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ADVANCED STUDY OF SPECTRAL AND HYPERFINE STRUCTURE PARAMETERS FOR Li-LIKE MULTICHARGED IONS WITHIN RELATIVISTIC THEORY

The relativistic many-body perturbation theory with the optimized Dirac zeroth approximation is applied to calculation of some fundamental characteristics of the hyperfine structure of middle and heavy 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 performance of the gauge invariance principle. There are listed the calculated values of derivatives of the one-electron characteristics, including the hyperfine structure parameters, on nuclear radius for the Li-like multicharged ions with the corresponding analysis.

1. Introduction

In the last few decades a study of energy, spectral and radiation properties of the multicharged ions has a subject of significant interest for many physical, astrophysical and chemical applications. The levels energies, transitions probabilities, oscillator strengths and so on are very important in atomic physics (spectroscopy, spectral lines theory), astrophysics, plasma physics, laser physics, quantum electronics. They are very much needed in research of thermonuclear reactions, where the ionic radiation is one of the primary loss mechanisms and so on. The spectral lines belonging to the radiation of many multicharged ions have been identified in both solar flares and nonflaring solar active regions, observed in high-temperature plasmas, such as pinches and laser-produced plasmas, and in beam-foil spectra.

The multiple observations of satellite lines of the He-, Li-, Be-like multicharged ions in the solar corona and in laboratory plasmas have emphasized the need for accurate values of the energetic and spectroscopic parameters for multicharged ions (c.f.[1-15]).

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.

Howver, it is well known that 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 Z40 an expansion into double series of the PT on the parameters 1/Z, αZ (α 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 meth-

ods 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.[1-15]). In this work the relativistic many-body perturbation theory with the optimized Dirac zeroth approximation (e.g.[13-15]) is applied to calculation of some fundamental characteristics of the hyperfine structure of middle and heavy Li-like multicharged ions. There are listed the calculated values of derivatives of the one-electron characteristics, including the hyperfine structure parameters, on nuclear radius for the Li-like multicharged ions with the corresponding analysis. It should be noted that the Li-like ions was always a subject of intensive theoretical and experimental studying (e.g. [1-4, 13-15, 18]).

2. Relativistic theory of determination hyperfine structure parameters

The theoretical basis of the RMBPT with the Dirac-Kohn-Sham zeroth approximation was in details presented in papers [13-15] (see [2-4] too), and here we will only present the essential features. As usually, we use the charge distribution in atomic (ionic) nucleus $\rho(r)$ in the Gaussian approximation:

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

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

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

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 [2]:

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

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:

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

(here α_i ,α_j are the Dirac matrices, ω_{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.[2-4].

In Refs. [2-4,17-22] 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 $1s^2$nlj. Formally they fall into one-electron Dirac equations for the orbitals $1s$1s and nlj with the potentials:

$$V(r)=2V(r\vee 1s)+V(r\vee \mathrm{nlj})+V_x(r)+V(r\vee R) \tag{8}$$

$V(r\vee R)$ includes the electrical and the polarization potentials of the nucleus; the components of the self-consistent Hartree-like potential, $V_{\mathrm{ex}}$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

$$V(r)=V(r\vee 1s)+V(r\vee \mathrm{nlj}) \tag{9}$$

and in the equation for the nlj orbital

$$V(r)=2V(r\vee 1s) \tag{10}$$

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 [13-15,18-20].

The used expression for $\rho(r\vee 1s)$ 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) $2V^{(1)}(r\vee 1s)=V_{\mathrm{scr}}$ 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. [2-4,13-24].

3. Results and Conclusions

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

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

$$W_\mu=0{,}5\ AC,$$

$$\Delta=-(4/3)(4\chi-1)(I+1)/[i(I-1)(2I-1)],$$

$$C=F(F+1)-J(J+1)-I(I+1). \tag{11}$$

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:

$$A=\{[(4{,}32587)10^{-4}Z^2\chi g_I]/(4\chi^2-1)\}(RA)_{-2}, \tag{12}$$

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

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (in Barn); radial integrals are defined as follows [4,18]:

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

$$(RA)_{-3}=\int_0^\infty drr^2[F^2(r)+G^2(r)]U(1/r^3,R) \tag{13}$$

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). In table 1 there are listed the calculated values of derivatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2l,3l,4l (l=0) states of the Li-like ions with minimally possible valus of j:

$$d\langle|V|\rangle/dR=Z^3DV\ (\mathrm{cm}^{-1}/\mathrm{cm});$$

$$d\langle|U|\rangle/dR=Z^5DU \text{ (cm}^{-1}\text{/cm)}, \quad (14)$$

$$dA/dR=Z^4g_IDA \text{ (cm}^{-1}\text{/cm)}.$$

Here 1cm^{-1} is an energy unit and 1cm is a length unit.

