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Behaviours of the excited states $1s^2np$ along lithium isoelectronic sequence from Z=11 to 20*

Hu Mu-Hong(胡木宏) and Wang Zhi-Wen(王治文)†

School of Physics and Electronic Technology, Liaoning Normal University, Dalian 116029, *China*

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Based on the obtained energy values of $1s^2np$ ($n \leq 9$) states for lithium-like systems from Z=11 to 20 (by the authors of this paper: Hu M H and Wang Z W 2004 *Chin. Phys.* **13** 662), this paper determines the quantum defects, as slowly varying function of energy, of this Rydberg series. Using them as input, it can predict the energies of any highly excited states below the ionization threshold for this series according to the quantum defect theory. The regularities of variation for quantum defects of the series along this isoelectronic sequence are physically analysed and discussed. The screening parameters, which are equal to the effective screening charge of the core-electrons, are also obtained.

Keywords: lithium-like system, excited state, quantum defect, screening parameter
PACC: 3130, 3110, 3270

1. Introduction

As we know, the study of structure and property for multicharged ions has been a subject of considerable interest for many fields, such as astrophysics, plasma physics and laser design. Most of the relative atomic 'data' that are tabulated for use as input reference data for these fields are generated by theoretical calculations, not measured in experiments.[1] Especially, the energies (including fine structures) and transition probabilities of the excited states for these systems have to be provided by theoretical predictions.[2] On other hand, from the point of view of theory, an important problem is how the electronic properties of the system quantitatively change as the nuclear charge Z is increased along the isoelectronic sequence, because this kind of variation reflects the regularities of variation for the relative importance of various interactions (physical effects) in the system along isoelectronic sequence. Zilitis studied the highly excited states of the isoelectronic sequences of lithium and potassium by using a semi-empirical method.[3,4] Recently, we have reported the calculated results of the $1s^2ns$, $1s^2nd$ and $1s^2nf$ states of lithium isoelectronic sequence.[5–9]

Not long ago, the energy and fine structure of $1s^2np$ ($n \leq 9$) states for the lithium isoelectronic sequence from Z =11 to 20 were calculated by using the full-core plus correlation (FCPC) method.[10] In the present paper based on the numerical results in Ref.[10] we will determine the quantum defects, as slowly varying function of energy, of Rydberg series $1s^2np$ for lithium-like ions from Z= 11 to 20. Using them as input, we can predict the energy of any highly excited states below the ionization thresholds of the systems for this series according to quantum defect theory (QDT). The regularities of variation for quantum defects of the series along this isoelectronic sequence are physically analysed and discussed. In order to inspect the physical meaning of these regularities still further, the screening parameters of nuclear charges are also obtained. The results in this paper will be useful to understand the behaviours of $1s^2np$ series along the isoelectronic sequence in the whole discrete energy region.

2. Method of theoretical analysis

For the configuration $1s^2nl$ of lithium-like systems, the excitation threshold of $1s^2$-core is higher. In energy region from discrete levels to the first ionization threshold of the ion, the interaction between channels converging to different ionization limits can be neglected. Single-channel QDT can be used to describe the behaviours of highly excited states of the systems. The basic physical picture of this theory is

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†Corresponding author. E-mail: zwwang@online.ln.cn, zh.w.wang@163.com

that in the large r region the system can be considered as a hydrogenic system in which a valence electron moves in the Coulombic field of the $1s^2$-core, and in the small r region the short-range non-Coulombic interaction between the valence electron and the electrons in the core results in the quantum defects in principal quantum numbers of discrete states, or the phase shifts in the wavefunctions of continuum states. According to QDT,[11,12] the quantum defect μ_n of $1s^2np$ states for the ions can be determined by

$$E_n = -\frac{(Z-N+1)^2}{2(n-\mu_n)^2} \quad \text{(in a.u.)}, \qquad (1)$$

where Z is nuclear charge and N= 3 is the number of electrons in the system. In Ref.[10], the non-relativistic energies of $1s^2np$ ($n \leq 9$) states for lithium-like ions from Z=11 to 20 were calculated by using FCPC method, the corrections to the energies from relativistic and QED effects were evaluated, and the term energies E_n of $1s^2np$ ($n \leq 9$) states were obtained. Because of non-complete screening of the core electrons to nuclear charge, the binding energy of the system is larger than that of the hydrogen-like system with the same Z, and the value of quantum defect, μ_n, is always positive.

