Ionization energies and term energies of the ground states $1s^2 2s$ of lithium-like systems*

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We extend the Hamiltonian method of the full-core plus correlation (FCPC) by minimizing the expectation value to calculate the non-relativistic energies and the wave functions of $1s^2 2s$ states for the lithium-like systems from $Z = 41$ to 50. The mass-polarization and the relativistic corrections including the kinetic-energy correction, the Darwin term, the electron–electron contact term, and the orbit–orbit interaction are calculated perturbatively as first-order correction. The contribution from quantum electrodynamic (QED) is also explored by using the effective nuclear charge formula. The ionization potential and term energies of the ground states $1s^2 2s$ are derived and compared with other theoretical calculation results. It is shown that the FCPC methods are also effective for theoretical calculation of the ionic structure for high nuclear ion of lithium-like systems.

Keywords: lithium-like systems, full core plus correlation, ionization energy, term energy

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1. Introduction

The research on the structures and properties of highly ionized atomic systems is of fundamental importance in atomic physics and plays an important role in other fields such as astrophysics, plasma physics, and laser physics. In addition, this subject also provides a challenge to theoretical work because there are significant differences between the features of these systems and of neutral or lowly ionized systems.[1,2] In recent years, there have been several reports of calculations of energies and oscillator strengths for lithium-like ions.[3–6] Particularly, the high-precision energies and oscillator strengths of $1s^2 2s$ and $1s^2 2p$ for Li-like systems up to $Z = 50$ were given by Yan *et al.*[3] using the Hylleraas-type variational method and the $1/Z$ expansion method. However, for lithium-like ions with higher Z, particularly for their excited states, there is little information available in literatures.

An elegant and complete variation approach, namely, the full core plus correlation (FCPC) method has been developed by Chung.[7] This method has been successfully applied to atomic systems with a $1s^2$ core.[8–11] In the FCPC method, a large predetermined multi-configuration interaction (CI) $1s^2$-core wave function is used as a single term in the total wave function of the three-electron system. The effect of the valence electron is accounted for by multiplying the core wave function with a linear combination of single-particle Slater orbitals. The relaxation of the core and other possible correlations are described by another larger CI wave function. Many elaborate calculations for the dipole polarizabilities,[12] the quadrupole and octupole polarizabilities,[13] the total atomic scattering factors,[14] and the hyperfine structure[15] of lithium isoelectronic sequence ($Z \leq 20$) have been carried out. Recently, this method has also been applied to the excited states $1s^2 nl$ (l = s, d, and f, $n \leq 5$) of lithium-like systems for $Z = 11$–20[16] and the ground states of the systems with $Z = 21$–30.[17] Later on, this method was used to calculate the energy and fine structure of $1s^2 np$ states,[18] and the dipole oscillator strengths for $1s^2 2p$–$1s^2 nd$ and $1s^2 3d$–$1s^2 nf$ ($n \leq 9$) transitions of lithium-like systems with $Z = 11$–20.[19,20] A natural extension is to test this method on the system with higher nuclear charge and in the higher energy region.

In this paper, we extend the Hamiltonian method of the full-core plus correlation by minimizing the expectation value to calculate the non-relativistic energies, relativistic correction, and quantum electronic dynamics of high ionization ($Z = 41$–50) $1s^2 2s$ state for the like-lithium atomic systems. The absolute energies, ionization potential, and term energies of the ground states $1s^2 2s$ are given and compared with other theoretical calculation results.

