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The hyperfine structure of the $1s^2ns^2S$ and $1s^2np^2P$ states ($n = 2, 3, 4$, and 5) for the lithium isoelectronic sequence

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Abstract. The non-relativistic hyperfine structure parameters, the *Fermi* contact, the spin-dipolar, the orbital and the electronic quadrupole terms, of the lithium-like ground state and low-lying states, $1s^2ns^2S$ and $1s^2np^2P$ ($n = 2$, 3, 4, and 5), are calculated with the full core plus correlation (FCPC) wave functions. With the 794- and 1185-term Slater-type expansions, the *Fermi* contact interactions of the 2^2S and 2^2P states in ^{7}LiI are determined to be 2.90313 a.u. and -0.21359 a.u., respectively. By using the global identities, the *Fermi* contact term is also given for the ground state in LiI. The typical patterns of convergence of the expectation values of the *Fermi* contact interaction for the lithium $1s^22s$ and $1s^22p$ states are analyzed. The contribution from the core polarization is examined. The calculated results of the lithium-like systems from LiI to NeVIII are compared with the previous theoretical results obtained with other methods, and with the experimental data available in the literature.

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1 Introduction

Hyperfine structure of three-electron systems has been studied extensively over the past two decades [1–8]. Experimentally, some properties of the atomic nucleus can be obtained by investigating the hyperfine structure of the atomic energy levels. The nuclear electric quadrupole moment, which is difficult to measure directly with nuclear physics techniques, can be determined using the measured hyperfine structure splitting and the accurate theoretical results [9]. On the other hand, with development of the experimental methods, the hyperfine structure constants have been measured to very high precision for the light elements. For example, the experimental value of the $A_{1/2}$ of the $2s^2S$ state in ^{7}LiI is 401.7520433(5) MHz [1]. It is accurate to about 1 par per 10^6 (ppm). Recently, Windholz *et al.* reported the results of the Laser-Atomic-Beam(LAB) measurement for the hyperfine structure constants of the 2^2S and 2^2P states in ^{6,7}Li with a somewhat lower accuracy of 10% [7]. From the theoretical point of view, the accurate theoretical calculation of the hyperfine structure is necessary to interpret these experimental data.

Up to now, the most sophisticated theoretical calculations of the hyperfine structure parameters for the light atoms have been carried out using many-body perturbation theory(MBPT) and its relativistic version(RMBPT) by Lindgren and coworkers [10–12], variational wave function in Hylleraas coordinates [13–19], as well as a large-scale multiconfiguration Hartree-Fock method by Sundholm and Olsen [9] and Fischer *et al.* [20,21]. The latter method has been applied extensively determined the various atomic properties. As mentioned by Yan *et al.* [22], Lindgren's MBPT results of *Fermi* contact terms for the 2^2S and 2^2P states disagree significantly with the experimental data and other theoretical results. The discrepancy arises from the truncated particle wave function summation from one set of diagrams [23]. Very recently, Drake *et al.* developed a variational technique for the lithium atom with multiple basis sets in Hylleraas coordinates [24, 25]. Their result for hyperfine structure constant of the 2^2S state in LiI is very close to McKenzie's non-relativistic limit, 2.9060(3) a.u. [26]. Though the *Fermi* contact terms of LiI and BeII were discussed in detailed in reference [22], other hyperfine structure parameters were not given. Also, the large-scale multiconfiguration Hartree-Fock(MCHF) method provides an alternative and effective approach to calculate the hyperfine structure constants. Recently, MCHF calculations of ^{7}LiI were reported by Calsson *et al.* [20] and other authors. Their results for the $1s^22s$ state are in very good agreement with experiments.

Recently, Chung has developed an elegant and complete variational approach, namely, the full core plus correlation(FCPC) method [27]. This method has been successfully applied to three- and four-electron systems with the $1s^2$-core. Many elaborate calculations, especially, for the oscillator strenghts, show that FCPC wave functions have a reasonable behavior over the whole configuration space [28–30]. As is well known, the theoretical calculations of the hyperfine structure parameters depend sensitively on

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the behavior of the wave function in the proximity of the nucleus. In addition, core polarization effects for the low l states need to be included in the nonrelativistic wave function. In other words, a careful treatment of the correlation effect is necessary if we make definitive comparison with measurements for the 2^2P state. The purpose of this work is to calculate the hyperfine structure parameters of the $1s^2ns$ and $1s^2np$ states ($2 \leq n \leq 5$) for the lithium-like systems from $Z = 3$ to 10 by using the FCPC method, and to provide furthermore a re-examination of the quality of our FCPC wave functions.

