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Calculations on the hyperfine constants of the ground states for lithium-like system*

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In this paper a relativistic many-body perturbation calculation is performed to calculate the hyperfine constants of the ground states for lithium-like isoelectronic sequence. Zeroth-order hyperfine constants are calculated with Dirac–Fock wavefunctions, and the finite basis sets of the Dirac–Fock equations are constructed by B splines. With the finite basis sets, the core polarization and the correlation effect are evaluated.

Keywords: hyperfine constant, many-body perturbation calculation, lithium-like ion
PACC: 3510F, 3130G, 3115

1. Introduction

With the development of experimental researches of the new optical frequency standards, studies of the hyperfine structure have become more and more important.[1−3] The hyperfine structure is caused by the interaction between the electrons and the electromagnetic multipole moments of the nucleus. Through the study of hyperfine structures, one can obtain both the information of nuclear structure and the electronic properties of atoms. During the last few decades, various experimental techniques, such as atomic-beam magnetic resonance method,[4−6] cascade anticrossing spectroscopy,[7] and collinear fast beam-laser spectroscopy,[8−10] have been used to measure the hyperfine structure of different atoms. Simultaneously, many theoretical methods including multiconfiguration Hartree–Fock (MCHF),[11] configuration-interaction methods,[12] multiconfiguration Dirac–Fock (MCDF),[13] many-body perturbation theory,[14] and so on,[15−17] have been developed for accurate calculations on hyperfine interactions.

Many-body perturbation theory (MBPT) provides a powerful and systematic method (with well-defined levels of perturbation) to calculate the properties of many-electron systems. The effective operator form of MBPT was developed and applied to calculate hyperfine structures by Garpman *et al.*[18,19] Lindgren[20] has presented a nonrelativistic coupled-cluster calculation of the energy levels and hyperfine constants of neutral lithium in which he sums infinite sets of MBPT terms and obtains very close agreement with experiments. Blundell *et al*[21] reported relativistic all-order MBPT calculations of energies and matrix elements for Li and Be^+. However, systematic studies of hyperfine constants for lithium-like ions are still needed for explaining experiments.

In this paper, we carry out a relativistic MBPT calculation for lithium-like isoelectronic sequence ($Z = 3 - 9$). The orbital energies are calculated with Dirac–Fock wavefunctions, and the finite basis sets of the Dirac–Fock equations are constructed by B splines. With the finite basis sets, the core polarization and the correlation effect are calculated, and the hyperfine structure constants of the ground states for lithium-like isoelectronic sequence ($Z = 3 - 9$) are obtained to display the systematic regularity of the system. The results are compared with those of other accurate calculations as well as with available experimental data.

2. Theory and method

The relativistic Hamiltonian for an atomic system is given by

$$H = H_0 + V, \tag{1}$$

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with

$$H_0 = \sum_{i=1}^{N}[c\boldsymbol{\alpha}_i\cdot\boldsymbol{p}_i+(\beta_i-1)c^2+V_{\rm nuc}(r_i)]+\sum_{i=1}^{N}u(r_i), \quad (2)$$

and

$$V = \sum_{i<j}\frac{1}{r_{ij}} - \sum_{i=1}^{N}u(r_i). \quad (3)$$

The contribution from the hyperfine interaction to the Hamiltonian can be represented by an expansion in multipoles of order K,

$$H_{\rm hfs} = \sum_{K=1}^{\infty}\boldsymbol{T}^{(K)}\cdot\boldsymbol{M}^{(K)}, \quad (4)$$

where $\boldsymbol{T}^{(K)}$ and $\boldsymbol{M}^{(K)}$ are spherical tensor operators of rank K in the electronic and nuclear space respectively.[22]

For single-electron system outside closed shells, the generalized hyperfine structure constants are[23]

$$\begin{aligned} A_K &= \langle\gamma jj|T_0^{(K)}|\gamma jj\rangle M_0^{(K)} \\ &= \begin{pmatrix} j & K & j \\ -j & 0 & j \end{pmatrix}\langle\gamma j\|T^{(K)}\|\gamma j\rangle M_0^{(K)}. \end{aligned} \quad (5)$$

For the magnetic-dipole hyperfine constant, $K = 1$. In the relativistic case, the traditionally used magnetic dipole hyperfine constant is

$$\begin{aligned} a = \frac{A_1}{Ij} &= \frac{\mu_{\rm I}}{Ij}\langle\gamma jj|T_0^{(1)}|\gamma jj\rangle \\ &= \frac{\mu_{\rm I}}{Ij}\begin{pmatrix} j & 1 & j \\ -j & 0 & j \end{pmatrix}\langle j\|T^{(1)}\|j\rangle, \end{aligned} \quad (6)$$

where I, $\mu_{\rm I}$ and j are the nuclear spin, magnetic-dipole moment, and total angular momentum of the electrons respectively.