For highly excited states with $n \geq 10$, quantum defects, μ_n, should be a smooth function of energy and can be expressed in the following form:

$$\mu_n(E) = \mu_0 + h_1 E + h_2 E^2. \qquad (2)$$

The coefficients μ_0, h_1, and h_2 of this series are determined by fitting the values μ_n of $1s^2np$ states with $n \leq 9$ obtained from Eq.(1). Firstly, we let $\mu \approx \mu_0$, and put it into Eq.(1). Then E_n and μ_n can be refined by an iteration procedure. Finally, the quantum defect and term energy are obtained. Once these coefficients are obtained, the term energy of any highly excited states ($n \geq 10$) below the ionization threshold of the system can be predicted by solving the set of Eqs.(1) and (2) with an iteration method.

Along an isoelectronic sequence, the electronic cloud is pulled into a more tightly bound configuration and the size of the system is shrunk as the increase of nuclear charge Z. This is the most important reason which results in the variations of the structure and property for atomic system along the isoelectronic sequence. In order to inspect this physical picture further, we can investigate the screening parameters of nuclear charge, which are closely interrelated to actual electric field experienced by valence electron in system. To do so, Eq.(1) can be rewritten as

$$E_n = -\frac{Z^{*2}}{2n^2} = -\frac{(Z-S)^2}{2n^2} \quad \text{(in a.u.)}, \qquad (3)$$

where $Z^* = Z - S$ is called as effective nuclear charge and S is the screening parameters which represent the effective screening charge of the electrons in the core. Starting from this equation, we can easily discuss the variations of S values in $1s^2np$ states as the increase of n and Z respectively.

3. Results and discussion

Based on our calculated term energy and fine structure of $1s^2np$ ($n \leq 9$) states for the lithium-like ions from Z=11 to 20 in Ref.[10], the energies of $1s^2np_{1/2,3/2}$ ($n \leq 9$) states for these ions, and the quantum defects, μ_n, of these states can be determined from Eq.(1). The results are given in Table 1. It is seen from this table that, as expected, the μ_n values, which are rather small, smoothly vary, and quickly tend to the constants with the increasing of n along $1s^2np$ series for every given ion. In addition, the quantum defects of $2p_{1/2}$ states are smaller than those of $2p_{3/2}$ states because the binding energies of the former are larger than those of the latter. As a typical example, the variation of quantum defects μ_n with principal quantum number in $1s^2np_{1/2,3/2}$ states of Na IX (Z=11) ion is plotted in Fig.1.

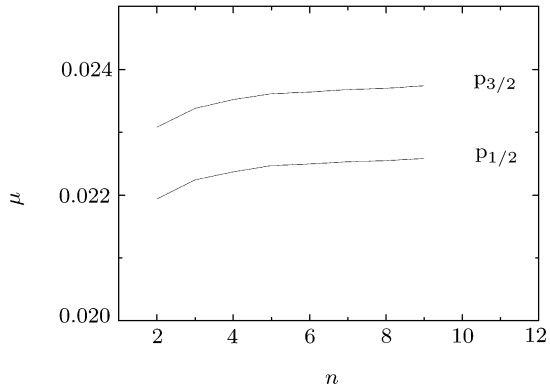


Fig.1. The quantum defects of $1s^2np_{1/2}$ and $1s^2np_{3/2}$ ($2 \leq n \leq 9$) states for Na IX ion.

Table 1. The quantum defects of $1s^2np_{1/2,3/2}$ ($2 \le n \le 9$) states for lithium-like systems from Z=11 to 20.

