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O. Yu. Khetselius, A. L. Mykhailov, E. A. Efimova, R. E. Serga

Odessa State Environmental University, L'vovskaya str.15, Odessa-9, 65016, Ukraine
E-mail: okhetsel@gmail.com

WAVELENGTHS AND OSCILLATOR STRENGTHS FOR Li-LIKE MULTICHARGED IONS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

The relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation is applied to calculation of the radiative transitions wavelengths and oscillator strengths 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. An accurate treatment of the QED perturbation theory fourth order (a second order of the atomic perturbation theory) Feynman diagrams (whose contribution into the energy shift imaginary part (radiation width) for the multi-electron atoms accounts for multi-body correlation effects) is performed. The obtained data on the radiative transition wavelengths and oscillator strengths for some transition in spectra of the Li-like multicharged ions are analyzed and compared with alternative theoretical and experimental results.

1. Introduction

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 [1-30].

There have been sufficiently many reports of theoretical and experimental studies of energies and oscillator strengths for the Li-like ions and other alkali-like ions (see, for example, [7-15]). Banglin Deng et al [12] presented the calculated wavelengths, oscillator strengths, transition probabilities, and line strengths for Li-like ions (Z = 7–30) in the framework of the relativistic configuration-interaction formalism using MCDF wave functions and considering the Breit interaction, QED and nuclear mass corrections. A critical evaluation and compilation of the spectroscopic parameters for Li-like ions (Z=3-28) was undertaken by Martin and Wiese [153-156]. Bièmont [30] applied fully variational nonrelativistic HF wave functions in computing 1s2n2L (n<8=s,p,d,f; 3<Z<22) Li-like states]. Aglitskii et al [121] experimentally observed the Lα wavelengths of Li-like ions (Z = 19–26) in laser-produced plasmas. Theoretical approach to studying the spectroscopic characteristics of the heavy multicharged ions (Li-like ions) within the RMBPT with the model potential zeroth approximation is developed by Ivanov-Ivanova [119-125]. Fully relativistic computing the wavelengths and oscillator strengths from excitation of Li-like ions (Z = 8–92) have been given by Zhang et al. [53]. Nahar [54] applied the Breit–Pauli R-matrix method to calculations of the wavelengths, transition probabilities, and oscillator strengths for a number of the Li-like ions with the nuclear charge Z=6-68. The relativistic quantum defect method has been used by Martin et al [55] to calculate the oscillator strengths for a number of radiative transitions between low-lying states in the Li-like ions for Z < 45. The energy levels and hy-

perfine constants of neutral lithium were studied by Lindgren[9] within a nonrelativistic coupled-cluster method, by Guan-Wang [47] within the effective operator form of MBPT etc. Relativistic all-order MBPT calculations of energies and matrix elements for Li and Be+ were reported in Ref. [44]. Wu Xiao-Li et al [50] have performed the relativistic MBPT calculation for lithium-like isoelectronic sequence (Z=3−9) within the DF method with using the finite basis sets of the Dirac–Fock equations, constructed by B splines.

Chen Chao and Wang Zhi-Wen [48] applied a full core plus correlation method with using multiconfiguration interaction wave functions to computing the nonrelativistic values of the oscillator strengths for a number of transitions into the Rydbers states along the LiI isoelectronic sequence. The Hylleraas-type variational method and the 1/Z expansion method have been used also to obtain the non-relativistic calculations data on the energies and oscillator strengths of $1s22s, 1s22p$ for Li-like systems up to Z = 50 [41-51].

In this paper the relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation is applied to calculation of the radiative transitions wavelengths and oscillator strengths for some Li-like multicharged ions. The relativistic, exchange-correlation and other corrections are accurately taken into account.

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 [26,27,93-102], 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:

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

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

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

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 [33]:

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

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 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 will be taken into account in the first two orders of the PT [93-102].

In Ref. [127,128] it has been proposed "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 details of procedure can be found in Ref. [126-134]. As in Ref. [127, 134], let us examine the multi-electron atomic ion with one quasiparticle in the first excited state, connected with the ground state by the electric dipole radiation transition. In the QED PT zeroth order we use the one-electron bare potential $V_N(r)+V_X(r)+V_C(r)$. As usual, the perturbation operator is as follows:

$$-V_{Xc}(r) - J_{\mu}(x) A^{\mu}(x) \qquad (8)$$

where A – vector-potential of the electromagnetic field, J – current operator.