In order to evaluate second- and third-order perturbation diagrams, a complete set of single-particle states are needed. We construct a complete finite basis set of the Dirac–Fock equations by B splines. Numerical techniques employing B splines are recognized as extremely powerful tools for computational problems in physics. Details of B splines can be found in the book of deBoor[24] and the formalism underlying our computational procedure can be found in Refs.[25,26].

Following Lindgren and Morrison,[19] the contribution of the core polarization to the hyperfine interaction can be calculated to all orders:

$$\begin{aligned} \Delta_{nj}^K = 2\sum_{ark}&(-1)^{k+j_m+j_r-1}(2j+1)[(2j_r+1)(2j_a+1)]^{1/2} \\ &\times[\,(-1)^{(3j_a+j_r+K)}\frac{\delta(k,K)}{2K+1}\begin{pmatrix} j & k & j \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{pmatrix} j_r & k & j_a \\ -1/2 & 0 & 1/2 \end{pmatrix}R^k(mr,na) \\ &-(-1)^{2j+K}\begin{pmatrix} j & k & j_a \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{pmatrix} j_r & k & j \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{Bmatrix} j & K & j \\ j_r & k & j_a \end{Bmatrix}R^k(mr,an)\,]\,\overline{h_a^r}^{(N)}, \end{aligned} \quad (7)$$

$$(\varepsilon_a-\varepsilon_r)\overline{h_a^r}^{(N)} = \langle r\|T^K\|a\rangle + \sum_{bsk}[G_1X^k(rb,as)-G_2X^k(br,as)]\overline{h_a^r}^{(N-1)}, \quad (8)$$

and

$$\overline{h_a^r}^{(0)} = \frac{\langle r\|T^K\|a\rangle}{\varepsilon_a-\varepsilon_r}. \quad (9)$$

With Eqs.(7)–(9), we use an iterative procedure to carry out the core polarization to all orders.

According to Lindgren and Morrison, the diagrams involving at least one double excitation are called the lowest-order correlations which are third-order hyperfine diagrams. There are 65 such correlation diagrams. The algebraic expression for one of these diagrams shown in Fig. 1 is

$$\begin{aligned} a_m^+a_n^+\sum_{rsta}&\frac{\langle m|T_Q^K|t\rangle\langle ta|r_{12}^{-1}|rs\rangle\langle rs|r_{12}^{-1}|na\rangle}{(\varepsilon_m-\varepsilon_t)(\varepsilon_n+\varepsilon_a-\varepsilon_r-\varepsilon_s)} = a_m^+a_n^+\sum_{rstak}\delta(j_t,j)\frac{(2j_r+1)(2j_a+1)(2j_s+1)}{2k+1} \\ &\times\begin{pmatrix} j & k & j_r \\ -1/2 & 0 & 1/2 \end{pmatrix}^2\begin{pmatrix} j_a & k & j_s \\ -1/2 & 0 & 1/2 \end{pmatrix}^2\frac{\langle m\|T^K|t\rangle R^k(ta,rs)R^k(rs,na)}{(\varepsilon_m-\varepsilon_t)(\varepsilon_n+\varepsilon_a-\varepsilon_r-\varepsilon_s)}, \end{aligned} \quad (10)$$

where T_Q^K is the hyperfine operator. The other expressions, such as $R^k(ta, rs)$, $X^k(rb, as\cdots)$, can be found in our former work. [25] In our program, we calculate all 65 such diagrams. In addition to the 65 diagrams, there are numerous second- and higher-order correlation diagrams, which need a lot of time to evaluate and are expected to be small.[27] Therefore, in order to estimate the effects of these diagrams, we only evaluate a few of them and the estimated values are included in our results. In order to get higher precision, we treat the atomic nuclei as Fermi nuclei,[28] not point charges, and the Gaussian integral is used in our programs.