Table 1 Derivatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2s,3s,4s states of the Li-like ions: $d\langle|V|\rangle/dR=Z^3DV$, $d\langle|U|\rangle/dR=Z^5DU$, $dA/dR=Z^4g_IDA$

nlj Z		30	41	59
$2s_{1/2}$	*DV*	20+11	41 +11	121 +12
	DU	14+06	16 +06	20 +06
	DA	19+06	24 +06	44 +06
$3s_{1/2}$	*DV*	60+10	12 +11	35 +11
	DU	42+05	44 +05	60 +05
	DA	56+05	74 +05	12 +06
$4s_{1/2}$	*DV*	24+10	51 +10	13 +11
	DU	17+05	18 +05	24 +05
	DA	23+05	30 +05	55 +05
nlj Z		69	79	92
$2s_{1/2}$	*DV*	223 +12	415 +12	967 +12
	DU	25 +06	36 +06	64 +06
	DA	63 +06	101 +07	197 +07
$3s_{1/2}$	*DV*	65 +11	122 +12	293 +12
	DU	81 +05	10 +06	18 +06
	DA	18 +06	29 +06	57 +06
$4s_{1/2}$	*DV*	26 +11	50 +11	121 +12
	DU	32 +05	47 +05	80 +05
	DA	81 +05	11 +05	23 +05

Let us remember that here V is a potential of the elctron-nuclear interaction and U is the Serber-Uehling vacuum-polarization potential. Considered value of full moment is j=3/2 for deriviative of the constant B on nuclear radius $\partial B/\partial R$ and value j=3/2 for other operators. It should be noted that the corresponding characteristics are less sensitive to the nuclear size for states with the large values of moment j. In any case cited effects are not observed in the modern experiment. In table 2 we present the calculated values of derivatives of the hfs constant B on nuclear radius (in cm^{-1}/cm); $dB/dR= -Z^4QDB/[I(2I-1)]$.

Table 2 Deriviatives of the hfs constant B on nuclear radius (in cm^{-1}/cm) $dB/dR= -Z^4QDB/[I(2I-1)]$.

Nlj	*Z*	20	41	59
$2p_{3/2}$	*DB*	02+02	11+02	17+02
$3p_{3/2}$	*DB*	19+01	37+01	57+01
$4p_{3/2}$	*DB*	03+01	11+01	21+01
nlj	*Z*	69	79	92
2p3/2	*DB*	27+02	40+02	71+02
3p3/2	*DB*	95+01	15+02	27+02
4p3/2	*DB*	38+01	60+02	12+02

Let us note that for derivatives in tables 1,2 the main member of degree dependence upon a charge Z is separated. The remained Z-dependence is directly connected with relativistic and nuclear (the finite nuclear charge) effects in the one-electron functions.

References

1. Grant I. *Relativistic Quantum Theory of Atoms and Molecules.* Oxford, 2007.
2. Glushkov, A.V. *Relativistic Quantum theory. Quantum mechanics of atomic systems*. Astroprint: Odessa, 2008.
3. Glushkov, A.V. *Relativistic and correlation effects in spectra of atomic systems*. Astroprint: Odessa, 2006.
4. Khetselius, O.Yu. *Hyperfine structure of atomic spectra*. Astroprint: Odessa, 2008.
5. Khetselius, O.Yu. Atomic parity non-conservation effect in heavy atoms and observing P and PT violation using NMR shift in a laser beam: To precise theory. *J. Phys.: Conf. Ser.* 2009, *194,* 022009
6. Khetselius, O.Yu. Hyperfine structure of radium. *Photoelectronics*. 2005, *14,* 83.
7. Khetselius, O.. Relativistic perturbation theory calculation of the hyperfine

