the $Z=2$ and 3 data or the $Z=2, 3$, and 4 data for the $2l/2l'$ states from Ref. 18 for a two-parameter or a three-parameter fitting to the quantum defect. From these parameters the energies of the corresponding states are then calculated for $Z=5$ and compared with the results of Ref. 18. In Table III we show such a comparison for all the $2l/2l'$ states. We first

TABLE IV. Binding energies of the $3l/3l'$ states for $Z=5$ calculated using the fitting procedure as compared with the calculations of Lipsky *et al.* (Ref. 18).

State	Two term		Three term		Ref. 18
	Double-Rydberg formula	Quantum-defect theory	Double-Rydberg formula	Quantum-defect theory	
$(2,0)^+ 1S^e$	69.11	69.01	69.11	69.11	69.11
$3P^o$	68.89	68.79	68.89	68.89	68.90
$1D^e$	68.27	68.16	68.27	68.27	68.27
$3F^o$	67.23	67.13	67.24	67.25	67.24
$(1,1)^+ 1P^o$	67.51	67.40	67.50	67.51	67.50
$3D^e$	66.78	66.67	66.78	66.79	66.78
$1F^o$	66.38	66.30	66.34	66.34	66.34
$3P^e$	67.73	67.62	67.73	67.74	67.73
$1D^o$	67.11	67.01	67.13	67.13	67.13
$3F^e$	65.49	65.43	65.54	65.54	65.54
$(0,2)^+ 1D^e$	65.87	65.80	65.88	65.89	65.88
$3D^o$	65.97	65.90	65.99	65.99	65.99
$(0,0)^+ 1S^e$	65.77	65.68	65.75	65.76	65.75
$3P^o$	65.40	65.34	65.43	65.43	65.43
$1D^e$	63.01	63.02	62.99	62.98	62.99
$(-1,1)^+ 1P^o$	62.21	62.32	62.17	62.16	62.18
$3P^e$	63.80	63.93	63.88	63.88	63.89
$(-2,0)^+ 1S^e$	59.43	60.49	59.53	59.42	59.57

note that the three-term fittings using the two different formulas give practically identical results and agree with the calculation of Ref. 18. To assess which formula works better for the intrashell doubly excited states, we look at the fitted energies using the two-parameter fitting. In Table III we see that the results fitted with the

double-Rydberg formula are generally more accurate. Thus we believe that the double-Rydberg formula (3) should be used to parametrize the energy levels for intrashell excited states. A similar comparison is made for the $3/3l'$ intrashell doubly excited states, as shown in Table IV. The double-Rydberg formula again works better.

TABLE V. Screening charge σ and the quantum-defect parameters a , b , and c for intrashell doubly excited states of heliumlike ions. The states are labeled by N , K , and T quantum numbers; the fourth column gives the spin, L , and parity of the state.