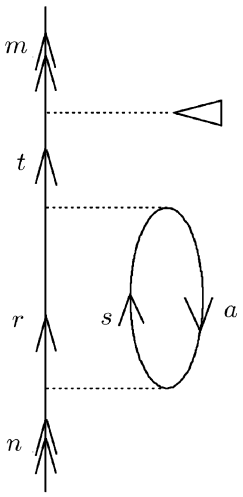


Fig.1. One of the 65 lowest-order correlation diagrams.

3. Results and discussion

In this paper we calculate the Dirac–Fock orbital energies for the lithium-like isoelectronic sequence ($Z = 3 - 9$) with the finite basis sets constructed by B splines. The results are given in Table 1 and Table 2. From Table 1 and Table 2, we can see that our results for lithium and orbital energies of $n = 2$ states and 3s state for lithium-like ions ($Z = 4 - 9$) are in very close agreement with the accurate theoretical data of Lindgren,[20] who calculated energies using Brueckner orbitals within the framework of non-relativistic MBPT, and with the zeroth-order Dirac–Hartree–Fock energies of Johnson *et al*,[21,29,30] who evaluated these energies in relativistic second- and third-order MBPT. This indicates that the wavefunctions in this work are quite accurate and reliable to evaluate the core polarization and the correlation effect in the hyperfine interactions.

Table 1. Orbital energies of ^{7}Li (units of a.u.).

state[a)]	This work	Lindgren[b)]	Johnson *et al*[c)]
2s	−0.196320	−0.196304	−0.19632
2p*	−0.128638		−0.12864
2p	−0.128636		−0.12864
3s	−0.073801		−0.07380
3p*	−0.056772		−0.05677
3p	−0.056771		−0.05677
3d*	−0.055562		−0.05556
3d	−0.055562		−0.05556

[a)] Notation: $p^* = p_{1/2}$, $p = p_{3/2}$, etc. [b)] Ref.[20], [c)] Ref.[29].

In Table 3, the hyperfine structure constants a for the ground states of the system are given. $H(1)$ is the Dirac–Fock contribution, $H(2)$ is the complete polarization, $H(3)$ is the first-order correlation, and 'Total' is $H(1) + H(2) + H(3)$. From Table 3, we can see that our total results for Li and Be^+ agree with the experimental data [31,32] at the level of a few percent, and are also compatible with the theoretical work [20,21] in which the core polarization and the pair correlation are evaluated essentially to all orders of perturbation theory. The difference between our data and other theoretical ones is mainly due to the fact that only the first-order correlation effect is taken into account in the total results. However, the Dirac–Fock contributions to the constant a are 284.43 MHz for Li and −497.89 MHz for Be^+ in this work. They agree very well with the values obtained in Ref.[21], which are 284.65 MHz and –498.23 MHz respectively. As mentioned above, the second- and higher-order correlation diagrams need a lot of time to evaluate. We consider only a few of them and give the estimated values of second- and higher-order correlation effects $H(4)$ in column 8 of Table 3, and 'Final' is 'Total' + $H(4)$. The differences between the final results and the experimental data for Li and Be^+ are less than one percent. Since the relativistic wavefunctions are quite reliable in our method, more accurate data could be expected to be given for heavier atoms for which relativistic effects become more appreciable.

Table 3 also shows the contributions from different parts of the hyperfine operator to the final results of the hyperfine structure constant a. We can see that the Dirac–Fock contribution to the constant a increases with increasing Z. Figure 2 shows this relation. This is because the Dirac–Fock contribution comes from the central-field model. In an isoelectronic sequence, the central-field from the nucleus plays a more and more important role when the atomic number Z of the nucleus increases.

Table 2. Orbital energies of lithium-like isoelectronic sequence ($Z = 4 - 9$) (units of a.u.).

