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THE HYPERFINE STRUCTURE AND OSCILLATOR STRENGTHS PARAMETERS FOR SOME HEAVY ELEMENTS ATOMS AND IONS: REVIEW OF DATA BY RELATIVISTIC MANY-BODY PERTURBATION THEORY CALCULATION

The energies and hyperfine structure constants for some heavy Li-like multicharged ions are calculated within the relativistic many-body perturbation theory formalism with a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections. The magnetic inter-electron interaction is accounted for in the lowest order on α^2 (α is the fine structure constant) parameter. The Lamb shift polarization part is taken into account in the modified Uehling-Serber approximation. The Lamb shift self-energy part is accounted for effectively within the generalized Ivanov-Ivanova non-perturbative procedure. The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized one-particle approximation are used for computing the Li-like ions (Z=11-42,69,70) and Cs energies and oscillator strengths, in particular, of radiative transitions from the ground state to the low-excited and Rydberg states $2s_{1/2}$ – $np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12) in the Li-like ions. A comparison of the calculated oscillator strengths with available theoretical and experimental data is performed.

1. Introduction

The research on the spectroscopic and structural properties of the heavy neutral and highly ionized atoms has a fundamental importance in many fields of atomic physics (spectroscopy, spectral lines theory), astrophysics, plasma physics, laser physics and so on (see, for example, refs. [1-22]). One could also mention here the important astrophysical applications. The experiments on the definition of hyperfine splitting also enable to refine the deduction of nuclear magnetic moments of different isotopes and to check an accuracy of the various computational models employed for the theoretical description of the nuclear effects.

The multi-configuration relativistic Hartree-Fock (RHF) and Dirac-Fock (DF) approaches (see, for example, refs. [3-5, 8-18] are the most reliable versions of calculation for multi-electron systems with a large nuclear charge. Usually, in these calculations the one- and two-body relativistic effects are taken into account practically precisely. It should be given the special attention to three very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed in the Oxford and German-Russian groups etc ("GRASP", "Dirac"; "BERTHA", "QED", "Dirac") (see refs. [3-5, 8-18] and references there). The useful overview of the relativistic electronic structure theory is presented in refs. [12, 13,17-20] from the QED point of view.

In the present paper the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized one-particle approximation are used for computing the Li-like ions (Z=11-42,69,70) and Cs energies and oscillator strengths, in particular, of radiative transitions from the ground state to the low-excited and Rydberg states $2s_{1/2}$ – $np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12) in the Li-like ions. Review of data and a comparison of the calculated oscillator strengths with different available theoretical and experimental data is presented.

2. Relativistic method to computing hyperfine structure parameters of atoms and multicharged ions

Let us describe the key moments of the approach (more details can be found in refs. [11, 14, 20-23]). The electron wave functions (the PT zeroth basis) are found from solution of the relativistic Dirac equation with potential, which includes ab initio mean-field potential, electric, polarization potentials of a nucleus. The charge distribution in the Li-like ion is modelled within the Gauss model. The nuclear model used for the Cs isotope is the independent particle model with the Woods-Saxon and spin-orbit potentials (see refs. [24]). Let us consider in details more simple case of the Li-like ion. We set the charge distribution in the Li-like ion nucleus *r(r)* by the Gaussian function:

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

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

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

Consider the DF type equations for a three-electron system $1s^2nlj$. Formally they fall into one-electron Dirac equations for the orbitals 1s and *nlj* with the potential:

$$V(r) = 2V(r|1s) + V(r|nlj) + V_{ex}(r) + V(r|R) \quad (3)$$

$V(r|R)$ includes the electrical and the polarization potentials of the nucleus; the components of the Hartree potential (in the Coulomb units):

