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HYPERFINE STRUCTURE PARAMETERS FOR Li-LIKE MULTICHARGED IONS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

Abstract. The relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation is applied to calculation of the hyperfine structure parameters for some Li-like multicharged ions. The relativistic, exchange-correlation and other corrections are accurately taken into account. The optimized relativistic orbital basis set is generated in the optimal many-body perturbation theory approximation with fulfilment of the gauge invariance principle. The obtained data on the hyperfine structure parameters of the Li-like multicharged ions are analyzed and compared with alternative theoretical and experimental results.

1. Introduction

In last years a studying the spectra of heavy and superheavy elements atoms and ions is of a great interest for further development as atomic and nuclear theories (c.f.[1-12]). Theoretical methods used to calculate the spectroscopic characteristics of heavy and superheavy ions may be divided into three main groups: a) the multi-configuration Hartree-Fock method, in which relativistic effects are taken into account in the Pauli approximation, gives a rather rough approximation, which makes it possible to get only a qualitative idea on the spectra of heavy ions. b) The multi-configuration Dirac-Fock (MCDF) approximation (the Desclaux program, Dirac package) [1-4] is, within the last few years, the most reliable version of calculation for multielectron systems with a large nuclear charge; in these calculations one- and two-particle relativistic effects are taken into account practically precisely.

The calculation program of Desclaux is compiled with proper account of the finiteness of the nucleus size; however, a detailed description of the method of their investigation of the role of the nucleus size is lacking.

In the region of small Z (Z is a charge of the nucleus) the calculation error in the MCDF approximation is connected mainly with incomplete inclusion of the correlation and exchange effects which are only weakly dependent on Z; c) In the study of lower states for ions with $Z \leq 40$ an expansion into double series of the PT on the parameters 1/Z, aZ (a is the fine structure constant) turned out to be quite useful. It permits evaluation of relative contributions of the different expansion terms: non-relativistic, relativistic, QED contributions as the functions of Z.

Nevertheless, the serious problems in calculation of the heavy elements spectra are connected with developing new, high exact methods of account for the QED effects, in particular, the Lamb shift (LS), self-energy (SE) part of the Lamb shift, vacuum polarization (VP) contribution, correction on the nuclear finite size for superheavy elements and its account for different spectral properties of these systems, including calculating the energies and constants of the hyperfine structure, deriviatives of the one-electron characteristics on nuclear radius, nuclear electric quadrupole, magnetic dipole moments etc (c.f.[1-10]).

In this paper the relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation [11-19] is applied to calculation of the hyperfine structure parameters for Li-like multicharged ions. The relativistic, exchange-correlation and nuclear effects corrections are accurately taken into account with using the consistent and high precise procedures (c.g. [11-17]).

2. Relativistic many-body perturbation theory with optimized zeroth approximation and energy approach

The theoretical basis of the RMBPT with the Dirac-Kohn-Sham zeroth approximation was widely discussed [11-17], and here we will only present the essential features. As usually, we use the charge distribution in atomic (ionic) nucleus $r(r)$ in the Gaussian approximation:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right) \qquad (1)$$

where $\gamma = 4/pR^2$ and R is the effective nucleus radius. The Coulomb potential for the spherically symmetric density $r(r)$ is:

$$V_{nucl}(r|R) = -\left((1/r)\int_0^r dr' r'^2 \rho\left(r'|R\right) + \int_r^\infty dr' r' \rho\left(r'|R\right)\right) \qquad (2)$$

Further consider the Dirac-like type equations for the radial functions F and G (components of the Dirac spinor) for a three-electron system $1s^2nlj$. Formally a potential $V(r|R)$ in these equations includes electric and polarization potentials of the nucleus, V_X is the exchange inter-electron interaction (in the zeroth approximation). The standard Kohn-Sham (KS) exchange potential is [13]:

$$V_X^{KS}(r) = -(1/\pi)[3\pi^2\rho(r)]^{1/3}. \qquad (3)$$

In the local density approximation the relativistic potential is [33]:

$$V_X[\rho(r),r] = \frac{\delta E_X[\rho(r)]}{\delta\rho(r)}, \qquad (4)$$

where $E_X[\rho(r)]$ is the exchange energy of the multielectron system corresponding to the homogeneous density $\rho(r)$, which is obtained from a Hamiltonian having a transverse vector potential describing the photons. In this theory the exchange potential is [3,4]:

$$V_X[\rho(r),r] = V_X^{KS}(r)\cdot\{\frac{3}{2}\ln\frac{[\beta+(\beta^2+1)^{1/2}]}{\beta(\beta^2+1)^{1/2}} - \frac{1}{2}\}, \qquad (5)$$

where $\beta = [3\pi^2\rho(r)]^{1/3}/c$, c is the velocity of light. The corresponding one-quasiparticle correlation potential

$$V_C[\rho(r),r] = -0.0333\cdot b\cdot\ln[1+18.3768\cdot\rho(r)^{1/3}], \qquad (6)$$

(here b is the optimization parameter; see below).