N	K	T	State	σ	a	b	c
2	1	0	$^1S^e$	0.2626	0.033	0.030	0.021
2	1	0	$^3P^o$	0.2774	0.023	0.019	0.042
2	1	0	$^1D^e$	0.3162	-0.115	0.096	0.140
2	0	1	$^1P^o$	0.3244	-0.125	0.129	0.085
2	0	1	$^3P^e$	0.3244	-0.007	-0.008	0.100
2	-1	0	$^1S^e$	0.3651	-0.247	-0.090	0.493
3	2	0	$^1S^e$	0.2500	0.085	0.062	0.003
3	2	0	$^3P^o$	0.2554	0.079	0.062	0.009
3	2	0	$^1D^e$	0.2673	0.040	0.100	0.008
3	2	0	$^3F^o$	0.2887	-0.016	0.150	0.020
3	1	1	$^1P^o$	0.2860	0.006	0.152	-0.019
3	1	1	$^3D^e$	0.3030	-0.020	0.142	0.021
3	1	1	$^1F^o$	0.3354	-0.265	0.512	-0.121
3	1	1	$^3P^e$	0.2860	0.042	0.093	0.015
3	1	1	$^1D^o$	0.3030	0.031	0.076	0.048
3	1	1	$^3F^e$	0.3354	-0.051	0.085	0.143
3	0	0	$^1S^e$	0.3198	-0.105	0.264	-0.041
3	0	0	$^3P^o$	0.3313	-0.084	0.137	0.086
3	0	0	$^1D^e$	0.3586	-0.366	0.581	-0.076
3	0	2	$^1D^e$	0.3273	-0.044	0.137	0.040
3	0	2	$^3D^o$	0.3273	-0.026	0.106	0.051
3	-1	1	$^1P^o$	0.3638	-0.461	0.647	-0.099
3	-1	1	$^3P^e$	0.3638	-0.142	0.017	0.254
3	-2	0	$^1S^e$	0.3873	-0.717	0.559	0.306
4	3	0	$^1S^e$	0.2434	0.133	0.067	
4	3	0	$^3P^o$	0.2462	0.124	0.077	
4	3	0	$^1D^e$	0.2520	0.100	0.100	
4	3	0	$^3F^o$	0.2615	0.065	0.136	
4	3	0	$^1G^e$	0.2760	-0.010	0.214	
4	3	0	$^3H^o$	0.2981	-0.073	0.261	
4	2	1	$^1P^o$	0.2685	0.075	0.131	
4	2	1	$^3D^e$	0.2760	0.051	0.164	
4	2	1	$^1F^o$	0.2887	-0.017	0.221	
4	2	1	$^3G^e$	0.3086	-0.084	0.269	
4	2	1	$^3P^e$	0.2685	0.082	0.126	
4	2	1	$^1D^o$	0.2760	0.075	0.137	
4	2	1	$^3F^e$	0.2887	0.042	0.171	
4	2	1	$^1G^o$	0.3086	-0.001	0.201	
4	1	2	$^1D^e$	0.2965	0.025	0.187	
4	1	2	$^3F^o$	0.3123	0.024	0.170	
4	1	2	$^3D^o$	0.2965	0.028	0.185	
4	1	2	$^1F^e$	0.3123	0.019	0.174	
4	1	0	$^1S^e$	0.2933	-0.003	0.210	
4	1	0	$^3P^o$	0.2981	-0.004	0.212	
4	1	0	$^1D^e$	0.3086	-0.064	0.265	
4	0	3	$^1F^o$	0.3266	-0.030	0.234	
4	0	3	$^3F^e$	0.3266	-0.017	0.221	
4	0	1	$^1P^o$	0.3244	-0.146	0.328	
4	0	1	$^3P^e$	0.3244	-0.076	0.268	

TABLE VI. Quantum-defect parameters a , b , and c for intershell doubly excited states of the $2l3l'$ types.

A	K	T	State	a	b	c
1	1	0	$^1S^e$	0.904	0.220	0.889
1	1	0	$^3P^o$	0.827	0.033	1.033
1	1	0	$^1D^e$	0.339	-0.369	1.641
1	0	1	$^1P^o$	-0.080	0.598	0.572
1	0	1	$^3P^e$	0.384	-0.156	0.875
1	-1	0	$^1S^e$	-0.795	0.513	0.044
-1	1	0	$^3S^e$	1.262	0.290	0.670
-1	1	0	$^1P^o$	1.147	0.274	0.659
-1	1	0	$^3D^e$	0.806	0.291	0.580
-1	0	1	$^3P^o$	0.752	0.236	0.334
-1	0	1	$^1P^e$	0.811	0.199	0.334
-1	-1	0	$^3S^e$	0.217	0.154	-0.405
0	-1	0	$^3P^o$	-0.050	-0.459	-0.559
0	-1	0	$^1P^o$	-0.528	-0.021	0.009
0	0	1	$^3D^e$	0.274	0.176	-0.472
0	0	1	$^1D^e$	-0.344	1.031	-0.566
0	0	1	$^3D^o$	0.137	0.075	0.009
0	0	1	$^1D^o$	0.447	0.170	-0.581
0	1	0	$^3F^o$	0.459	0.180	-0.236
0	1	0	$^1F^o$	-0.521	1.537	-0.490