2. Theory

The essential point of the FCPC method is to use a bulky predetermined $1s^2$-core wave function as a single term in the total wave function of the three-electron system. The relaxation of the core and the other possible correlations is described by another large CI wave function. The wave function of the lithium-like system with $1s^2$ core is given by

$$\Psi(1,2,3) = A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i \mathrm{e}^{-\beta r_3}\mathrm{Y}_{l(i)}(3)\chi(3)\right.$$

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$$+\sum_i C_i \Phi_{n(i),l(i)}(1,2,3)\Big], \tag{1}$$

where A is the anti-symmetrization operator, and $[\psi_{1s1s}(1,2)]$ is a predetermined $1s^2$-core wave function, and its expression can be found in Ref. [7]. The second term on the right-hand side of Eq. (1) describes the relaxation of the $1s^2$-core and the other possible correlations $\phi_{n(i),l(i)}$ are the basis set of three-electron system.[7,9–11]

The non-relativistic energies of a lithium-like system are calculated by (in units of a.u.)

$$H_0 = \sum_{i=1}^{3}\left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right] + \sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}. \tag{2}$$

The non-relativistic energies of the three-electron system are calculated by minimizing the expectation value of H_0

$$\delta E_0 = \delta\langle H_0\rangle = \delta\frac{\langle\psi|H_0|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{3}$$

In order to calculate accurately the non-relativistic energy, it is necessary to consider the contribution of energy from the higher component of the angular momentum (high L). For this reason, we calculate them by extrapolating the deviation of $1s^2$ ionic variational energy relative to the precise value (Drake), i.e.,

$$\begin{aligned} E_{\text{nonre}}(1s^2 2s) &= E_{\text{upper}}(1s^2 2s) + \Delta E_{\text{higher}-l}(1s^2) \\ &\quad + \Delta E_{\text{higher}-l}(1s^2 2s). \end{aligned} \tag{4}$$

Among them, $E_{\text{upper}}(1s^2 2s)$, $\Delta E_{\text{higher}-l}$, and $\Delta E_{\text{higher}-l}(1s^2 2s)$ are the variational energy of three electronic systems, the correction caused by $1s^2$-ion insufficient number, and the correction of high angular momentum, respectively. The $E_{\text{nonre}}(1s^2 2s)$ is the non-relativistic energy of the system.

The correlation from the relativistic and mass-polarization effects is given by

$$\Delta E = \langle\psi|H_1 + H_2 + H_3 + H_4 + H_5 + H_6 + H_7|\psi\rangle. \tag{5}$$

The total energy is

$$E_{\text{tot}} = E_0 + \Delta E. \tag{6}$$

The correction of the relativistic perturbation to the kinetic energy is

$$H_1 = \frac{1}{8c^2}\sum_{i=1}^{3} p_i^4, \tag{7}$$

where $c = 137.036$, and the Darwin term is

$$H_2 = \frac{Z\pi}{2c^2}\sum_{i=1}^{3}\delta(r_i). \tag{8}$$

The electron–electron contact term is

$$H_3 = -\frac{\pi}{c^2}\sum_{\substack{i,j=1\\ i<j}}^{3}\left[1 + \frac{8}{3}\boldsymbol{s}_i\cdot\boldsymbol{s}_j\right]\delta(r_{ij}). \tag{9}$$

The orbit–orbit interaction term is

$$H_4 = -\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i<j}}^{3}\frac{1}{r_{ij}}\left[\boldsymbol{p}_i\cdot\boldsymbol{p}_j + \frac{\boldsymbol{r}_{ij}(\boldsymbol{r}_{ij}\cdot\boldsymbol{p}_i)\cdot\boldsymbol{p}_j}{r_{ij}^2}\right]. \tag{10}$$

The spin–orbit interaction term is

$$H_5 = \frac{Z}{2c^2}\sum_{i=1}^{3}\frac{\boldsymbol{l}_i\cdot\boldsymbol{s}_i}{r_{ij}}. \tag{11}$$

The term which describes the interaction between spin and other orbits is

$$H_6 = -\frac{1}{2c^2}\sum_{i\neq j}^{3}\left[\frac{1}{r_{ij}^3}(\boldsymbol{r}_i - \boldsymbol{r}_j)\times\boldsymbol{p}_j\right]\cdot(\boldsymbol{s}_i + 2\boldsymbol{s}_j). \tag{12}$$