In Section 2 we give a brief account of the theory. The numerical results, including *Fermi* contact, spin-dipolar, orbital and electric quadrupole terms, and the discussion is presented in Section 3. A conclusion is given in Section 4.

2 Theory

The hyperfine structure of the atomic levels is caused by the interaction between the electrons and the electromagnetic multiple moments of the nucleus. The hyperfine interaction Hamiltonian can be represented be a multiple expression [20,31]

$$H_{\mathrm{hys}} = \sum_{k=1} T^{(k)} \cdot M^{(k)}, \tag{1}$$

where $T^{(k)}$ and $M^{(k)}$ are spherical tensor operators of rank k in the electronic and nuclear space, respectively. The $k = 1$ term represets the magnetic-dipole interaction between the magnetic field generated be the electrons and nuclear magnetic dipole moments, the $k = 2$ term the electric quadrupole interaction between the electric field gradient from the electrons and the non-spherical charge distribution of the nucleus. The contributions from higher-order terms are much smaller and can offen be neglected.

In the non-relativistic framework, the electronic tensor operators, in atomic units, can be written as

$$\begin{aligned} T^{(1)} = & \frac{\alpha^2}{2} \sum_{i=1}^{3} \left[2 g_l r_i^{-3} l_i^{(1)} - \sqrt{10} g_{\mathrm{s}} \left\{ s_i^{(1)} C_i^{(2)} \right\}^{(1)} r_i^{-3} \right. \\ & \left. + \frac{8\pi}{3} g_{\mathrm{s}} s_i^{(1)} \delta(\mathbf{r}_i) \right] \end{aligned} \tag{2}$$

and

$$T^{(2)} = -\sum_{i=1}^{3} r_i^{-3} C_i^{(2)}, \tag{3}$$

where α is fine structure constants, $g_l = 1 - m/M$ and $g_{\mathrm{s}} = 2.0023193$ are the orbital and electron spin g factors (taking into account the normal mass effect and QED effect), respectively. δ is the three-dimensional delta function. M is the nuclear mass.

Generally, the uncoupling and the coupling hyperfine parameters, in a.u., are defined as [20]:

$$a_{\mathrm{c}} = \left\langle \gamma L M_L S M_S \left| \sum_{i=1}^{3} 2 s_0^{(1)}(i) r_i^{-2} \delta(r_i) \right| \gamma L M_L S M_S \right\rangle, \quad (\textit{Fermi} \text{ contact}) \tag{4}$$

$$a_{\mathrm{sd}} = \left\langle \gamma L M_L S M_S \left| \sum_{i=1}^{3} 2 s_0^{(1)}(i) C_0^{(2)}(i) r_i^{-3} \right| \gamma L M_L S M_S \right\rangle, \quad (\text{spin}-\text{dipolar}) \tag{5}$$

$$a_l = \left\langle \gamma L M_L S M_S \left| \sum_{i=1}^{3} l_0^{(1)}(i) r_i^{-3} \right| \gamma L M_L S M_S \right\rangle, \quad (\text{orbital}) \tag{6}$$

$$b_{\mathrm{q}} = \left\langle \gamma L M_L S M_S \left| \sum_{i=1}^{3} 2 C_0^{(2)}(i) r_i^{-3} \right| \gamma L M_L S M_S \right\rangle, \quad (\text{electric quadrupole}) \tag{7}$$

and

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)(2J+1)]^{1/2}} \left\langle \gamma J \left\| T^{(1)} \right\| \gamma J \right\rangle, \tag{8}$$

$$A_{J-1,J} = \frac{\mu_I}{I} \frac{1}{[J(2J-1)(2J+1)]^{1/2}} \left\langle \gamma J - 1 \left\| T^{(1)} \right\| \gamma J \right\rangle, \tag{9}$$

$$B_J = 2Q \left[\frac{2J(J-1)}{(2J+1)(2J+2)(2J+3)} \right]^{1/2} \left\langle \gamma J \left\| T^{(2)} \right\| \gamma J \right\rangle, \tag{10}$$

where $M_L = L$ and $M_S = S$. In these expressions, μ_I and Q are the nuclear magnetic moment and the nuclear quadrupole moment, respectivily. I is the nuclear spin and J is the atomic electronic angular moment.