structure parameters for some heavy-element isotopes. *Int. Journ. Quant. Chem.* 2009, *109,* 3330-3335.
8. Khetselius, O.Yu. Relativistic calculation of the hyperfine structure parameters for heavy elements and laser detection of the heavy isotopes. *Phys.Scripta.* 2009, *135,* 014023.
9. Khetselius, O.Yu. Optimized relativistic many-body perturbation theory calculation of wavelengths and oscillator strengths for Li-like multicharged ions. Adv. Quant. Chem. 2019, *78*, 223-251.
10. Khetselius O.Yu.; Gurnitskaya, E.P. Sensing the hyperfine structure and nuclear quadrupole moment for radium. *Sensor Electr. and Microsyst. Techn.* 2006, *2,* 25-29.
11. Khetselius, O.Yu.; Gurnitskaya, E.P. Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi. *Sensor Electr. and Microsyst. Techn.* 2006, *3,* 35-39.
12. Khetselius, O.Yu. *Quantum structure of electroweak interaction in heavy finite Fermi-systems.* Astroprint: Odessa, 2011.
13. Khetselius O.Yu., Glushkov A.V., Ternovsky E.V., Buyadzhi V.V., Mykhailov O.L. Hyperfine and Electroweak Interaction in Heavy Finite Fermi-Systems and Parity Non-conservation Effect. In*: Mammino L., Ceresoli D., Maruani J., Brändas E. (eds) Advances in Quantum Systems in Chemistry, Physics, and Biology. Ser.: Progress in Theor. Chem. and Phys.*, Cham: Springer. 2020, Vol.32, P.65-81.
14. Khetselius O., Mykhailov, A. Relativistic calculation of wavelengths and E1 oscillator strengths in li-like multicharged ions and gauge invariance principle. *Photoelectronics.* 2020, *29*, 134-142.
15. Mykhailov O.L., Efimova E., Ternovsky E.V., Serga I., Hyperfine structure parameters for Li-like multicharged ions within relativistic many-body perturbation theory *Photoelectronics*. 2019, *28*, 113-120.
16. Svinarenko, A.A. Study of spectra for lanthanides atoms with relativistic many-body perturbation theory: Rydberg resonances. *J. Phys.: Conf. Ser.* 2014, *548,* 012039.
17. Ivanova, E.P.; Ivanov, L.N.; Glushkov, A.V.; Kramida, A.E. High order corrections in the relativistic perturbation theory with the model zeroth approximation, Mg-Like and Ne-Like Ions. *Phys. Scripta* 1985, *32,* 513-522.
18. Ivanov, L. N.; Ivanova, E. P.; Aglitsky, E. V. Modern Trends in the Spectroscopy of Multicharged Ions. *Phys. Rep*. 1988, *166,* 315-390.
19. Glushkov, A.V.; Ivanov, L.N. Radiation decay of atomic states: atomic residue polarization and gauge noninvariant contributions. *Phys. Lett. A* 1992, *170,* 33-36.
20. Glushkov A.V.; Ivanov, L.N. DC strong-field Stark effect: consistent quantum-mechanical approach. *J. Phys. B: At. Mol. Opt. Phys.* 1993, *26,* L379-386.
21. Glushkov, A.V. Spectroscopy of atom and nucleus in a strong laser field: Stark effect and multiphoton resonances. *J. Phys.: Conf. Ser*. 2014, *548*, 012020
22. Glushkov A., Spectroscopy of cooperative muon-gamma-nuclear processes: Energy and spectral parameters *J. Phys.: Conf. Ser.* 2012, *397,* 012011
23. Glushkov, A. Multiphoton spectroscopy of atoms and nuclei in a laser field: relativistic energy approach and radiation atomic lines moments method// Adv. Quant.Chem. (Elsevier), 2018, *7*8, doi.org/10.1016/bs.aiq.2018.06.004
24. Glushkov, A.V., Khetselius, O.Yu., Svinarenko A.A., Buyadzhi, V.V., Ternovsky, V.B, Kuznetsova, A., Bashkarev, P Relativistic perturbation theory formalism to computing spectra and radiation characteristics: application to heavy element. *Recent Studies in Perturbation Theory*, ed. D. Uzunov (InTech) 2017, 131-150.

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Summary. The relativistic many-body perturbation theory with the optimized Dirac zeroth approximation is applied to calculation of some fundamental characteristics of the hyperfine structure of middle and heavy 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 performance of the gauge invariance principle. There are listed the calculated values of derivatives of the one-electron characteristics, including the hyperfine structure parameters, on nuclear radius for the Li-like multicharged ions with the corresponding analysis.

Keywords: Relativistic theory, spectral and hyperfine structure parameters, Li-like multicharged ions

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УДОСКОНАЛЕНИЙ АНАЛІЗ ПАРАМЕТРІВ СПЕКТРІВ ТА НАДТОНКОЇ СТРУКТУРИ Li-ПОДІБНИХ БАГАТОЗАРЯДНИХ ІОНІВ В МЕЖАХ РЕЛЯТИВІСТСЬКОЇ ТЕОРІЇ

Резюме. Релятивістська багаточастинкова теорія збурень з оптимізованим нульовим наближенням Дірака застосована для обчислення фундаментальних характеристик надтонкої структури середніх і важких Li-подібних багатозарядних іонів. Релятивістські, обмінно-кореляційні та інші поправки враховані ефективно. Оптимізований релятивістський орбітальний базис генерується в оптимальному наближенні багаточастинкової теорії збурень із застосуванням принципу калібрувальної інваріантності. Наведені розрахункові значення похідних одноелектронних характеристик, у тому числі, параметрів надтонкої структури, від радіуса ядра для ряду Li-подібних багатозарядних іонів з відповідним аналізом.

Ключові слова: релятивістська теорія, параметри спектрів та надтонкої структури, Li-подібні багатозарядні іони

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