Further one may treat the lowest order multielectron effects, in particular, the gauge dependent radiative contribution for a certain class of the photon propagator calibration. The contribution of the QED PT fourth order diagrams A into the ImδE accounts for the exchange-polarization effects. In fact it describes the collective effects and is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution). This value is considered to the typical electron correlation effect, whose minimization is a reasonable criterion in searching the optimal one-electron basis of PT. All the gauge non-invariant terms are multi-electron by their nature (the particular case of the gauge non-invariance manifestation is the non-coincidence of the oscillator strengths values, obtained in the approximate calculations with the "length" and "velocity" transition operator forms). Quite complicated calculation of contribution of the QED PT fourth order polarization diagrams into Im δE gives the following result [127]:

Here, f is the boundary of the closed shells; $n \geq f$ indicates the unoccupied bound and the upper continuum electron states; $m \leq f$ indicates the finite number of states in the core and the states of the negative continuum (accounting for the electron vacuum polarization).

$$\mathrm{Im}\delta E_{ninv}(\alpha - s; b) = -C \int\int\int\int dr_1 dr_2 dr_3 dr_4$$
$$\sum_{\substack{n>f \\ m\leq f}} \left(\frac{1}{\omega_{mn} + \omega_{\alpha s}} + \frac{1}{\omega_{mn} - \omega_{\alpha s}} \right) \cdot$$
$$\cdot \psi_{\alpha}^{+}(r_1) \psi_{m}^{+}(r_2) \psi_{s}^{+}(r_4) \psi_{n}^{+}(r_3) \frac{1 - \alpha_1 \alpha_2}{r_{12}} \qquad (9)$$
$$\{ [(\alpha_3 \alpha_4 - \alpha_3 n_{34} \alpha_4 n_{34}) / r_{14}] \cdot$$
$$\cdot sin[\omega_{\alpha n}(r_{12} + r_{34})] + \omega_{\alpha n} cos[\omega_{\alpha n}(r_{12} + r_{34})]$$
$$(1 + \alpha_3 n_{34} \alpha_4 n_{34}) \} \cdot \psi_m(r_3) \psi_{\alpha}(r_4) \psi_n(r_2) \psi_s(r_1).$$

The expression (9) can be represented in the form of terms:

$$\sum_{\substack{n>f \\ m\leq f}} < \alpha m | W_1 | ns >< sn | W_2 | m\alpha > /(\omega_{mn} \pm \omega_{\alpha s}) \qquad (10)$$

with four different combinations of operators and (see details in Refs. [127-129]). The sum over n can be calculated by the method of differential equations. The minimization of the density functional ImδE leads to the integral differential equation for the ρ_c, that can be numerically solved. This step allows to determine the optimization parameter b. In Ref. [127] the authors elaborated a simplified computational procedure. We have used more sophisticated method, presented in Ref. [131313]. It presents for first time the full consistent realization of the optimization approach within our version of the RMBPT.

The key elements of the relativistic energy approach to computing radiation widths and oscillator strengths for atomic systems are presented in Refs. [13-13]. Let us remind that an initial general energy formalism combined with an empirical model potential method in a theory of atoms and multicharged ions has been developed by Ivanov-Ivanova et al [119-125], further more general ab initio gauge-invariant relativistic approach has been presented in [127,128]. We use the optimized version of this formalism with our construction of one-quasiparticle representation. In the energy approach [124-126] the imaginary part of electron energy shift of an atom is connected with the radiation decay pos-

sibility (transition probability). An approach, based on the Gell-Mann and Low formula with the QED scattering matrix, is used in treatment of the relativistic atom. The total energy shift of the state is usually presented in the form:

$$\delta E = \mathrm{Re}\delta E + \mathrm{i}\Gamma/2 \qquad (11)$$

where Γ is interpreted as the level width, and the decay probability P = Γ. For the α-s radiation transition the imaginary part of electron energy in the lowest order of perturbation theory is determined as [124]:

$$\mathrm{Im}\,\delta E = -\frac{1}{4\pi}\sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n\alpha n}, \qquad (12)$$

where $\omega_{\alpha n}$ is a frequency of the α-n radiation, (α>n>f) for electron and (α<n<f)

for vacancy. The matrix element V is determined as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (13)$$

The separated terms of the sum in (34) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha n} = \frac{1}{4\pi}V^{|\omega_{\alpha n}|}_{\alpha n\alpha n}. \qquad (36)$$

The corresponding oscillator strength: $gf=\lambda^2\Gamma_{\alpha n}/6.67\times10^{15}$, where g is the degeneracy degree, λ is a wavelength in angstroms (Å). 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].

3. Results and Conclusions

In table 1 we list our computational results on the wavelengths and oscillator strengths gf (upper number in the line "Our work": data, obtained without using the optimized basis set and accounting for the exchange-polarization corrections; lower number in the line "Our work" – with using the optimized basis set and accounting for the exchange-polarization corrections) for $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in the Li-like ions with Z=21,22. In Table 1 the data on the wavelengths, oscillator strengths, calculated by Banglin Deng et al [52] (in the framework of the relativistic configuration-interaction formalism using multiconfiguration DF wave functions and considering the Breit interaction, QED and nuclear mass corrections), Zhang et al (the Dirac-Fock-Slater method and disturbed wave approximation), Martin et al (the relativistic quantum defect method),Nahar (ab initio calculations including relativistic effects employing the Breit-Pauli R-matrix method) and the NIST data [10-14] are listed too. The data by Banglin Deng et al [12] are obtained in the length gauge, and the ratios (V/L; in %) of the velocity and length gauges data to check the accuracy of calculations are listed. We also present our values of the gauge non-invariant contribution (Ninv; in %). Comparison of the presented data shows that the agreement between the theoretical data and experimental results is more or less satisfactory.