state[a]	2s	2p*	2p	3s	3p*	3p	3d*	3d
				$^{9}Be^{+}$				
This work	−0.666183	−0.519447	−0.519406	−0.266523	−0.228427	−0.228414	−0.222297	−0.222294
Other theo.[b]	−0.666183	−0.519447	−0.519406	−0.266523				
				$^{11}B^{2+}$				
This work	−1.390127	−1.167352	−1.167158	−0.571939	−0.513170	−0.513112	−0.500238	−0.500224
Other theo.[c]	−1.390126	−1.167352	−1.167158					
				$^{13}C^{3+}$				
This work	−2.365898	−2.068823	−2.068242	−0.989177	−0.909976	−0.909803	−0.889383	−0.889340
Other theo.[c]	−2.365898	−2.068823	−2.068242					
				$^{15}N^{4+}$				
This work	−3.592973	−3.222506	−3.221143	−1.518015	−1.418496	−1.418093	−1.389735	−1.389632
Other theo.[c]	−3.592973	−3.222506	−3.221143					
				$^{17}O^{5+}$				
This work	−5.071312	−4.627921	−4.625184	−2.158422	−2.038630	−2.037822	−2.001307	−2.001092
Other theo. [c]	−5.071312	−4.627921	−4.625184					
				$^{19}F^{6+}$				
This work	−6.801084	−6.284988	−6.280044	−2.910444	−2.770387	−2.768928	−2.724121	−2.723724
Other theo.[c]	−6.801084	−6.284988	−6.280043					

[a] Notation: $p^* = p_{1/2}$, $p = p_{3/2}$, etc. [b] Ref. [21], [c] Ref.[30].

Table 3. Contributions from different parts of the hyperfine operator to the a factors of the ground states for lithium-like isoelectronic sequence ($Z = 3 - 9$) (units of MHz). $H(1)$ is the Dirac–Fock contribution, $H(2)$ complete polarization, $H(3)$ the first-order correlation, and 'Total' is $H(1)+H(2)+H(3)$. $H(4)$ is the estimated second- and higher-order correlations, and 'Final' is 'Total' $+H(4)$.

Isotope	I	μ_I	$H(1)$	$H(2)$	$H(3)$	Total	$H(4)$	Final	$H(1)$/Final	Other theo.	Exp.
^{7}Li	3/2	3.2564	284.43	95.34	13.88	393.65	5.69	399.34	71.23%	403.53[a] 402.47[b]	401.75[c]
$^{9}Be^{+}$	3/2	−1.1775	−497.89	−110.62	−12.06	−620.57	−4.98	−625.55	79.59%	−625.63[b]	−625.01[d]
$^{11}B^{2+}$	3/2	2.6886	3036.88	504.30	44.37	3585.55	18.22	3603.77	84.27%		
$^{13}C^{3+}$	1/2	0.7024	4921.91	652.52	48.28	5622.71	19.69	5642.40	87.23%		
$^{15}N^{4+}$	1/2	−0.2832	−3546.76	−391.28	−25.00	−3963.04	−10.64	−3973.68	89.26%		
$^{17}O^{5+}$	5/2	−1.8938	−7691.31	−726.57	−40.88	−8458.75	−15.38	−8474.13	90.76%		
$^{19}F^{6+}$	1/2	2.6289	80923.62	6685.40	336.06	87945.08	161.85	88106.93	91.85%		

[a] Ref.[20], [b] Ref.[21], [c] Ref.[31], [d] Ref.[32].

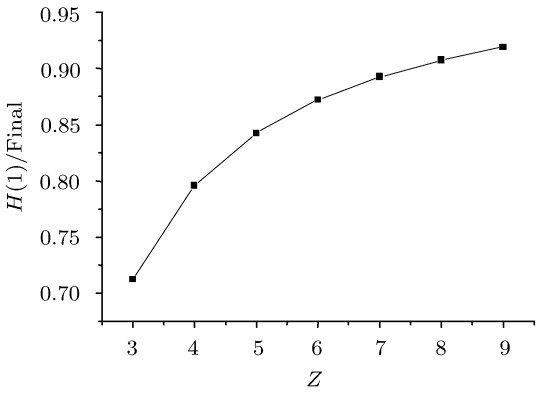


Fig.2. The Dirac–Fock contribution to the a factor increases with Z.

4. Conclusions

In this work we have performed a relativistic MBPT calculation for lithium-like isoelectronic sequence ($Z = 3 - 9$), where the orbital energies and hyperfine constants of the ground states are evaluated. The relativistic wavefunctions used in this work are quite accurate to calculate the core polarization and the correlation effect in the hyperfine interactions. The principal discrepancy between our results and experiments is due to the uncalculated higher-order correlation effects. It is believed that the accuracy of these calculations could be improved by including the

omitted effects perturbatively. We hope that our theoretical results will be useful for analysing future experiments.

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