The mass-polarization term is

$$H_7 = -\frac{1}{M}\sum_{i<j}^{3}\nabla_i\cdot\nabla_j. \tag{13}$$

In the calculation of the fine structure, the LS coupling scheme is used.[21] In this paper, contribution from quantum electrodynamics (QED) is also included by using the effective nuclear charge and Hydrogen formula as follows:

$$\Delta E_{\text{QED}} = \frac{4Z_{\text{eff}}^4\alpha^3}{3\pi n^2}\left\{\frac{19}{30} - 2\ln(\alpha Z_{\text{eff}}) - \ln[K(n,0)]\right\}, \tag{14}$$

where α is the fine-structure constant, Z_{eff}^4 is the effective charge of hydrogen ions, and the Bethe number $K(n,0)$ is from Ref. [22]. The total energies of $1s^2$-core and three-electron systems are given by

$$E_{\text{tot}} = E_{\text{nonre}} + \Delta E_{\text{re}}, \tag{15}$$

where ΔE_{re} is the relativistic correction obtained from the first perturbation. The ionization energies of three electronic system $1s^2 2s$ states are given by the total energy difference of $1s^2$-core and three electronic systems, namely,

$$E_{\text{IP}} = E_{\text{tot}}(1s^2\,{}^1\text{S}) - E_{\text{tot}}(1s^2 2s^2\text{S}) - \Delta E_{\text{QED}}. \tag{16}$$

3. Results and discussion

In this work, a 222-term core wave function with seven l components is utilized. Though the number of terms is not substantial enough, this does not lead to a substantial effect on our calculations because the IP is determined by subtracting the energy of the three-electron system from that of the $1s^2$ core. To calculate the $1s^2 2s$ energy, we use eight terms and 771 terms of $\phi_{n(i)l(i)}(1,2,3)$ with 13 partial waves in Eq. (1). The corresponding Rydberg constant is taken from Ref. [22]. The deviation caused by ion of insufficient number has good offset effect in the calculation of the ionization energy. Thus,

the calculation results which have extremely high precision are given, and we greatly reduce the amount of calculation.

In order to compare the convergence, the same $1s^2$-core wave functions are used in all calculations of lithium-like $1s^22s$ systems. The 222-term $1s^2$-core wave function, 771-term three-electron system wave function, and full-core plus correlation variational energy are obtained by Eq. (3). Our calculated results of the non-relativistic energies of $1s^22s$ states are listed in Table 1. We find that the correlation effect of the valence electron and $1s^2$-core is huge, and the convergence of energy and wave function is slow because of great contribution of angular momentum wave to energy.

Table 1. Energy convergence for the $1s^2$-core and the $1s^22s$ states of lithium-like systems.