$$V(r|i) = \frac{1}{Z}\int d\vec{r}'\rho(r|i)/|\vec{r}-\vec{r}'| \quad (4)$$

Here $\rho(r|i)$ is the distribution of the electron density in the state $|i>$, V_{ex} is the exchange inter-electron interaction. The main exchange effect will be taken into account if in the equation for the valent electron orbital we assume $V(r) = V(r|core) + V(r|nlj)$ and in the equation for the *nlj* orbital $V(r) = 2V(b, r|core)$ (here b is the optimization parameter; see below). 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 [11, 12,15]. A procedure of taking into account the radiative QED corrections is in details given in the refs. [11,14,20-22]. Regarding the vacuum polarization effect let us note that this effect is usually taken into consideration in the first PT theory order by means of the Uehling-Serber potential. This potential is usually written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp(-2rt/\alpha Z)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \quad (5)$$

where $g=r/(aZ)$. In our calculation we use more exact approach [22]. The Uehling potential, determined as a quadrature (6), may be approximated with high precision by a simple analytical function. The use of new approximation of the Uehling potential permits one to decrease the calculation errors for this term down to 0.5 – 1%. A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova (see refs. [11]). It is supposed that for any ion with *nlj* electron over the core of closed shells the sought value may be presented in the form:

$$E_{SE}(Z, nlj) = 0.027148\frac{\xi^4}{n^3} f(\xi, nlj)\left(cm^{-1}\right), \quad (6)$$

The parameter $x=(E_R)^{1/4}$, E_R is the relativistic part of the bounding energy of the outer electron; the universal function $f(\xi, nlj)$ does not depend on the composition of the closed shells and the actual potential of the nucleus. The energies of electric quadruple and magnetic dipole interactions are defined by a standard way with the hyperfine structure constants, usually expressed through the standard radial integrals [27]:

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

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

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (in Barn); $(RA)_{-2}$, $(RA)_{-3}$ are the radial integrals usually defined as follows:

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

$$(RA)_{-3,} = \int_0^\infty drr^2[F^2(r) + G^2(r)U(1/r^2, R) \cdot \qquad (8)$$

The radial parts *F* and *G* of the Dirac function two components for electron, which moves in the potential *V(r;R)+U(r;R),* are determined by solution of the Dirac equations. To define the hyperfine interaction potentials $U(1/r^n,R)$, we use the method by Ivanov et al [11]. The key elements of the optimized relativistic energy approach to computing oscillator strengths are presented in [1,15,29]. Let us remind that an initial general energy formalism combined with an empirical model potential method has been developed by Ivanov-Ivanova et al [11], further more general ab initio gauge-invariant relativistic approach has been presented in [12], where the calibration of the single model potential parameter b has been performed on the basis of the special *ab initio* procedure within relativistic energy approach [12] (see also [1529,30]). All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93). The details of the used method can be found in the references [1,11,14,21-24].

4. Results and Conclusions

Firstly we present the results of computing the oscillator strengths of transitions in spectra of the Li-like ions (Z=11-42,69,70). There are considered the radiative transitions from ground state to the low-excited and Rydberg states, particularly, $2s_{1/2}$ – $np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12). To test the obtained results, we compare our calculation results of the oscillator strengths values for some Li-like ions with the known theoretical and tabulated results [29,31]. As an example, in table 1 we present the computed oscillator strength values for the $2s_{1/2} - 2p_{1/2,3/2}$ transitions in Li-like ions S^{13+}, Ca^{17+}, Fe^{23+}, Zn^{27+}, Zr^{37+}, Mo^{39+}, Sn^{47+}, Tm^{66+}, Yb^{67+}. The DF calculation data by Zilitis [31b] and the "best" compillated (experimental) data [31a] for the low-Z Li-like ions are listed in table 1 for comparison too. Note that the experimental data on the oscillator strengths for many (especially, high-Z) Li-like ions are missing.

Overall, there is a physically reasonable agreement of the listed data. The important

features of the approach used are using the optimized one-particle representation and account for polarization effects. It should be noted that an estimate of the gauge-non-invariant contributions (the difference between the oscillator strengths values calculated with using the transition operator in the form of "length" and "velocity") is about 0.3%, i.e., the results obtained with different photon propagator gauges (Coulomb, Babushkon, Landau) are practically equal. In Table 2 we present our results (RMPT) of computing the reduced matrix elements (atomic units) of different radiative transitions in the ^{133}Cs spectrum [1,30b]. The experimental (Exp) and other theoretical (SD- the results of computing within the relativistic DF single-double approximation [4a]; DF, RHFc – the Dirac-Fock and relativistic

Table 1

Oscillator strengths of the $2s_{1/2} - 2p_{1/2,3/2}$ transitions in Li-like ions.