		μ_n				μ_n	
Z	n	$p_{1/2}$	$p_{3/2}$	Z	n	$p_{1/2}$	$p_{3/2}$
11	2	0.02308	0.02194	16	2	0.01832	0.01561
	3	0.02338	0.02224		3	0.01890	0.01618
	4	0.02352	0.02237		4	0.01920	0.01647
	5	0.02361	0.02247		5	0.01938	0.01665
	6	0.02364	0.02250		6	0.01951	0.01678
	7	0.02368	0.02253		7	0.01960	0.01688
	8	0.02370	0.02255		8	0.01967	0.01694
	9	0.02374	0.02258		9	0.01975	0.01702
12	2	0.02159	0.02027	17	2	0.01789	0.01479
	3	0.02203	0.02062		3	0.01858	0.01546
	4	0.02215	0.02074		4	0.01891	0.01580
	5	0.02224	0.02082		5	0.01913	0.01601
	6	0.02229	0.02088		6	0.01928	0.01615
	7	0.02234	0.02093		7	0.01940	0.01625
	8	0.02237	0.02096		8	0.01947	0.01635
	9	0.02240	0.02099		9	0.01965	0.01636
13	2	0.02053	0.01884	18	2	0.01759	0.01407
	3	0.02090	0.01920		3	0.01838	0.01484
	4	0.02108	0.01938		4	0.01877	0.01523
	5	0.02119	0.01948		5	0.01902	0.01547
	6	0.02126	0.01956		6	0.01919	0.01564
	7	0.02132	0.01961		7	0.01931	0.01576
	8	0.02136	0.01966		8	0.01938	0.01583
	9	0.02139	0.01969		9	0.01947	0.01594
14	2	0.01961	0.01761	19	2	0.01739	0.01342
	3	0.02005	0.01804		3	0.01829	0.01431
	4	0.02026	0.01824		4	0.01864	0.01466
	5	0.02039	0.01837		5	0.01902	0.01503
	6	0.02048	0.01846		6	0.01922	0.01522
	7	0.02055	0.01853		7	0.01941	0.01541
	8	0.02061	0.01859		8	0.01954	0.01554
	9	0.02059	0.01857		9	0.01962	0.01562
15	2	0.01888	0.01654	20	2	0.01730	0.01286
	3	0.01939	0.01703		3	0.01831	0.01386
	4	0.01964	0.01728		4	0.01883	0.01436
	5	0.01979	0.01743		5	0.01914	0.01467
	6	0.01990	0.01754		6	0.01936	0.01489
	7	0.01998	0.01762		7	0.01953	0.01505
	8	0.02005	0.01769		8	0.01963	0.01515
	9	0.02010	0.01777		9	0.01971	0.01522

Table 2 gives the values of expansion coefficients in Eq.(2) for quantum defects of $1s^2np$ ($2 \le n \le 9$) states for the lithium-like ions from Z=11 to 20. By using these quantum defects, as smoothly varying function of energy, and the iteration method described above, we can recalculate the ionization potentials of

$1s^2np$ ($6 \leq n \leq 9$) states for these ions. The results are given in the columns marked by 'semi-exp.' of Table 3. The corresponding results[10] calculated from FCPC method are also listed in this table for comparison. As can be seen from this table, the agreement between them is up to five or six digits. This indicates that the energy of any highly excited states $1s^2np$ ($n \geq 10$) below the ionization threshold of the system can be accurately predicted by this iteration method with the quantum defects determined above, as input.

Table 2. The coefficients in the expansions of quantum defects for $1s^2np$ ($2 \leq n \leq 9$) states of lithium-like systems from Z=11 to 20.

Z	μ_0	h_1	h_2
11	2.300233×10^{-2}	-1.175095×10^{-4}	7.403628×10^{-6}
12	2.151261×10^{-2}	-1.223508×10^{-4}	8.403139×10^{-6}
13	2.029333×10^{-2}	-1.125338×10^{-4}	5.241725×10^{-6}
14	1.928802×10^{-2}	-9.334102×10^{-5}	2.714148×10^{-6}
15	1.853903×10^{-2}	-1.037689×10^{-4}	2.957018×10^{-6}
16	1.795001×10^{-2}	-1.103650×10^{-4}	2.930980×10^{-6}
17	1.750388×10^{-2}	-1.117703×10^{-4}	2.558865×10^{-6}
18	1.716776×10^{-2}	-1.119732×10^{-4}	2.235147×10^{-6}
19	1.733806×10^{-2}	-2.035824×10^{-4}	6.097066×10^{-6}
20	1.686761×10^{-2}	-1.197995×10^{-4}	1.968495×10^{-6}

Table 3. The comparison of ionization potentials for $1s^2np$ states of lithium-like systems from Z=11 to 20 from semi-empirical and FCPC methods.