By using standard tensor-operator technique, the correspondence between uncoupling and coupling parameters of the present atomic configurations can be written:

$$A_{1/2} = \frac{C \mu_I}{3I} g_{\mathrm{s}} a_{\mathrm{c}}, \quad (\text{for } {}^2\text{S state}) \tag{11}$$

$$A_{1/2} = \frac{C \mu_I}{3I} \left[4 g_l a_l - 10 g_{\mathrm{s}} a_{\mathrm{sd}} - \frac{1}{3} g_{\mathrm{s}} a_{\mathrm{c}} \right], \tag{12}$$

$$A_{3/2} = \frac{C \mu_I}{3I} \left[2 g_l a_l - g_{\mathrm{s}} a_{\mathrm{sd}} + \frac{1}{3} g_{\mathrm{s}} a_{\mathrm{c}} \right], \quad (\text{for } {}^2\text{P state}) \tag{13}$$

$$A_{1/2,3/2} = \frac{C \mu_I}{3I} \left[g_l a_l + \frac{5}{4} g_{\mathrm{s}} a_{\mathrm{sd}} - \frac{1}{3} g_{\mathrm{s}} a_{\mathrm{c}} \right], \tag{14}$$

$$B_{3/2} = -D Q b_q, \tag{15}$$

where $A_{1/2}$, $A_{3/2}$, $A_{1/2,3/2}$ and $B_{3/2}$ are expressed in MHz, the uncoupling constants in atomic units and μ_I in nuclear magnetron (μ_N), respectively. In equations (11), (12), (13), (14) and (15), C and D are the conversion factors from a.u. to MHz. They are 95.41067 and 2.3497×10^5, respectively. So that our results calculated from these equations can be compared with the experimental data which are mostly given in MHz.

In practice, it is difficult to obtain a wave function at small separations with good quality. On the other hand, as long as Ψ is the true eigenfunction of the non-relativistic Hamiltonian, it satisfies the electron-nuclear cusp condition introduced by Kato [32] and Steiner [33], namely,

$$\frac{\partial\rho(\mathbf{r})}{\partial r}|_{r=0} = -2Z\rho(0) = -2Z\left\langle\delta(\mathbf{r}_i)\right\rangle, \tag{16}$$

where $\rho(\mathbf{r})$ is the charge density.

Hiller *et al.* suggested that the average of the operator involving a $\delta(\mathbf{r})$ function may be replaced by that of a global operator [34]. These identities are applied to the calculation of the electron-electron, electron-nucleus contact interactions and *Fermi* contact term, *etc.*

For the our case, we recast a_c as follows:

$$\begin{aligned} a_c &= \left\langle\Psi\left|\sum_{i=1}^{3}2s_0^{(1)}(i)r_i^{-2}\delta(r_i)\right|\Psi\right\rangle \\ &= 8\pi\left\langle\Psi\left|\sum_{i=1}^{3}s_{iZ}\delta(\mathbf{r}_i)\right|\Psi\right\rangle \\ &= 4\left\langle\Psi\left|\sum_{i=1}^{3}s_{iZ}\left(\frac{\partial V}{\partial r_i}-\frac{\mathbf{l}_i^2}{r_i^3}\right)\right|\Psi\right\rangle \end{aligned} \tag{17}$$

where

$$V = \sum_{i=1}^{3}\left(\frac{-Z}{r_i}\right) + \frac{1}{2}\sum_{i\neq j}^{3}\frac{1}{r_{ij}}\cdot \tag{18}$$

We may use an identical global operator form to replace the delta function form in the *Fermi* contact interaction. Of couse, in practice only an approximate wave function are available. So that equation (17) is no longer exactly valid. In other words, the agreement between the values calculated from equation (4) and equation (17) becomes an important judgement of the quality of the wave functions used.

