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RELATIVISTIC CALCULATION OF WAVELENGTHS AND E1 OSCILLATOR STRENGTHS IN LI-LIKE MULTICHARGED IONS AND GAUGE INVARIANCE PRINCIPLE

The spectral wavelengths and oscillator strengths for $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in the Li-like multicharged ions with the nuclear charge Z=28,30 are calculated on the basis of the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized Dirac-Kohn-Sham one-particle approximation and gauge invariance principle performance. The comparison of the obtained results with available theoretical and experimental (compilated) data is performed. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth order that significantly provides a physically reasonable agreement between theory and precise experiment.

1. Introduction

The development of new directions in the The study of spectroscopic and structural 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. [1-10].

However, a study of the spectral characteristics of heavy atoms and ions in the Rydberg states has to be more complicated as it requires a necessary accounting for the relativistic, exchange-correlations effects and possibly the QED corrections for superheavy atomic systems. The simultaneous correct accounting of relativistic, quantum electrodynamic (QED), and many-particle correlation effects is essential [11–40]. The results of calculating the characteristics of atomic processes based on modern theoretical methods often differ several times.

The difference in the values of the transition amplitudes, the oscillator strengths, and the radiation widths for heavy atoms using various expressions for the photon propagator reaches 5–30% (we are essentially talking about the non-fulfillment of the principle of gauge invariance when calculating physical quantities) [11-18]. From the point of view of applications for the majority of the most important atomic systems, there is very often partially or completely missing information on their energy, radiation or/and autoionization characteristics (heavy atoms, atoms of alkaline-earth elements, lanthanides and actinides).

In this paper The spectral wavelengths and oscillator strengths for $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in the Li-like multicharged ions with the nuclear charge Z=28,30 are calculated on the basis of the combined relativistic energy approach and

relativistic many-body perturbation theory with the zeroth order optimized Dirac-Kohn-Sham one-particle approximation and studying an effect of the gauge invariance on the transition amplitude values for some Li-like multicharged ions.

2. Relativistic theory of multicharged ions

In Refs. [2-5,.8,16-25] the fundamentals of the relativistic many-body PT formalism have been in detail presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In Refs. [16-24] there is realized a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix *M* diagonalization. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the *M*. The complex secular matrix *M* is represented in the form:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \qquad (1)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}, M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. The optimized 1-QP representation is the best one to determine the zeroth approximation. In the relativistic energy approach, which has received a great application during solving numerous problems of atomic, molecular and nuclear physics (e.g., see Refs. [16-54]), the imaginary part of electron energy shift of an atom is directly connected with the radiation decay possibility (transition probability). An approach, using the Gell-Mann and Low formula with the QED scattering matrix, is used in treating the relativistic atom. The total energy shift of the state is usually presented in the form:

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

where Γ is interpreted as the level width, and the decay possibility P = Γ. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [16-20]:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \qquad (3)$$

where (α>n>f) for electron and (α<n<f) for vacancy. The matrix element is determined as follows:

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega| r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (4)$$

where ω_{ij} is the transition frequency; α_i ,α_j are the Dirac matrices. The separated terms of the sum in (1) represent the contributions of different channels and a probability of the dipole transition

Naturally, the physical values should not depend on the calibration of the photonic propagator. In general form, it can be written as

$$D = D_T + C \cdot D_L,$$
$$D_T = \frac{\delta_{\mu\nu}}{k_0^2 - k^2},$$
$$D_L = \frac{k_\mu k_\nu}{k_0^2 - k^2} \qquad (5)$$

where the term D_T is corresponding to exchange by transverse photons, D_L — longitudinal ones, C is the gauge constant. contribution of the main exchange-correlation (the second and higher orders of the atomic perturbation theory or fourth etc of the QED perturbation theory) diagrams to imaginary part of an electron energy shift looks like [17]:

$$\mathrm{Im}\, E_{ninv}(\alpha - s \mid A_d) = -C\frac{e^2}{4\pi}\iiint\int dr_1 dr_2 dr_3 dr_4$$

$$\sum\left(\frac{1}{\omega_{mn}+\omega_{\alpha_s}} + \frac{1}{\omega_{mn}-\omega_{\alpha_s}}\right)\Psi^+_\alpha(r_1)\Psi^+_m(r_2)\Psi^+_s(r_3)\cdot$$

$$\cdot \Psi_n^+(r_4)(1-\alpha_1\alpha_2)/r_{12} \cdot \{[(\alpha_3\alpha_4 - (\alpha_3 n_{34})(\alpha_4 n_{34}))/r_{34} \cdot$$

$$\sin[\omega_{\alpha_n}(r_{12}+r_{34}) + \omega_{\alpha_n} \cdot \cos[\omega_{\alpha_n}(r_{12}+r_{34})](1+(\alpha_3 n_{34})$$

$$(\alpha_4 n_{34}))]\}\Psi_m(r_3)\Psi_\alpha(r_4)\Psi_n(r_2)\Psi_s(r_1) \qquad (6)$$

Expression (6) can be represented as an a sum:

$$\Sigma \langle \alpha m | W_1 | ns \rangle \langle sn | W_2 | m\alpha \rangle / (\omega_{mn} \pm \omega_{\alpha s}) \qquad (7)$$

with (4) different operator combinations W_1, W_2. The sum over n can be calculated by the method of differential equations. The index m numbers a finite number of states occupied in the core and the state of the real continuum. The continuum-related part describes the vacuum polarization of the electron field and leads to divergent integrals in the non-renormalizable theory. Its contribution to the main contribution has an additional order of smallness (αZ^2). The minimization of the density functional $\mathrm{Im}\delta E$ 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. [8] the authors elaborated a simplified computational procedure.