Method	DF [31b]	DF [31b]	[31c]	[31c]	[30b]	[30b]
Ion	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{3/2}$	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{3/2}$	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{3/2}$
S^{13+}	0.0299	0.0643	0.030	0.064	0.0301	0.0641
Ca^{17+}	0.0234	0.0542	0.024	0.054	0.0236	0.0541
Fe^{23+}	0.0177	0.0482	0.018	0.048	0.0179	0.0481
Zn^{27+}	0.0153	0.0477	–	–	0.0156	0.0475
Zr^{37+}	0.0114	0.0543	–	–	0.0118	0.0540
Mo^{39+}	–	–	0.011	0.056	0.0107	0.0556
Sn^{47+}	0.0092	0.0686	–	–	0.0095	0.0684
Tm^{66+}	–	–	–	–	0.0071	01140
Yb^{67+}	0.0067	0.1170	–	–	0.0069	0.1167

Table 2

The reduced dipole matrix elements (a.u.) of some transitions in the Cs (see text)

Tran-Sition	SD [4a]	Scaled [4a]	DF [4b]	RHF [4c]	RHF[4d]	QDA [21c]	RMPT [1,30b]	Exp.
$6p_{1/2}$-6s	4.482	4.535	4.510	4.494	-	4.282	4.486	4.4890(7)
$6p_{3/2}$-6s	6.304	6.382	6.347	6.325	-	5.936	6.320	6.3238(7)
$7p_{1/2}$-6s	0.297	0.279	0.280	0.275	0.2825	0.272	0.283	0.284(2)
$7p_{3/2}$-6s	0.601	0.576	0.576	0.583	0.582	0.557	0.582	0.583(9)
$8p_{1/2}$-6s	0.091	0.081	0.078	-	-	0.077	0.087	-
$8p_{1/2}$-6s	0.232	0.218	0.214	-	-	0.212	0.225	-
$6p_{1/2}$-7s	4.196	4.243	4.236	4.253	4.237	4.062	4.231	4.233(22)
$6p_{3/2}$-7s	6.425	6.479	6.470	6.507	6.472	6.219	6.478	6.479(31)
$7p_{1/2}$-7s	10.254	10.310	10.289	10.288	10.285	9.906	10.308	10.308(15)
$7p_{3/2}$-7s	14.238	14.323	14.293	14.295	14.286	13.675	14.322	14.320(20)

Table 3

The hyperfine structure constants of some Li-like ions: $A=Z^3 g_I \overline{A}$ (cm^{-1}) and $B=\frac{Z^3 Q}{I(2I-1)}\overline{B}(mm^{-1})$

nlj	Z	20	69	79	92
3s	$\overline{A}$	26 –03	51 –03	63 –03	90 –03
4s	$\overline{A}$	15 –03	19 –03	24 –03	36 –03
$2p_{1/2}$	$\overline{A}$	25 –03	56 –03	71 –03	105 –02
$3p_{1/2}$	$\overline{A}$	81 –04	16 –03	20 –03	31 –03
$4p_{1/2}$	$\overline{A}$	32 –04	72 –04	91 –04	11 –03
$2p_{3/2}$	$\overline{A}$	50 –04	67 –04	71 –04	72 –04
	$\overline{B}$	9 –04	13 –04	15 –04	17 –04
$3p_{3/2}$	$\overline{A}$	13 –04	19 –04	21 –04	22 –04
	$\overline{B}$	31 –05	51 –05	55–05	62 –05
$4p_{3/2}$	$\overline{A}$	62 –05	89 –05	92 –05	8 –04
	$\overline{B}$	10 –05	20 –05	22 –05	26 –05
$3d_{3/2}$	$\overline{A}$	88 –05	10 –04	11 –04	12 –04
	$\overline{B}$	51 –06	9 –05	10 –05	11 –05
$4d_{3/2}$	$\overline{A}$	35 –05	51 –05	55 –05	58 –05
	$\overline{B}$	12 –06	44 –06	50 –06	56 –06
$3d_{5/2}$	$\overline{A}$	36 –05	48 –05	50 –05	52 –05
	$\overline{B}$	21 –06	38 –06	39 –06	40 –06
$4d_{5/2}$	$\overline{A}$	15 –05	19 –05	20 –05	21 –05
	$\overline{B}$	59 –07	15 –06	16 –06	17 –06
$4f_{5/2}$	$\overline{A}$	06–05	12 –05	13 –05	14 –05
	$\overline{B}$	16 –07	53 –07	58 –07	63 –07