We now turn to the description of the wave function used in this work. According to the FCPC method [27–30], the wave function for the three-electron systems with a $1s^2$-core can be written as

$$\begin{aligned}\Psi(1,2,3) =& A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i e^{-\beta r_3}Y_{LM_L}(3)\chi_{SM_S}(3)\right.\\ &\left.+\sum_i C_i\Phi_{n(i),l(i)}(1,2,3)\right],\end{aligned} \tag{19}$$

where A is an antisymmetrization operator. Φ_{1s1s} is a predetermined $1s^2$-core wave function which is represented by a CI basis set, *i.e.*,

$$\begin{aligned}\Phi_{1s1s}(1,2) =& A\sum_{kn,l}C_{knl}r_1^k r_2^n\exp(-\beta_l r_1-\rho_l r_2)\\ &\times Y_l(1,2)\chi(1,2).\end{aligned} \tag{20}$$

Table 1. Convergence study of the nonrelativistic *Fermi* contact term (a_c) for the lithium $1s^22s^2S$ and $1s^22p^2P$ states.(in a.u.)

Angular component	No. of terms	2^2S	Angular component	No. of terms	2^2P
core +2s	9	2.329506	core +2p	8	0.000000
(0,0)0,0	165	0.545335	(0,1)1,2	120	0.000000
$(0,0)\,0,0^a$	22	−0.125613	$(0,1)\,1,2^a$	81	0.004406
(0,1)1,1	123	0.134529	$(1,2)\,1,0^a$	35	0.000003
$(0,1)\,1,1^a$	22	0.000606	(1,2)1,0	35	0.000015
(1,0)1,1	34	−0.000233	$(0,0)\,0,1^a$	93	−0.198533
(0,2)2,2	162	0.013299	$(1,0)\,1,0^a$	125	−0.022337
$(0,2)\,2,2^a$	32	0.000002	(0,2)2,3	56	0.000136
(0,3)3,3	50	0.003322	$(0,2)\,2,3^a$	56	0.001439
(0,4)4,4	32	0.001265	(0,3)3,4	56	0.000027
(0,5)5,5	34	0.000090	$(0,3)\,3,4^a$	55	0.000395
(0,6)6,6	34	0.001373	(0,4)4,5	56	0.000035
(1,2)1,1	35	−0.000935	$(0,4)\,4,5^a$	55	0.000146
$(1,2)\,1,1^a$	20	0.000695	(0,5)5,6	56	0.000018
(2,3)1,1	20	−0.000075	$(0,5)\,5,6^a$	56	0.000065
Total	794	2.90313	(0,6)6,7	56	0.000010
			$(0,6)\,6,7^a$	56	0.000033
			(1,1)0,1	34	0.000577
			(1,1)2,3	13	0.000002
			(1,2)1,2	34	0.000068
			(1,3)2,3	13	−0.000005
			(2,3)1,0	35	0.000000
			Total	1185	−0.21359

[a] In these angular components the spins of the first two electrons couple into a triplet.

The angular part is

$$Y_l(1,2) = \sum_m\left\langle lm,l-m|0,0\right\rangle Y_{lm}(\theta_1,\varphi_1)Y_{l-m}(\theta_2,\varphi_2). \tag{21}$$

$\chi(1,2)$ is a two-electron singlet spin function. The linear and non-linear parameters in equation (20) are determined by optimizing the energy of the He-like 1s1s system. The factor multiplying with Φ_{1s1s} is a linear combination of the Slater type orbitals for the valance electron. The second term on the right-hand side of equation (19) descibes the core relaxation and the intershell correlation in the three-electron system. The basis function is chosen as

$$\Phi_{n(i),l(i)}(1,2,3) = \varphi_{n(i)}(R)Y_{l(i)}^{LM}(\hat{R})\chi_{SM_S}. \tag{22}$$

The radial and angular basis functions are

$$\varphi_{n(i)}(R) = \prod_{j=1}^{3}r_j^{n_j}\exp(-\beta_j r_j) \tag{23}$$

and

$$\begin{aligned}Y_{l(i)}^{LM}(\hat{R}) =& \sum_{m_j}\left\langle l_1m_1l_2m_2|l_{12}m_{12}\right\rangle\left\langle l_{12}m_{12}l_3m_3|LM\right\rangle\\ &\times\prod_{j=1}^{3}Y_{l_jm_j}(\Omega_j),\end{aligned} \tag{24}$$

respectively, where $l(i)$ represents the set of l_1, l_2, l_{12} and l_3. The angular component is simply denoted as

$$l_i = [(l_1, l_2)l_{12}, l_3], \qquad (25)$$

where l_{12} and l_3 coupling into L is implicitly implied. Using a similar notation, the doublet spin function can be represented by

$$\chi_{SM_s} = [(s_1, s_2)s_{12}, s_3]. \qquad (26)$$

It has two possible spin doublets

$$\chi_1 = [(s_1, s_2)0, s_3], \qquad (27)$$

$$\chi_2 = [(s_1, s_2)1, s_3]. \qquad (28)$$

In the present work, these FCPC wave functions for the n^2S and n^2P ($n = 2$, 3, 4 and 5) states of Li-like systems are obtained by using the variational method. The hyperfine structure parameters of these states are calculated by using our FCPC wave function determined above.