The contribution of the main exchange-correlation (the second and higher orders of the atomic perturbation theory or fourth etc ones of the QED perturbation theory) to imaginary part of an electron energy shift is determined by the polarizability of an atomic core, which is related to the electronic core density ρ_c. The expression (6) can be represented an a functional of the density ρ_c.

Under calculating the matrix elements (2) one should use the expansion for potential $\sin|\omega|r_{12}/r_{12}$ on spherical functions as follows [16-20]:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0}^{\infty} (\lambda) J_{\lambda+1/2}(|\omega|r_1) J_{\lambda+1/2}(|\omega|r_2) P_\lambda(\cos \widehat{r_1 r_2}), \qquad (8)$$

where J is the Bessel function of first kind and $(\lambda) = 2\lambda + 1$. Substitution of the expansion (5) to matrix element of interaction gives as follows [14]:

$$V_{1234}^{\omega} = [(j_1)(j_2)(j_3)(j_4)]^{1/2} \sum_{\lambda\mu} (-1)^{\mu} \begin{pmatrix} j_1 j_3 & \lambda \\ m_1 - m_3 & \mu \end{pmatrix} \times$$

$$\times \mathrm{Im}\{Q_\lambda^{Qul}(1234) + Q_\lambda^{Br}(1234)], \qquad (9)$$

where j_i is the total single electron momentums, m_i – the projections; Q^{Qul} is the Coulomb part of interaction, Q^{Br} - the Breit part. Their detailed definitions are presented in Refs. [10-11,18,19]. The relativistic wave functions are calculated by solution of the Dirac equation with the potential, which includes the "outer electron- ionic core" potential and exchange-polarization potential [20]. In fact, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $\mathrm{Im}\Delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels. According to [11, 18], "in the fourth order of QED PT (the second order of the atomic PT) there appear the diagrams, whose contribution to the $\mathrm{Im}\Delta E_{ninv}$ accounts for correlation effects and this contribution is determined by the electromagnetic potential gauge (the gauge dependent contribution)". The accurate procedure for minimization of the functional $\mathrm{Im}\delta E_{ninv}$ leads to the Dirac-Kohn-Sham-like equations for the electron density that are numerically solved by the Runge-Cutta standard method It is very important to know that the regular realization of the total scheme allows to get an optimal set of the 1QP functions and more correct results in comparison with so called simplified one, which has been used in Refs. [11-13] and reduced to the functional minimization using the variation of the correlation potential parameter b. Other details can be found in Refs. [8,16,17].

The adequate, precise computation of radiative parameters of the heavy Rydberg alkali-metal atoms within relativistic perturbation theory requires an accurate accounting for the multi-electron exchange-correlation effects (including polarization and screening effects, a continuum pressure etc). These effects within our approach are treated as the effects of the perturbation theory second and

higher orders. Using the standard Feynman diagrammatic technique one should consider two kinds of diagrams (the polarization and ladder ones), which describe the polarization and screening exchange-correlation effects. The detailed description of the polarization diagrams and the corresponding analytical expressions for matrix elements of the polarization interelectron interaction (through the polarizable core of an alkali atom) potential is presented in Refs. [16-40].

An effective approach to accounting for the polarization diagrams contributions is in adding the effective two-quasiparticle polarizable operator into the perturbation theory first order matrix elements. In Ref. [21] the corresponding non-relativistic polarization functional has been derived. More correct relativistic expression has been presented in the Refs. [22,8] and used in our theory.

The corresponding two-quasiparticle polarization potential looks as follows:

$$V_{pol}^{d}(r_1 r_2) = X \left\{ \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'| \cdot |r' - r_2|} - \right.$$

$$\left. - \int \frac{dr' \left(\rho_c^{(0)}(r')\right)^{1/3} \theta(r')}{|r_1 - r'|} \int \frac{dr'' \left(\rho_c^{(0)}(r'')\right)^{1/3} \theta(r'')}{|r'' - r_2|} \Big/ \left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle \right\} \quad (10a)$$

$$\left\langle \left(\rho_c^{(0)}\right)^{1/3} \right\rangle = \int dr \left(\rho_c^{(0)}(r)\right)^{1/3} \theta(r), \quad (10b)$$

$$\theta(r) = \left\{ 1 + \left[3\pi^2 \cdot \rho_c^{(0)}(r) \right]^{2/3} / c^2 \right\}^{1/2}, \quad (10c)$$

where ρ_c^0 is the core electron density (without account for the quasiparticle), X is numerical coefficient, c is the light velocity. The contribution of the ladder diagrams (these diagrams describe the immediate interparticle interaction) is summarized by a modification of the perturbation theory zeroth approximation mean-field central potential (look [2,8]), which includes the screening (anti-screening) of the core potential of each particle by the two others. All computing was performed with using the modified PC code "Superatom-ISAN" (version 93).