Hartree —Fock method data with accounting for the second order correlation corrections; QDA-the data by the perturbation theory with the quantum defect approximation) [4,21,29,30] data are listed too.

In table 3 we present the calculated data of the hyperfine structure constants for some Li-like ions. There are presented results for the parameters: $A=Z^3 g_I \overline{A}$ and $B=\frac{Z^3 Q}{I(2I-1)}\overline{B}(mm^{-1})$.

In table 4 the experimental (A^{Exp}) and theoretical data of the magnetic dipole constant A (MHz) for the valent states of ^{133}Cs atom (I=7/2, g_i=0.7377208) are presented (from Ref. [1,5,29]). The theoretical results are obtained on the basis of the standard RHF (A^{RHF}) calculation, the RHF ($A^{RHF}+dA$) calculation with taking into account the PT second and higher corrections (look Refs. [5,15,29] and references therein) and the RMPT (A^{RMPT}) calculation (our data). The analysis shows

Table 4

The values (in MHZ) of the hyperfine structure constant A for valent states of the ^{133}Cs isotope: A^{Exp} - experiment; A^{RHF} - the RHF calculation data; $A^{RHF}+dA^{RHF}$ - the RHF calculation data with taking into account the PT second and higher orders contributions [5]; A^{RMPT} – the RMPT calculation data [29] (look details in Refs.[5,15,29]).

State	A^{RHF} [5]	dA [5]	$A^{RHF}+dA$ [5]	dA^{RMPT} [29]	A^{RMPT} [29]	A^{Exp}
$6s_{1/2}$	1426,81	864,19	2291,00	870,96	2294,45	2298,16
$7s_{1/2}$	392,05	151,99	544,04	152,45	545,480	545,90(9)
$6p_{1/2}$	161,09	131,58	292,67	130,08	292,102	291,90(13)
$7p_{1/2}$	57,68	35,53	94,21	35,64	94,317	94,35(4)
$6p_{3/2}$	23,944	25,841	49,785	26,322	50,205	50,275(3)
$7p_{3/2}$	8,650	7,605	16,255	7,920	16,590	16,605(6)
$5d_{3/2}$	---	---	---	7,802	16,422	---

that taking into account the correlation and QED corrections is important to reach the physically reasonable agreement between theoretical and experimental data.

The fundamental reason of physically reasonable agreement between theory and experiment is connected with the correct taking into account the inter-electron correlation effects, nuclear (due to the finite size of a nucleus), relativistic and radiative corrections. The key difference between the results of the RHF, RMPT methods calculations is explained by using the different schemes of taking into account the inter-electron correlations. The contribution of the PT high order effects and nuclear contribution may reach the units and even dozens of MHz and should be correctly taken into account. So, it's necessary to take into account more correctly the spatial distribution of the magnetic moment inside a nucleus (the Bohr-Weisskopf effect), the nuclear-polarization corrections etc too.