Z	states	semi-exp.	FCPC[10]	Z	states	semi-exp.	FCPC[10]
11	6p	1.1336290	1.1336279	16	6p	2.738327	2.738348
	7p	0.8319675	0.8319686		7p	2.010176	2.010199
	8p	0.6364558	0.6364557		8p	1.538082	1.538106
	9p	0.5025592	0.5025612		9p	1.214682	1.214711
12	6p	1.3988300	1.3988271	17	6p	3.142971	3.142988
	7p	1.0266750	1.0266759		7p	2.307282	2.307307
	8p	0.7854508	0.7854527		8p	1.765446	1.765481
	9p	0.6202355	0.6202385		9p	1.394260	1.394292
13	6p	1.6918820	1.6918868	18	6p	3.575546	3.575574
	7p	1.2418370	1.2418446		7p	2.624896	2.624935
	8p	0.9501024	0.9501080		8p	2.008503	2.008536
	9p	0.7502797	0.7502873		9p	1.586232	1.586276
14	6p	2.0128020	2.0128187	19	6p	4.036213	4.036119
	7p	1.4774630	1.4774831		7p	2.963176	2.963134
	8p	1.1304160	1.1304372		8p	2.267386	2.267367
	9p	0.8926950	0.8927031		9p	1.790706	1.790689
15	6p	2.3616140	2.3616293	20	6p	4.524650	4.524671
	7p	1.7335760	1.7335956		7p	3.321756	3.321807
	8p	1.3264090	1.3264318		8p	2.541772	2.541817
	9p	1.0474960	1.0475232		9p	2.007414	2.007450

It is also seen from Table 1 that the μ_n values for every given state monotonically decrease as the increasing of Z along the isoelectronic sequence. This change is made clear by considering the following fact: the electronic cloud of $1s^2$-core is shrunk much more than that of valence electron as Z increases. As an example, the variation of quantum defects of $1s^22p_{1/2}$ and $1s^22p_{3/2}$ states with the increase of Z along this isoelectronic sequence from Z=11 to 20 is shown in Fig.2.

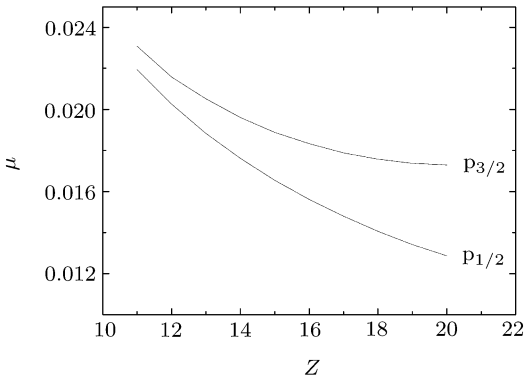


Fig.2. The variation of quantum defects of $1s^22p_{1/2}$ and $1s^22p_{3/2}$ states with the increase of Z along the isoelectronic sequence.

From the viewpoint of the screening effect from nuclear charge, one can see the same physical picture as described above. Table 4 gives the screening parameters in $1s^2np_{1/2,3/2}$ states for lithium-like systems from Z=11 to 20. It is noted from this table that the screening parameters in $1s^2np_{1/2}$ states are larger than those in $1s^2np_{3/2}$ states for a given ion. In other words, the actual electric fields seen by valence electrons in $1s^2np_{1/2}$ states are stronger than those in $1s^2np_{3/2}$ states. These are the inevitable consequence of the following fact: the binding energies of the former are larger than those of the latter. As the increase of n, the S values of $1s^2np_{1/2}$ and $1s^2np_{3/2}$ states for a given system weakly increase and tend to the constants. In Fig.3 the variation of screening parameters in $1s^2np_{1/2,3/2}$ states with the increase of n for Na IX (Z=11) ion is depicted as a typical example. In Fig.4, the variation of screening parameters S in $1s^22p_{1/2,3/2}$ states for these ions along the sequence is depicted. It is seen from this figure that the values of S inferred from Eq.(3) are approximately independent of Z, especially at larger Z. There is the similar behaviour for other$1s^2np_{1/2,3/2}$ ($n > 2$) states of these ions. These numerical results are completely consistent with the physical picture reflected in Fig.2 and the arguments about the properties of highly ionized atoms given in Ref.[13].

Table 4. The screening parameters of $1s^2np_{1/2,3/2}$ states for lithium-like systems from Z=11 to 20.

Z	n	$p_{1/2}$	$p_{3/2}$	Z	n	$p_{1/2}$	$p_{3/2}$
11	2	2.1039	2.0987	16	2	2.1282	2.1093
	3	2.0701	2.0667		3	2.0882	2.0775
	4	2.0529	2.0503		4	2.0672	2.0577
	5	2.0425	2.0404		5	2.0543	2.0466
	6	2.0355	2.0338		6	2.0452	2.0392
	7	2.0305	2.0290		7	2.0392	2.0338
	8	2.0267	2.0254		8	2.0344	2.0296
	9	2.0237	2.0226		9	2.0307	2.0265
12	2	2.1080	2.1014	17	2	2.1342	2.1109
	3	2.0733	2.0687		3	2.0929	2.0773
	4	2.0554	2.0519		4	2.0709	2.0593
	5	2.0448	2.0416		5	2.0574	2.0480
	6	2.0372	2.0348		6	2.0482	2.0404
	7	2.0319	2.0299		7	2.0416	2.0348
	8	2.0280	2.0261		8	2.0365	2.0307
	9	2.0249	2.0233		9	2.0328	2.0273