We have tested this procedure for some higher- Z elements and compared results with those available from Bachau. We conclude that the present procedure is quite adequate in predicting the energies accurate to the order of 0.01 eV. To assist with the prediction of energy levels for other heliumlike ions, we show the calculated parameters a , b , and c and the σ calculated from (2) in Table V for the $nlnl'$ ($n=2-4$) intrashell states. Using these parameters in Eqs. (3) and (4) would allow the calculation of the energy levels of the $nlnl'$ intrashell doubly excited states to an accuracy of the order of 0.01–0.05 eV for any Z until relativistic effects become important. We remark that the parameters a , b , and c are obtained from the data of Ref. 18 for $Z=2, 3$, and 4 for the $2l2'$ and $3l3l'$ states. For the $4l4l'$ intrashell states only a subset of positive K is given using a two-parameter formula. There are less extensive data available for the latter set. We used $Z=1$

results from Ref. 20 and $Z=7$ results from Ref. 19 to find a and b for the $4l4l'$ states.

IV. INTERSHELL STATES

We applied the quantum-defect formula (5) to analyze the energy levels of the $2l3l'$ states. Using the data for $Z=2, 3$, and 4 from Ref. 18 we calculated the parameters a , b , and c for the quantum defect for each state. The results are given in Table VI. Using these parameters and Eq. (5), we calculated the energies of $2l3l'$ states of Ne^{8+} measuring from the $1s$ threshold for Ne^{9+} . These energies correspond to the Auger energies for each state if such transitions are allowed. We compare our results with the calculations of Karim *et al.*²² where they calculated the energy of each state using a single configuration in a Hartree-Fock-Slater potential. In Table VII we show the Auger energies calculated using the fitted quantum-defect parameters and using the $(K, T)^A$ classification, and compare the results with those of Karim *et al.* Discrepancies of a fraction of 1 eV to several eV's can be seen. We believe that the present results are more accurate since CI mixings were not considered in the calculations of Karim *et al.*

It is worthwhile to discuss the systematics of the energy levels of intershell doubly excited states. We show in Fig. 1 the energy levels of the $2l3l'$ states of Ne^{8+} ordered according to the $(K, T)^A$ designations. We first note that the rotor structure for the $(1,0)^+$ and the $(1,0)^-$ groups. For each given $A=+1, -1$, or 0 group, we also note that states with the most positive K have the lowest energies. For the same K and T , the $A=-1$ states have lower energies than the $A=+1$ states. We note that in the $2l3l'$ manifold, any state with $A=-1$ is the lowest member of the Rydberg ${}_n(K, T)_N^-$ series, while the state with $A=+1$ belongs to the second member of the ${}_n(K, T)_N^+$ series, with $n=N=2$ state being the first member of the series. We also note that for $A=0$ states, the singlet and triplet states for each K and T occur in pairs; the triplet state has lower energy than the singlet state if the parities of the states are given by $\pi=(-1)^L$. For states where $\pi=(-1)^{L+1}$ the opposite is true. Such spectroscopic regularity can be expected for any inter-

TABLE VII. Auger electron energies of heliumlike neon calculated from the $1/Z$ expansion of the quantum defect vs results from Ref. 22. The states are designated using the correlated classification scheme as well as the single-particle notation. Blank entries under Karim *et al.* indicate states which do not decay via autoionization.