Angular component	No. of terms	$-\Delta E$/a.u.				
		$Z=41$	$Z=42$	$Z=43$	$Z=44$	$Z=45$
(0,0)	49	1655.50044716	1737.87544303	1822.25043899	1908.62543502	1997.00043113
(1,1)	42	0.026280866	0.026285666	0.026290128	0.026294590	0.026298739
(2,2)	36	0.003796752	0.003797257	0.003797597	0.003814764	0.003816229
(3,3)	30	0.001034153	0.001034827	0.001035487	0.001036083	0.001036664
(4,4)	25	0.000383601	0.000383883	0.000384155	0.000384388	0.000384641
(5,5)	20	0.000164074	0.000163581	0.000167229	0.000167340	0.000167441
(6,6)	20	0.000084057	0.000084094	0.000084184	0.000084241	0.000084299
Total	222	1655.53219066	1737.90719234	1822.28219777	1908.65721643	1997.032219
Cor+3s	9	1849.59128236	1941.94345209	2036.54562879	2133.39782412	2232.49999869
((0,0),0)	124	0.000898489	0.000900864	0.000902156	0.000901997	0.000903652
((0,1),1)	175	0.005313760	0.005320748	0.005327139	0.005332474	0.005338119
((0,2),2)	125	0.000572567	0.000573618	0.000574721	0.000574896	0.000575722
((0,3),3)	116	0.000133002	0.000132919	0.000133486	0.000133865	0.000134204
((0,4),4)	62	0.000044515	0.000044679	0.000046007	0.000046135	0.000046167
((0,5),5)	60	0.000020070	0.000020970	0.000021748	0.000021783	0.000215197
((0,6),6)	30	0.000009032	0.000009475	0.000010709	0.000010690	0.000010797
((0,1),1)	20	0.000000988	0.000001067	0.000001003	0.000001147	0.000001101
((1,0),1)	15	0.000000798	0.000000338	0.000000308	0.000000204	0.000000130
((0,2),2)	10	0.000000548	0.000000899	0.000000114	0.000000112	0.000001245
((1,2),1)	9	0.000000146	0.000000134	0.000000115	0.000000108	0.000000103
((0,0),0)	8	0.000000051	0.000000026	0.000000012	0.000000018	0.000000025
((2,3),1)	8	0.000000001	0.000000002	0.000000008	0.000000009	0.000000003
Total	771	1849.59827633	1941.95045783	2036.55264734	2133.40484873	2232.50703148
Angular component	No. of terms	$-\Delta E$/a.u.				
		$Z=46$	$Z=47$	$Z=48$	$Z=49$	$Z=50$
(0,0)	49	2087.37542729	2179.75042352	2274.12541979	2370.50041609	2468.87541242
(1,1)	42	0.026302746	0.026306547	0.026310215	0.026313718	0.026317081
(2,2)	36	0.003817749	0.003819106	0.003820293	0.003821365	0.003822334
(3,3)	30	0.001037246	0.001037786	0.001038309	0.001038810	0.001039285
(4,4)	25	0.000384869	0.000385051	0.000385305	0.000385501	0.000385703
(5,5)	20	0.000167556	0.000167651	0.000167754	0.000167845	0.000167937
(6,6)	20	0.000084353	0.000084385	0.000084446	0.000084501	0.000084552
Total	222	2087.40722181	2179.78222404	2274.15722611	2370.53222783	2468.90722932
Cor+3s	9	2333.85217425	2437.46169923	2543.30652690	2651.40870416	2761.76088241
((0,0),0)	124	0.000905251	0.000906801	0.000908337	0.000909667	0.000910857
((0,1),1)	175	0.005343192	0.005348040	0.005352752	0.005357098	0.005361138
((0,2),2)	125	0.000574862	0.000575272	0.000575680	0.000576006	0.000576286
((0,3),3)	116	0.000134977	0.000135266	0.000135647	0.000135976	0.000136358
((0,4),4)	62	0.000045108	0.000045113	0.000045098	0.000045072	0.000044978
((0,5),5)	60	0.000019410	0.000019260	0.000019092	0.000018920	0.000018717
((0,6),6)	30	0.000018091	0.000017883	0.000017656	0.000017416	0.000017169
((0,1),1)	20	0.000000617	0.000000566	0.000000534	0.000000536	0.000000559
((1,0),1)	15	0.000000406	0.000000368	0.000000332	0.000000312	0.000000301
((0,2),2)	10	0.000000080	0.000000055	0.000000038	0.000000025	0.000000016
((1,2),1)	9	0.000000090	0.000000078	0.000000070	0.000000064	0.000000057
((0,0),0)	8	0.000000021	0.000000027	0.000000047	0.000000039	0.000000046
((2,3),1)	8	0.000000001	0.000000003	0.000000002	0.000000001	0.000000002
Total	771	2333.85921635	2437.468747962	2543.31358219	2651.41576529	2761.76794889