The perturbation operator contains the relativistic potential of the interelectron interaction of the form:

$$V_{e-e}^{rel}(r_i,r_j) = \frac{\left(1-\alpha_i\alpha_j\right)}{r_{ij}}\exp(i\omega_{ij}r_{ij}), \qquad (7)$$

(here a_i, a_j are the Dirac matrices, w_{ij} is the transition frequency) with the subsequent subtraction of the exchange and correlation potentials. The rest of the exchange and correlation effects is taken into account in the first two orders of the PT (c.g.[3-5].

In Refs. [20-29] it was presented the effective relativistic formalism with ab initio optimization principle for construction of the optimal relativistic orbital basis set. The minimization condition of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of the atomic levels is used. The alternative versions are proposed in refs. [30-37].

The general scheme of treatment of the spectra for Li-like ion is as follows. Consider the Dirac-type equations for a three-electron system $1s^2nlj$. Formally they fall into one-electron Dirac equations for the orbitals $1s$ 1s and nlj with the potential:

$$V(r) = 2V(r|1s) + V(r|nlj) + V_x(r) + V(r|R) \qquad (8)$$

$V(r|R)$ includes the electrical and the polarization potentials of the nucleus; the components of the self-consistent Hartree-like potential, V_{ex} is the exchange inter-electron interaction (look below). The main exchange effect will be taken into account if in the equation for the $1s$ orbital we assume

$$V(r) = V(r|1s) + V(r|nlj) \qquad (9)$$

and in the equation for the nlj orbital

$$V(r) = 2V(r|1s) \qquad (10)$$

The rest of the exchange and correlation effects will be taken into account in the first two orders of the PT by the total inter-electron interaction [13-17].

The used expression for $\rho(r|1s)$ coincides with the precise one for a one-electron relativistic atom with a point nucleus. The finiteness of the nucleus and the presence of the second $1s$ electron are included effectively into the energy E_{1s}.

Actually, for determination of the properties of the outer nlj electron one iteration is sufficient. Refinement resulting from second iteration (by evaluations) does not exceed correlation corrections of the higher orders omitted in the present calculation.

The relativistic potential of core (the "screening" potential) $2V^{(1)}(r|1s) = V_{scr}$ has correct asymptotic at zero and in the infinity. The procedures for accounting of the nuclear, radiative QED corrections are in details presented in Refs. [3-5,14, 39-42].

3. Results and Conclusions

Energies of the quadruple (W_q) and magnetic dipole (W_m) interactions, which define a hyperfine structure, are calculated as follows [4]:

$$W_q = [D + C(C+1)]B,$$

$$W_m = 0,5\ AC,$$

$$D = -(4/3)(4c-1)(I+1)/[i(I-1)(2I-1)],$$

$$C = F(F+1) - J(J+1) - I(I+1). \qquad (16)$$

Here I is a spin of nucleus, F is a full momentum of system, J is a full electron momentum. Constants of the hyperfine splitting are expressed through the standard radial integrals:

$$A = \{[(4,32587)10^{-4}Z^2 cg_I]/(4c^2-1)\}(RA)_{-2}, \qquad (17)$$

$$B = \{7.2878\ 10^{-7}\ Z^3 Q/[(4c^2-1)I(I-1)\}\ (RA)_{-3},$$

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (in Barn); radial integrals are defined as follows:

$$(RA)_{-2} = \int_0^\infty dr r^2 F(r) G(r) U(1/r^2, R),$$

$$(RA)_{-3} = \int_0^\infty dr r^2 [F^2(r) + G^2(r)] U(1/r^3, R) \qquad (18)$$

and calculated in the Coulomb units ($=3,57$ $10^{20}Z^2 m^{-2}$; $= 6,174\ 10^{30}Z^3 m^{-3}$ for valuables of the corresponding dimension). The radial parts F and G of two components of the Dirac function for electron, which moves in the potential $V(r;R) + U(r,R)$, are determined by solution of the Dirac equations (look above).

We have carried out the calculation of constants of the hyperfine interaction: the electric quadruple constant B, the magnetic dipole constant A with inclusion of nuclear finiteness and the Uehling potential for Li-like ions (c.g. [3-5]).

In table 4 the calculation results for the constants of the hyperfine splitting for the lowest excited states of Li-like ions are presented.