3 Results and discussions

The same seven angular component 222 terms are used in the wave function for the 1s^2-core. For the 1s^2ns($2 \leq n \leq 5$) states in Li we chose the wave function with nine d_i terms and 794, 488, 575 and 399 terms in the $\Phi_{n(i),l(i)}$ of equation (19) for $n = 2$, 3, 4 and 5 respectively. Similarly, we chose the wave function with nine d_i terms and about 300-600 terms in the $\Phi_{n(i),l(i)}$ of equation (19) for the other Z systems. For the 1s^2np states from LiI to NeVIII, we used the wave function with eight d_i terms and about 1000-1200 terms in the $\Phi_{n(i),l(i)}$ of equation (19).

A detailed convergence chracteristic study of the *Fermi* contact term a_c for the lithium 1s^{2}2s and 1s^{2}2p states is given in Table 1. We see from this table that their convergence is rather fast. In addition, we also note that unlike the calculation of the energy and oscillator strength, the small oscillation of the convergence pattern for the *Fermi* contact term with increasing numbers of the partial wave function is encountered. Therefore, some considerable efforts have been spent to choose the relevant partial wave function in our present calculations. For this reason, our choice of the partial wave function differs slightly from the that in reference [30]. For the 2^{2}S state, the contribution from the second term of the equation (19) is very obvious. It provides about 20% of the total value of this term. The contributions to the enegy from the partial wave function $[(0,1)1,1]$, which differs from the 1s^{2}2s configuration in the angular symmetry, is most important [27]. This is in accordance with that in Fischer's MCHF approach [35]. But for the *Fermi* contact term, the other partial wave functions, $[(0,0)0,0]$, and $[(0,0)0,0]^*$, also provide the significant contributions. However, for the 2^{2}P state, a dramatic situation occurs if we note that the first term of equation (19) does not contribute to the *Fermi* contact term. In other words, the partial wave functions which describe the core relaxation and the intershell correlation have to be included in the total wave function.

Both the theoretical calculation and measurement of the hyperfine structure for the three-electron systems has received considerable attention in the literature. The most extensively studied hyperfine structure of the lithium-like systems is probably for LiI. Some typical theoretical results as well as experimental data of this property have been collected in Tables 2 and 3. The coupling constants corresponding to states for LiI are given in these tables. In Table 2 we also gave the calculated values of the *Fermi* contact term for the 2^{2}S state by using the global operator defined by equation (17). Although there is somewhat of a difference between our two results obtained by different equations, we tend towards considering that the result obtained by equation (4) is more reliable. As can be seen from the Table 1, the final *Fermi* contact term reported here appears to have converged to the fifth significant digit. It is fairly satisfactory, considering that the present variational calculation weights the energy important region away from the nucleus. In order to explain further this conclusion, the cusp condition has also been checked up by using FCPC wave functions. We found that the cusp ratio, $\frac{d\rho}{dr}|_{r=0}/-2\rho(0)$, is $3.0{-}1.84 \times 10^{-4}$ for the ground state of the lithium. This value is in very close agreement with the nuclear charge $Z = 3$. So we believe that the wave functions employed in this work can give self-consistent result, particularly, at the region near the nucleus. In the Hylleraas approach the expectation of the Hiller-Sucher-Feinberg operator cannot as yet be evaluated. To the best of our knowledge, there is only one similar consideration using the configuration interaction(CI) type wave function which is constructed from Slater-type orbitals for Li ground state by Bhatia and Sucher [43]. Their results are 3.0717 and 2.9014, by using equations (4) and (17), respectively. As can be seen from Table 2, the agreement between our corresponding results is better than that of Bhatia and Sucher. This means that our wave function used in the present work is reasonable and accurate in the full configuration space. The recent results of McKenzie [26], 2.90600, and of Yan *et al.* [22], 2.90592, are probably the most accurate in the literature. The uncertainty in the most accurate experimental datum, 2.906023(3), of Beckmann *et al.* is rather small [1]. Most of the theoretical values at most agree with the measured values to five significant figures. In addition, Yan *et al.* also gave the small corrections from the finite nuclear mass, size, relativistic and QED effects. Unfortunately, these corrections are in the wrong direction away from the experimental values. For the 2^{2}P state, our result of the *Fermi* contact term, -0.21359, is in excellent agreement with the experimental value of Orth *et al.*, $-0.2135(10)$. In contrast, most of the results from the MCHF and MBPT approach fall outside the experimental uncertainty. Note that the small changes of the uncoupling parameters could cause the obvious changes in the coupling parameters, considering that the multiplying factor $C\mu_I/3I$ is not a small quantity, as one can see from other theoretical results of Table 3.