Table 1.

The calculated wavelengths, oscillator strengths for $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in the Li-like ions with Z=21-30; V/L is the ratios of the velocity and length gauges values by Banglin Deng et al [12]; Ninv (in %) is the gauge non-invariant contribution (this work);

Z	Ref.	Wavelength (A)	Oscillator strength (gf, 10^{-1})	V/L; Ninv (%)
21	Banglin Deng et al	16.862	1.2392	V/L= 0.117
	NIST	16.861	1.2404	
	Zhang et al	16.856	1.250	
	Martin et al	-	1.24	
	This work	16.860	1.2835 1.2401	Ninv= 0.10
22	Banglin Deng et al	15.254	1.2484	V/L= 0.128
	NIST	15.253	1.2489	
	Zhang et al	15.249	1.259	
	Nahar	15.3	1.281	
	Martin et al		1.24	
	This work	15.252	1.2967 1.2492	Ninv= 0.11

The approach presented (with using the optimized relativistic PT) can provide sufficiently high accuracy and physically reasonable description of the corresponding wavelengths and oscillator strengths. 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 0.15%, i.e., the results for oscillator strengths obtained with using different photon propagator gauges (Coulomb, Babushkin, Landau) are practically equal. This is the evidence of a successful choice of the one-quasiparticle representation.

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O. Yu. Khetselius, A. L. Mykhailov, E. A. Efimova, R. E. Serga

THE HYPERFINE STRUCTURE OF HEAVY ELEMENTS ATOMS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

Summary

The relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation is applied to calculation of the radiative transitions wavelengths and oscillator strengths 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. An accurate treatment of the QED perturbation theory fourth order (a second order of the atomic perturbation theory) Feynman diagrams (whose contribution into the energy shift imaginary part (radiation width) for the multi-electron atoms accounts for multi-body correlation effects) is performed. The obtained data on the radiative transition wavelengths and oscillator strengths for some transition in spectra 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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О. Ю. Хецелиус, А. Л. Михайлов, Э. А. Ефимова, Р. Э. Серга

СВЕРХТОНКАЯ СТРУКТУРА ТЯЖЕЛЫХ АТОМОВ В РАМКАХ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме

Релятивистская многочастичная теория возмущений с оптимизированным нулевым приближением Дирака-Кона-Шэма применена для расчета длин волн радиационных переходов и сил осцилляторов для некоторых 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. Предложена процедура аккуратного учета вкладов, описываемых диаграммами Фейнмана четвертого порядка КЭД теории возмущений (второй порядок атомной теории возмущений), в мнимую часть энергетического сдвига атомных уровней (радиационные ширины) многоэлектронных атомов с целью учета многочастичных корреляционных эффектов. Полученные данные о длинах волн радиационного перехода и силах осциллятора для некоторого перехода в спектрах Li-подобных многозарядных ионов анализируются и сравниваются с альтернативными теоретическими и экспериментальными результатами.

Ключевые слова: Релятивистская многочастичная теория возмущений – оптимальное одноквазичастинкове представление – Силы осцилляторов – Энергетический подход – Корреляционные поправки

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О. Ю. Хецеліус, О. Л. Михайлов, Е. О. Ефімова, Р. Е. Сєрга

НАДТОНКА СТРУКТУРА ВАЖКИХ АТОМІВ В РАМКАХ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ

Резюме

Релятивістська багаточастинкова теорія збурень з оптимізованим нульовим наближенням Дірака-Кона-Шема застосована для розрахунку довжин хвиль радіаційних переходів і сил осциляторів для деяких 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. Запропоновано процедуру акуратного урахування вкладів, описуваних діаграмами Фейнмана четвертого порядку КЕД теорії збурень (другий порядок атомної теорії збурень), в уявну частину енергетичного зсуву атомних рівнів (радіаційні ширини) багатоелектронних атомів з метою врахування багаточастинкових кореляційних ефектів. Отримані дані по довжинам хвиль радіаційних переходів та силам осциляторів для деяких переходів у спектрах Li-подібних багатозарядних іонів, які порівнюються з альтернативними теоретичними і експериментальними результатами.

Ключові слова: Релятивістська багаточастинкова теорія збурень – Оптимальне одноквазічастинкове представлення – Сили осциляторів – Енергетичний підхід – Кореляційні поправки