State	Present results	Karim <i>et al.</i>	Independent-particle notation	State	Present results	Karim <i>et al.</i>	Independent-particle notation
$(1,0)^+ ^1S^e$	889.93	890.83	$2s3s$	$(1,0)^- ^3S^e$	886.61	887.83	$2s3s$
$^3P^o$	890.77	891.92	$2s3p$	$^1P^o$	887.69	889.08	$2p3s$
$^1D^e$	895.29	896.40	$2p3p$	$^3D^e$	890.76		$2p3p$
$(0,1)^+ ^1P^o$	898.05	899.27	$2s3p$	$(0,1)^- ^3P^o$	891.31	892.75	$2p3s$
$^3P^e$	894.79	897.36	$2p3p$	$^1P^e$	890.83		$2p3p$
$(-1,0)^+ ^1S^e$	903.78	905.29	$2p3p$	$(-1,0)^- ^3S^e$	896.04		$2p3p$
$(-1,0)^o ^3P^o$	898.76	900.23	$2p3d$	$(-1,0)^o ^1P^o$	902.15	903.52	$2p3d$
$(0,1)^o ^3D^e$	895.55	896.97	$2p3d$	$(0,1)^o ^1D^e$	899.92	901.49	$2p3d$
$(0,1)^o ^3D^o$	896.74		$2s3d$	$(0,1)^o ^1D^o$	894.10	895.68	$2p3d$
$(1,0)^o ^3F^o$	893.96	895.76	$2p3d$	$(1,0)^o ^1F^o$	900.91	902.71	$2p3d$

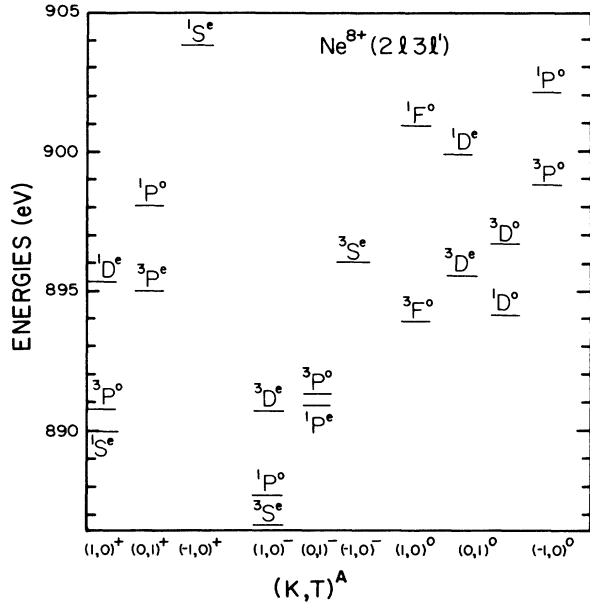


FIG. 1. Energy-level diagram of $2l3l'$ states of Ne^{8+} . Energies are measured from the $1s$ threshold of Ne^{9+} . The states are labeled according to the $(K, T)^A$ quantum numbers.

shell $nln'l'$ manifolds.

Using the quantum defect for each of the ${}_3(K, T)_2^A$ states, one can calculate the energy levels of the other members of the Rydberg series if one assumes the quantum defect along the series is a constant. For doubly excited states such an estimate is usually adequate if the accuracy of the Auger electron energies is limited to the order of 0.1 eV. Furthermore, using the energy diagram similar to Fig. 1 the relative positions of the doubly excited states are known. Such a procedure would allow the identification of the observed Auger spectra for the higher members of the Rydberg series even if accurate energies are not known.

Before leaving this section, we should point out that the quantum defects calculated from the parameters listed in Tables V and VI are negative for most states with negative K , in contrast with the familiar positive quantum defects in singly excited states. Such negative quantum defects are the results of correlations in doubly excited states. We note that for negative K states, the two electrons are on the same side of the nucleus and thus the Coulomb repulsion between the two electrons is larger than one would have expected from the averaged configurations. Similarly for positive K states one would expect a larger positive quantum defect because of the relative reduction of the Coulomb repulsion as the two electrons in this case tend to stay on opposite sides of the nucleus. For intrashell doubly excited states a negative quantum defect could also be due to the overestimate of the screening charge given in Eq. (2).