Table 4. (*Continued*)

Z	n	$p_{1/2}$	$p_{3/2}$	Z	n	$p_{1/2}$	$p_{3/2}$
13	2	2.1129	2.1036	18	2	2.1407	2.1126
	3	2.0766	2.0704		3	2.0980	2.0791
	4	2.0580	2.0533		4	2.0751	2.0609
	5	2.04662	2.0429		5	2.0609	2.0495
	6	2.03898	2.0359		6	2.0512	2.0417
	7	2.03350	2.0308		7	2.0441	2.0360
	8	2.02937	2.0270		8	2.0388	2.0317
	9	2.02614	2.0241		9	2.0346	2.0283
14	2	2.1177	2.1057	19	2	2.1478	2.1141
	3	2.0802	2.0722		3	2.1036	2.0811
	4	2.0608	2.0547		4	2.0792	2.0623
	5	2.0489	2.0441		5	2.0647	2.0511
	6	2.0410	2.0369		6	2.0545	2.0131
	7	2.0352	2.0317		7	2.0471	2.0374
	8	2.0309	2.0279		8	2.0415	2.0330
	9	2.0275	2.0248		9	2.0371	2.0295
15	2	2.1227	2.1075	20	2	2.1557	2.1157
	3	2.0840	2.0740		3	2.1099	2.0832
	4	2.0638	2.0562		4	2.0847	2.0646
	5	2.0515	2.0453		5	2.0689	2.0528
	6	2.0431	2.0380		6	2.0581	2.0147
	7	2.0371	2.0327		7	2.0502	2.0387
	8	2.0326	2.0875		8	2.0442	2.0341
	9	2.0290	2.0257		9	2.0394	2.0304

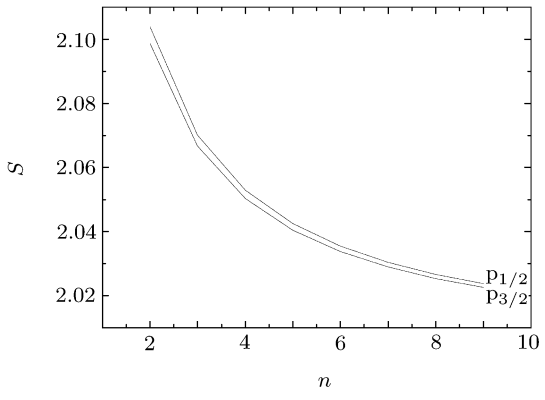


Fig.3. The screening parameters in $1s^2np_{1/2}$ and $1s^2np_{3/2}$ ($2 \le n \le 9$) states for Na IX ion.

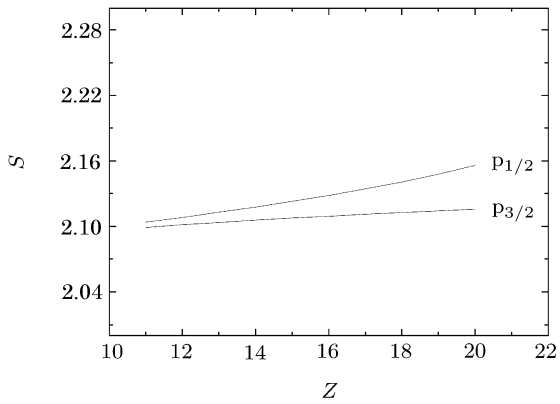


Fig.4. The screening parameters in $1s^22p_{1/2,3/2}$ states for lithium-like systems from Z=11 to 20.

4. Summary

In this paper, based on our numerical results about the energy for $1s^2np$ ($n \le 9$) of lithium-like ions from Z=11 to 20 obtained in Ref.[10], we aim at determining the quantum defects of Rydberg series $1s^2np$ for these ions, and thereby extrapolating our theoretical prediction about the energy of this series for the isoelectronic sequence to whole discrete energy region below the ionization thresholds of the systems according to QDT. The regularities of variation for quantum

defects and the screening parameters in $1s^2np_{1/2,3/2}$ states of the ions along the individual Rydberg series and the isoelectronic sequence are physically analysed and discussed, respectively. We hope that the results obtained in this paper would be useful to understand the behaviours of $1s^2np$ series along the isoelectronic sequence.

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