Using the wavefunctions obtained above, the non-relativistic energy of $1s^2$-core, the relativistic energy including the kinetic-energy correction, the Darwin term, the electron–electron contact, the orbit–orbit interaction, the mass polarization, and the total energy are shown in Table 2. The energy correction caused by $1s^2$-ion insufficient number and the correction of high angular momentum are given in Table 3. The relativistic correction items of three electronic system and the quantum electrodynamics correction $\Delta E_{\rm QED}$ about the valence electrons 2s are also listed in Table 3. Among them, the effect of the polarization items is relatively small, and mainly determined by the element. In this paper, ^{93}Nb, ^{96}Mo, ^{98}Te, ^{101}Ru, ^{103}Rh, ^{106}Pd, ^{108}Ag, ^{112}Cd, ^{115}In, and ^{119}Sn are calculated. We find that the change of relativistic kinetic-energy correction and Darwin term is very obvious with the nuclear charge Z. This is because the relativistic kinetic energy is closely related to the effective nuclear charge $Z_{\rm eff}$, and for the highly charged lithium-like ions ($Z = 41$–50) in this paper, the relativistic effect is more important, which is one of the important features of the highly charged ions, different from those medium and low charged ions.

Table 2. Non-relativistic energy, term energy of relativistic correction, and mass-polarization of $1s^22s$ ($Z = 41$–50) states (in units of a.u.).

Z	Variational energy	$\langle H_1 + H_2 \rangle$	$\langle H_3 \rangle$	$\langle H_4 \rangle$	$\langle H_{\rm MP} \rangle$	Total energy
41	1655.5322	–36.343065	0.4392247	–0.0070046	0.0000549	1691.4429
42	1737.9072	–40.052599	0.4724366	–0.0073584	0.0000553	1777.4947
43	1822.2822	–44.039930	0.5074807	–0.0077195	0.0000559	1865.8223
44	1908.6572	–48.317845	0.5441799	–0.0080894	0.0000559	1956.4389
45	1997.0322	–52.900080	0.5826718	–0.0084676	0.0000562	2049.3580
46	2087.4072	–57.800766	0.6229382	–0.0088543	0.0000565	2144.5938
47	2179.7822	–63.034331	0.6650211	–0.0092498	0.0000567	2242.1607
48	2274.1572	–68.615522	0.7089515	–0.0096539	0.0000570	2342.0734
49	2370.5322	–74.559395	0.7547788	–0.0100666	0.0000573	2444.3469
50	2468.9072	–80.881340	0.8025369	–0.0104878	0.0000575	2548.9965

Table 3. Correction of $1s^2$-core, contribution of high angular momentum, relativistic correction, and mass-polarization (in units of a.u.).

Z	Correction of $1s^2$-core	Contribution of high angular momentum	$\langle H_1 + H_2 \rangle$	$\langle H_3 \rangle$	$\langle H_4 \rangle$	$\langle H_{\rm MP} \rangle$
41	0.00025957	0.0000279	–41.558554	0.4800555	–0.0076214	0.0000638
42	0.00025956	0.0000292	–45.811359	0.5163325	–0.0080099	0.0000641
43	0.00025959	0.0000330	–50.384520	0.5546985	–0.0084041	0.0000645
44	0.00025960	0.0000329	–55.292544	0.5948867	–0.0088080	0.0000649
45	0.00025962	0.0000333	–60.549310	0.6370353	–0.0092208	0.0000652
46	0.00025961	0.0000557	–66.173189	0.6811450	–0.0096435	0.0000656
47	0.00025963	0.0000550	–72.180057	0.7272362	–0.0100751	0.0000659
48	0.00025963	0.0000543	–78.586658	0.7753546	–0.0105163	0.0000662
49	0.00025966	0.0000535	–85.411097	0.8255542	–0.0109668	0.0000665
50	0.00025968	0.0000527	–92.670323	0.8778726	–0.01142684	0.0000668