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Abstract

The energies and hyperfine structure constants for some heavy Li-like multicharged ions are calculated within the relativistic many-body perturbation theory formalism with a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections. The magnetic inter-electron interaction is accounted for in the lowest order on a^2 (a is the fine structure constant) parameter. The Lamb shift polarization part is taken into account in the modified Uehling-Serber approximation, the Lamb shift self-energy part - within the generalized Ivanov-Ivanova procedure. The combined relativistic energy approach and many-body perturbation theory with the zeroth order optimized one-particle approximation are used for computing the Li-like ions (Z=11-42,69,70) and Cs energies and oscillator strengths, in particular, of radiative transitions from the ground state to the low-excited and Rydberg states $2s_{1/2} – np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12) in the Li-like ions. A comparison of the calculated oscillator strengths with available theoretical and experimental data is performed.

Key words: Hyperfine structure – Oscillator strengths - Relativistic perturbation theory

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СВЕРХТОНКАЯ СТРУКТУРА И СИЛЫ ОСЦИЛЛЯТОРОВ РАДИАЦИОННЫХ ПЕРЕХОДОВ ДЛЯ РЯДА АТОМОВ И ИОНОВ ТЯЖЕЛЫХ ЕЛЕМЕНТИВ: ОБЗОР ДАННЫХ ВЫЧИСЛЕНИЙ НА ОСНОВЕ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме

Энергии и константы сверхтонкой структуры для некоторых тяжелых Li-подобных многозарядных ионов вычислены в рамках релятивистской многочастичной теории возмущений с эффективным с учетом обменно-корреляционных, релятивистских, ядерных и радиационных поправок. Магнитное межэлектронное взаимодействие учитывается в низшем порядке на a^2 (а постоянная тонкой структуры) параметру. Поляризационная часть сдвига Лэмба учитывается в модифицированном приближении Юлинга-Сербера, собственно-энергетическая часть сдвига Лэмба - эффективно в рамках обобщенной непертурбативной процедуры Иванова-Ивановой. Обобщенный релятивистский энергетический подход и многочастичная теории возмущений с оптимизированным нулевым приближением использованы для определения энергий, сил осцилляторов переходов в спектрах Cs, Li-подобных ионов (Z = 11-42,69,70) и, в частности, радиационных переходов из основного состояния в низшие возбужденные и ридберговские

$2s_{1/2}$ – $np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12) состояния в Li-подобных ионах. Проведено сравнение экспериментальных данных и результатов расчетов на основе различных теоретических методов.

Ключевые слова: Сверхтонкая структура, Силы осцилляторов, Релятивистская теория возмущений

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НАДТОНКА СТРУКТУРА І СИЛИ ОСЦИЛЯТОРІВ РАПДІАЦІЙНИХ ПЕРЕХОДІВ ДЛЯ ДЕЯКИХ АТОМІВ ТА ІОНІВ ВАЖКИХ ЕЛЕМЕНТІВЖ ОГЛЯД ДАНИХ ОБЧИСЛЕНЬ НА ОСНОВІ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ

Резюме

Енергії і константи надтонкої структури для деяких важких Li-подібних багатозарядних іонів обчислені в рамках релятивістської Багаточасткові теорії збурень з ефективним з урахуванням обмінно-кореляційних, релятивістських, ядерних і радіаційних поправок. Магнітна міжелектроннао взаємодія враховується в нижчому порядку на a^2 (a -стала тонкої структури) параметру. Поляризаційна частина зсуву Лемба враховується в модифікованому наближенні Юлінга-Сербера, власно-енергетична частина зсуву Лемба - ефективно в рамках узагальненої непертурбативної процедури Іванова-Іванової. Узагальнений релятивістський енергетичний підхід і багаточастинкова теорії збурень з оптимізованим “0” наближенням використані для визначення енергій і сил осциляторів переходів в спектрах Cs, Li-подібних іонів (Z = 11-42,69,70), зокрема, радіаційних переходів з основного стану в нижчі збуджені і ридберговскі $2s_{1/2}$ – $np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12) стани у Li-подібних іонах. Проведено порівняння експериментальних даних і даних обчислень на основі різних теоретичних методів.

Ключові слова: Надтонка структура, Сили осциляторів, Релятивістська теорія збурень