Table 2. Comparison of the nonrelativistic hyperfine parameter for the ^{7}Li 1s^{2}2s^{2}S state. The *Fermi* contact term (a_c) is expressed in atomic units and the $A_{1/2}$ in MHz.

Author	Method	Ref.	a_c	$A_{1/2}$
		Theory		
Larsson (1968)	100-term Hylleraas	[13]	2.906	401.74
Garpman *et al.* (1976)	MBPT	[11]	2.9065	401.81
Lindgren (1985)	MBPT	[12]	2.91726	403.31
King *et al.* (1986)	352-term Hylleraas	[16]	2.904	401.47
King (1989)	602-term Hylleraas	[17]	2.906359	401.79
King *et al.* (1990)	296-term Hylleraas	[18]	2.907051	401.89
Blundell *et al.* (1989)	all-order MBPT	[36]	2.9119	402.56
Mårtensson *et al.* (1990)	Coupled-Cluster	[37]	2.89819	400.67
Sundholm *et al.* (1990)	MCHF	[9]	2.9039	401.46
Esquivel *et al.* (1991)	CI	[38]	2.90856	402.10
McKenzie (1991)	1134-term Hylleraas	[26]	2.9060	401.75
Carlsson *et al.* (1992)	MCHF	[20]	2.9047	401.57
Tong *et al.* (1993)	MCHF	[21]	2.9051	401.62
Yan *et al.* (1996)	Extra-Hylleraas	[22]	2.90592	401.74
This work	FCPC(CI)[a]		2.90313	401.352
This work	FCPC(CI)[b]		2.89124	399.708
		Experiment		
Beckmann *et al.* (1974)	ABMR[c]	[1]	2.906023(3)	401.7520433(5)
Winholz *et al.* (1990)	LAB[d]	[7]	2.9064(18)	401.81(25)

[a] Obtained by using equation (4) in the text.
[b] Obtained by using equation (17) in the text.
[c] ABMR means Atomic Beam magnetic resonance.
[d] LAB means Laser Atomic Beam Spectroscopy.

In Table 4, we compare our results of the uncoupling constants for the lithium-like systems with those of Garpman *et al.* [11]. They have used an effective-operator form of the many-body theory to calculate the hyperfine structure. The effect of core polarization was included in their calculations. The experimental data of the hyperfine structure of the three-electron systems are available only for the 1s^{2}2s states of ^{6,7}LiI, ^{9}BeII, and ^{19}FVII, for the 1s^{2}2p states of ^{6,7}Li, ^{9}BeII, ^{11}BIII, and for the 1s^2ns ($n = 3$ and 4) of ^{7}LiI, we are not aware of any experimental results for other Z systems. For the 2^{2}S state in ^{9}BeII, ^{19}FVII, the measured values of $A_{1/2}$, $-625.008837048(10)$ MHz [44], and 88855(525) MHz [45], are in agreement with our present theoretical results, -624.5144 MHz and 89549.546 MHz, respectively. For the 2^{2}P state in ^{9}BeII, the measured value of $A_{1/2}$, $-118.6(3.6)$ MHz [46], also agree with our prediction, -117.24876 MHz. But the accuracy of the experimental value of $A_{3/2}$, $-19.2(28.6)$ MHz, is too low to draw any definite conclusion on the comparison with the theory. For the 2p^{2}P state in ^{11}BIII, the beam-gas Hanle technique of Kowalski *et al.* yields $A_{3/2} = 123.6(4.0)$ MHz [47]. Our calculated result is 119.185 MHz.