The non-relativistic FCPC energy of three-electron system $1s^22s$ are listed in Table 4. According to the non-relativistic energy, the relativistic term energy, and the quantum electrodynamics correction of the valence electrons 2s obtained above, as well as the FCPC ionization energies of $1s^22s$ ground states are calculated in Table 4. They are given together with the results of Ref. [3] for comparison. No experimental data are available for the systems for $Z =$ 41–50. Our calculated values are in agreement with the data in Refs. [3]. For example, the non-relativistic energies of $1s^22s$ states for Nb^{39+} ion obtained in this paper are -1849.59827633 a.u., the corresponding results of Yan *et al.*[3] are -1849.598580969 a.u. The relative discrepancies between them are within 10 ppm. The biggest discrepancy between them, ^{96}Mo ($Z = 42$), is 68 cm^{-1}. It seems to suggest that the non-relativistic energies of $1s^22s$ states obtained in this work are accurate and reliable enough. This also shows that our calculation method is suitable for the energy calculation of the higher nuclear charge.

Figure 1 shows the changing rule of the ionization energies obtained above with the nuclear charge Z. This shows that our results follow a well-behaved isoelectronic regularity. No experimental data are found for the system $1s^22s$ with $Z = 41$–50.

Table 4. Non-relativistic energy of $1s^2 2s$ ($Z = 41$–50), total energy, ionization energy, and other theoretical results (in units of cm^{-1}).

Z	Non-relativistic energy/a.u.	Non-relativistic energy/a.u.[a)]	QED correction/a.u.	Relativistic correction/a.u.	Total energy/a.u.	Ionization energy/a.u.
41	1849.59827633	1849.59858097	0.381672	41.0860561	1890.6005661	199.1592
42	1941.95045783	1941.95076496	0.423031	45.3029732	1987.1605876	209.6675
43	2036.55264734	2036.55294948	0.467756	49.8381611	2086.2881491	220.4676
44	2133.40484873	2133.40513449	0.516036	54.7064004	2187.9979936	231.5609
45	2232.50703148	2232.50731996	0.568062	59.9214303	2292.3037882	242.9477
46	2333.85921635	2333.85950585	0.624049	65.5016219	2399.2238771	254.6321
47	2437.46874796	2437.45435023	0.684203	71.4628300	2508.7740656	266.6155
48	2543.31358219	2543.31387881	0.748742	77.8217535	2620.9710078	278.8999
49	2651.41576529	2651.41606582	0.817902	84.5964431	2735.8327019	291.4882
50	2761.76794889	2761.76825316	0.891909	91.8038104	2853.3760102	304.3820

[a)] Ref. [3].

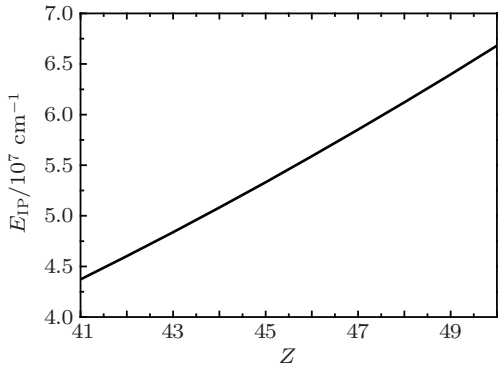


Fig. 1. Ionization potential of the ground states $1s^2 2s$ of lithium-like systems as a function of Z.

4. Conclusion

We have extended the FCPC method to calculate ionization energies and term energies for lithium-like atomic systems for $Z = 41$–50, with higher nuclear charge than that in previous literature.[23] Our calculated term energies agree well with the theoretical results obtained by $1/Z$ expansion method in Ref. [3]. The agreement of our results with the theoretical data available in the literature is usually better than a few hundred cm^{-1}. Our calculated ionization energies for lithium-like $1s^2 2s$ for $Z = 41$–50 follow a well-behaved isoelectronic trend. These results show that the FCPC method is effective for calculations involving lithium-like systems with higher nuclear charges.

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