V. EXTRAPOLATIONS ALONG THE DOUBLE-RYDBERG LADDERS

The ${}_n(K, T)_N^A$ classification scheme can be used to examine the systematics of energy levels along the double-

Rydberg ladders. For intrashell states the states in the ladder are those where the correlation patterns are almost the same but the "orbital" size of both electrons increases simultaneously. An example of such a ladder is the group of intrashell states ${}_N(N-1, \dots)_N^+ 1S^e$. (In the conventional notations, these states are labeled as $Ns^2 1S^e$.) Using the double-Rydberg formula (3), we can extrapolate the quantum defect along N for each fixed Z to obtain energies for the states in the ladder. For example, we can use the data in Table V to find the quantum defects for the states ${}_N(N-1, 0)_N 1S^e$ ($N=2, 3$, and 4) for a fixed Z . From these data we can fit the N dependence of the quantum defect to a quadratic equation for each ladder which can then be used to calculate the quantum defects for higher N 's. We have checked this procedure for states with positive K . The resulting N dependence of δ is quite small. In fact if we just use the quantum defect calculated for $N=4$, and compared with the quantum defect fitted using the aforementioned procedure, the difference in the energies of doubly excited states calculated using both methods is less than one part in 10^3 . For the purpose of estimating the energy levels of higher Z and higher N , we suggest that one can use the assumption of a constant δ along the double Rydberg ladder. Note that this method was used in the fitting procedure for calculating the energy levels of doubly excited states of He^- .^{15,16}

Such a method of estimating the energy levels of high-lying doubly excited states for high- Z ions is useful in the study of double-electron capture in the collision between multiply charged heavy ions with atoms at low energies. To estimate the principal quantum number of the intrashell doubly excited states populated in such collisions, we consider the simple curve-crossing model. The asymptotic potential curve in the entrance channel is given by E_i plus the polarization potential of the neutral target atom by the incident charge Z . The possible exit channels are doubly excited states with energies E_f plus the Coulomb repulsion between the heliumlike ion with charge $Z-2$ and the doubly ionized target. Transition occurs when the potential curves of the entrance and exit channels intersect. If the small polarization potential is neglected, then the crossing occurs when

$$E_i = E_f + 2(Z-2)/R_c. \quad (6)$$

Experimental evidence indicates that if R_c is in the range of 4–8 a.u., the transition probabilities are usually large. This is understood by the fact that if the crossing occurs at larger R_c , the crossing is more likely to be diabatic, while if the crossing occurs at smaller R_c , it is more likely to be adiabatic. If Eq. (3) is used to estimate the energies of the final states E_f , from Eq. (6) one can identify the doubly excited states populated in the collision. For the lowest member of the $NlNl'$ states, one can even set the quantum defect δ in Eq. (3) to be zero.

VI. SUMMARY AND DISCUSSION

In this article we show that the energy levels of intrashell doubly excited states can be easily expressed in a double Rydberg formula where the quantum defect can

be expressed as a two- or three-term $1/Z$ expansion. By determining the parameters from calculations carried out for low- Z ions, we show that the formula allows the calculation of energy levels of other ions along the isoelectronic sequence. For intershell states we show that the conventional quantum-defect theory can be applied where the quantum defect can be expanded also in powers of $1/Z$. The parameters shown in Tables V and VI are useful in calculating energy levels of any helium-like ions of interest.

We have not extended the analysis to other higher doubly excited states. For higher $nlnl'$ states existing calculations are not complete. Only the lower few states with positive K have been calculated. We believe that in future theoretical work, one does not need to extend the calculations to many Z 's. Instead, one should carry out extensive calculations only for two or three Z 's and use the method outlined here to calculate energy levels for

any other Z 's.

We also have not analyzed the dependence of the autoionization widths with the nuclear charge Z and with the K , T , and A quantum numbers. There is some evidence of simple systematics for autoionization widths, but definite conclusions are still not available since accurate calculations for widths are still rather scarce.

Energy levels of doubly excited states with $1s$ or $1s^2$ cores are also needed for experiments in the collision of multiply charged ions with atoms. A similar parametrization procedure like the present one is currently under study.

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