In Table 5, we give a comparison between present results and King's results for the other low-lying n^2S state. The Hylleraas-type variational calculations [19] of King agree to about three figures with our results. For the 3s^{2}S state of ^{7}LiI, our calculated $A_{1/2} = 93.251$ MHz. The agreement with the recent measured value of 94.68(22) MHz of Stevens *et al.* [23] is of the order of one percent. But is agrees well with an earlier measurement, 92(3) MHz [8]. Our value of $A_{1/2}$(4^{2}S, ^{7}LiI), 35.068 MHz, is in good agreement with the value measured, 36.4(4.0) MHz, using the method of Doppler-free two-photo spectroscopy [48].

4 Conclusion

In this work we have calculated the hyperfine structure constants of the ground state and low-lying excited states for the lithium isoelectronic sequence from $Z = 3$ to 10, by using the FCPC wave function. The results are well converged with the increasing numbers of the partial wave functions. The low angular-momentum components contribute much more than the higher ones. We have emphasized the importance of core polarization in the present paper. The careful choice for the partial wave functions is necessary to obtain an excellent agreement between the theory and the experiment. In other words, our present FCPC method is very flexible. The systematical improvement on the *Fermi* contact term, the spin-dipolar and the orbital terms is possible by optimizing the additional the partial wave functions. We find that our wave functions provide satisfactory results. The uncertainty of these

Table 3. Comparison of the nonrelativistic hyperfine parameters for the ^{7}Li 1s^{2}2p^{2}P state. The uncoupling constants *Fermi* contact ($a_{\rm c}$), spin-dipolar($a_{\rm sd}$), orbital(a_l), and electric quadrupole ($b_{\rm q}$) terms are expressed in atomic units, and the $A_{1/2}$, $A_{3/2}$, and $A_{1/2,3/2}$ in MHz.

Author	Method	Ref.	$a_{\rm c}$	$a_{\rm sd}$	a_l	$b_{\rm q}$	$A_{1/2}$	$A_{3/2}$	$A_{1/2,3/2}$
			Theory						
Nesbet (1970)	Bethe-Goldstone	[39]	−0.2146	−0.0135	0.0632	−0.0228	45.9935	−3.03534	11.9165
Lunell (1973)	SO-SCF	[40]	−0.2132	−0.0117	0.0588	−0.0235	42.2263	−3.32909	11.8595
Ahlenius *et al.* (1973)	78-term Hylleraas	[14]	−0.2162	−0.01342	0.0634	−0.02016	46.01186	−3.07042	12.0179
Ahlenius *et al.* (1978)	97-term Hylleraas	[15]	−0.2086	−0.01352	0.0628	−0.02236	45.63430	−2.81680	11.6090
Glass *et al.* (1976)	CI	[41]	−0.2129	−0.0138	0.0625	−0.0247	46.13676	−3.09506	11.7381
Garpman *et al.* (1976)	MBPT	[11]	−0.2070	−0.01332	0.06262	−0.022536	45.23440	−2.74025	11.5574
Lindgren (1985)	MBPT	[12]	−0.2208	−0.01348	0.06308	−0.02266	46.21848	−3.33485	12.1974
Sundholm *et al.* (1990)	MCHF	[9]	−0.2158	−0.01346	0.06303	−0.02253	45.94662	−3.10856	11.9671
Sundholm *et al.* (1990)	Semitheoretical	[9]	−0.2148	−0.01346	0.06307		45.91157	−3.05696	11.9237
Carlsson *et al.* (1992)	HF	[20]	0	−0.01171	0.05857	−0.02343	32.35185	−6.46262	2.01714
Carlsson *et al.* (1992)	MCHF	[20]	−0.2155	−0.01346	0.06305	−0.02255	45.93832	−3.09198	11.9546
Carlsson *et al.* (1992)	MCHF[a]	[20]	−0.2156	−0.01346	0.05304	−0.02255	45.94016	−3.09797	11.9585
Tong *et al.* (1993)	MCHF	[21]	−0.2175	−0.013341	0.06308	−0.02187	45.94890	−3.15236	12.0367
Yan *et al.* (1996)	Extra-Hylleraas	[22]	−0.2148						
This work	FCPC(CI)		−0.21359	−0.01341	0.06309	−0.02242	45.79295	−2.99186	11.87853
			Experiment						
Ritter (1965)	ODR[b]	[3]					46.17(35)		
Lyons *et al.* (1970)	Analysis of Exp	[42]	−0.2128	−0.0138	0.0626		46.159	−3.07	11.7404
Orth *et al.* (1975)	ODR[b]	[2]	−0.2135(10)	−0.01356(8)	0.0627(3)	−0.0232(30)	45.914(25)	−3.055(14)	11.823(81)
Nagourney *et al.* (1978)	LC[c]	[4]						−2.95(4)	
Shimizu *et al.* (1987)	LIF[d]	[5]						−3.08(4)	
Carlsson *et al.* (1989)	QB[e]	[6]						−3.08(4)	
Windholz *et al.* (1990)	LAB[f]	[7]					46.05(30)	−3.18(10)	