Analogous data for other states have been presented earlier (see ref. [5,20]). Our calculation showed also that a variation of the nuclear radius on several persents could lead to to changing the transition energies on dozens of thousands $10^3 cm^{-1}$.

Table 1.

Constants of the hyperfine electron-nuclear interaction: $A = Z^3 g_I\ \overline{A}$ **cm**$^{-1}$, $B = \dfrac{Z^3 Q}{I(2I-1)}\ \overline{B}$ **cm**$^{-1}$

nlj	Z	69	79	92
$2s$	$\overline{A}$	176 -02	215 -02	314 -02
$3s$	$\overline{A}$	51 –03	63 –03	90 –03
$4s$	$\overline{A}$	19 –03	24 –03	36 –03

$2p_{1/2}$	$\overline{A}$	56 –03	71 –03	105 –02
$3p_{1/2}$	$\overline{A}$	16 –03	20 –03	31 –03
$4p_{1/2}$	$\overline{A}$	72 –04	91 –04	11 –03
$2p_{3/2}$	$\overline{A}$	67 –04	71 –04	72 –04
	$\overline{B}$	13 –04	15 –04	17 –04
$3p_{3/2}$	$\overline{A}$	19 –04	21 –04	22 –04
	$\overline{B}$	51 –05	55–05	62 –05
$4p_{3/2}$	$\overline{A}$	89 –05	92 –05	8 –04
	$\overline{B}$	20 –05	22 –05	26 –05
$3d_{3/2}$	$\overline{A}$	10 –04	11 –04	12 –04
	$\overline{B}$	9 –05	10 –05	11 –05
$4d_{3/2}$	$\overline{A}$	51 –05	55 –05	58 –05
	$\overline{B}$	44 –06	50 –06	56 –06
$3d_{5/2}$	$\overline{A}$	48 –05	50 –05	52 –05
	$\overline{B}$	38 –06	39 –06	40 –06
$4d_{5/2}$	$\overline{A}$	19 –05	20 –05	21 –05
	$\overline{B}$	15 –06	16 –06	17 –06

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Summary. The relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation is applied to calculation of the hyperfine structure parameters for some Li-like multicharged ions. The relativistic, exchange-correlation and other corrections are accurately taken into account. The optimized relativistic orbital basis set is generated in the optimal many-body perturbation theory approximation with fulfilment of the gauge invariance principle. The obtained data on the hyperfine structure parameters of the Li-like multicharged ions are analyzed and compared with alternative theoretical and experimental results.

Keywords: Relativistic many-body perturbation theory – Optimal one-quasiparticle representation – Oscillator strengths –Energy approach – Correlation corrections

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ПАРАМЕТРЫ СВЕРХТОНКОЙ СТРУКТУРЫ ДЛЯ Li-ПОДОБНЫХ МНОГОЗАРЯДНЫХ ИОНОВ В РАМКАХ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме. Релятивистская многочастичная теория возмущений с оптимизированным нулевым приближением Дирака-Кона-Шэма применена для расчета параметров сверхтонкой структуры Li-подобных многозарядных ионов. Релятивистские, обменно-корреляционные и другие поправки учитываются в рамках последовательных процедур. Оптимизированный базис релятивистских орбиталей генерируется в последовательном нулевом приближении релятивистской многочастичной теории возмущений, исходя из условия выполнения принципа калибровочной инвариантности. Полученные данные для параметров сверхтонкой структуры для Li-подобных многозарядных ионов анализируются и сравниваются с альтернативными теоретическими и экспериментальными результатами.

Ключевые слова: Релятивистская многочастичная теория возмущений., сверхтонкая структура, литий-подобные ионы

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ПАРАМЕТРИ НАДТОНКОЇ СТРУКТУРИ ДЛЯ Li-ПОДІБНИХ БАГАТОЗАРЯДНИХ ІОНІВ В РАМКАХ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ

Резюме. Релятивістська багаточастинкова теорія збурень з оптимізованим нульовим наближенням Дірака-Кона-Шема застосована для розрахунку параметрів надтонкої структури для Li-подібних багатозарядних іонів. Релятивістські, обмінно-кореляційні та інші поправки

враховуються в рамках послідовних процедур. Оптимізований базис релятивістських орбіталей генерується в послідовному нульовому наближенні релятивістської багаточастинкової теорії збурень, виходячи з умови виконання принципу калібрувальної інваріантності. Отримані дані параметрів надтонкої структури для Li-подібних багатозарядних іонів порівнюються з альтернативними теоретичними і експериментальними результатами.

Ключові слова: Релятивістська багаточастинкова теорія збурень, надтонка структура, літій-подібні іони