[a] Corrected for relativistic, finite nuclear size, and finite nuclear mass effects.

[b] ODR means Optical Double Resonance.

[c] LC means Level Crossing.

[d] LIF means Laser Induced Fluorescence with delayed detection.

[e] QB means Quantum Beats.

[f] LAB means Laser-Atomic-Beam Spectroscopy.

Table 4. Comparison between different theoretical calculations of $a_{\rm c}$, $a_{\rm sd}$, a_l, $b_{\rm q}$ for the Li-like 1s^{2}2s and 1s^{2}2p configurations (in a.u.).

		2^2S	2^2P			
		$a_{\rm c}$	$a_{\rm c}$	$a_{\rm sd}$	a_l	$b_{\rm q}$
LiI	This work	2.90313	−0.21359	−0.01341	0.06309	−0.02242
	Ref. [11]	2.9085	−0.2070	−0.01332	0.06262	−0.02254
BeII	This work	12.49306	−1.07036	−0.10197	0.48509	−0.18422
	Ref. [11]	12.559	−1.0548	−0.10214	0.4832	−0.18312
BIII	This work	31.45032	−2.43966	−0.32285	1.53639	−0.59362
	Ref. [11]	31.56	−2.4105	−0.3222	1.539	−0.5936
CIV	This work	62.75126	−4.24652	−0.72193	3.46632	−1.35081
	Ref. [11]	62.91	−4.1625	−0.7208	3.466	−1.35
NV	This work	109.44747	−6.49565	−1.35185	6.52407	−2.55702
	Ref. [11]	109.61	−6.3735	−1.3498	6.525	−2.5548
OVI	This work	174.40823	−9.16048	−2.25818	10.95936	−4.29855
	Ref. [11]	174.63	−9.075	−2.26	10.97	−4.312
FVII	This work	267.45862	−12.23734	−3.49613	17.02184	−6.70673
	Ref. [11]	260.8	−12.12	−3.498	17.03	−6.712
NeVIII	This work	371.52344	−15.80422	−5.11818	24.96146	−9.85859
	Ref. [11]					

Table 5. Comparison between different theoretical calculations of the *Fermi* contact term (a_c) for the Li-like $1s^2ns$ ($n = 3$, 4, and 5) configurations. (in a.u.)

		3^2S	4^2S	5^2S
LiI	This work	0.67451	0.25366	0.12100
	Ref. [19]	0.67026	0.23065	0.113117
BeII	This work	3.18087	1.25071	0.61419
	Ref. [19]	3.17253	1.25229	0.61800
BIII	This work	8.33669	3.34097	1.65744
	Ref. [19]	8.32806	3.34148	
CIV	This work	17.02574	6.89190	3.44268
	Ref. [19]	17.01778	6.89443	
NV	This work	30.13893	12.39569	6.16654
	Ref. [19]	30.12749	12.29126	
OVI	This work	48.41444	19.98798	10.00637
	Ref. [19]	48.54534	19.90327	
FVII	This work	73.12239	30.05274	15.19325
	Ref. [19]	73.15853	30.10441	
NeVIII	This work	104.78986	43.23145	21.87968
	Ref. [19]	104.8572	43.26988	

results should be about five digits. Since we concentrate our attention on the non-relativistic hyperfine structure parameters, the small relativistic corrections are not computed in this work. Our results for Li is in good agreement with the recent Hylleraas calculations, and with the experimental data. For the other Z systems, at present very little experimental data is available in the literature. For these Li-like ions, our calculated values agree reasonably well with the other theoretical results in the literature. We hope that the present results may stimulate experimentalists to further their efforts to carry out measurements of these systems.

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