3. Results and conclusion

We applied the above described approach to compute the oscillator strengths (reduced dipole matrix elements) for a number of transitions in spectra of the heavy alkali atoms and corresponding ions.

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 $1s^2 2s$ ($^2S_{1/2}$) → $1s^2 3p$ ($^2P_{1/2}$) 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 [12] (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 [10-15] 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. 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" G1 and "velocity" G2) is about 0.1%. The theoretical data, obtained with using the different photon propagator gauges

(Coulomb and Babushkin ones) are practically equal.

Table 1.

The calculated wavelengths, oscillator strengths for $1s^2 2s\ (^2S_{1/2}) \rightarrow 1s^2 3p\ (^2P_{1/2})$ transitions in the Li-like ions with Z=28,30; 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.	Wave-length (A)	Oscillator strength (gf, 10^{-1})	V/L; Ninv (%)
28	Banglin Deng et al	9.104	1.2889	V/L~0.2
	NIST	9.105	-	
	Zhang et al	9.099	1.299	
	Nahar	9.1	1.339	
	Martin et al		1.28	
	This work	9.103	1.3285 1.2891	N_{inv}~0.1
30	Banglin Deng et al	7.859	1.2983	V/L~0.2
	Zhang et al	7.854	1.309	
	Martin et al		1.29	
	This work	7.858	1.3387 1.2985	N_{inv}~0.1
	Banglin Deng et al	7.859	1.2983	V/L~0.2

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RELATIVISTIC CALCULATION OF WAVELENGTHS AND E1 OSCILLATOR STRENGTHS IN Li-LIKE MULTICHARGED IONS AND GAUGE INVARIANCE PRINCIPLE

Summary. The spectral wavelengths and oscillator strengths for $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in the Li-like multicharged ions with the nuclear charge Z=28,30 are calculated on the basis of the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized Dirac-Kohn-Sham one-particle approximation and gauge invariance principle performance. The comparison of the obtained results with available theoretical and experimental (compilated) data is performed. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth order that significantly provides a physically reasonable agreement between theory and precise experiment

Key words: relativistic theory, radiative transitions, gauge invariance principle, lithium-like ions

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РЕЛЯТИВИСТСКИЙ РАСЧЕТ ДЛИН ВОЛН И E1 СИЛ ОСЦИЛЛЯТОРОВ В LI-ПОДОБНЫХ МНОГОЗАРЯДНЫХ ИОНАХ И ПРИНЦИП КАЛИБРОВОЧНОЙ ИНВАРИАНТНОСТИ

Резюме. Спектральные длины волн и силы осцилляторов для переходов $1s^22s\ (^2S_{1/2}) \rightarrow 1s^23p\ (^2P_{1/2})$ в Li-подобных ионах с зарядом ядра Z = 28,30 вычислены на основе комбинированного релятивистского энергетического подхода и релятивистской многочастичной теории возмущений с дирак-кон-шэмовским одночастичным нулевым приближением и условием соблюдения принципа калибровочноъ инвариантности в радиационных переходах. Проведено сравнение полученных результатов с имеющимися теоретическими и экспериментальными данными. Важный момент связан с аккуратным учетом вкладов сложных многочастичных обменных корреляционных (поляризационных) эффектов и с использованием оптимизированного одноквазичастичного представления в нулевом приближении релятивистской многочастичной теории возмущений, что определяет определенное согласие теории и эксперимента.

Ключевые слова: релятивистская теория, радиационные переходы, принцип калибровочной инвариантности, литий-подобные ионы

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РЕЛЯТИВІСТСЬКИЙ РОЗРАХУНОК ДОВЖИН ХВИЛЬ І E1 СИЛ ОСЦИЛЯТОРІВ В Li-ПОДІБНИХ БАГАТОЗАРЯДНИХ ІОНАХ ТА ПРИНЦИП КАЛІБРУВАЛЬНОЇ ІНВАРІАНТНОСТІ

Резюме. Спектральні довжини хвиль і сили осциляторів для переходів $1s^22s\ (^2S_{1/2}) \rightarrow 1s^23p\ (^2P_{1/2})$ в Li-подібних багатозарядних іонах з зарядом ядра Z = 28,30 обчислені на основі комбінованого релятивістського енергетичнго підходу і релятивістської багаточастинкової теорії збурень з дірак-кон-шемівським одночастинковим наближенням нульового порядку і умовою дотримання принципу калібровочно' інваріантності в радіаційних переходах. Проведено порівняння отриманих результатів з наявними теоретичними і експериментальними даними. Важливий момент пов'язаний з акуратним урахуванням внесків складних багаточасткових обмінних кореляційних (поляризаційних) ефектів і з використанням оптимізованого одноквазічастічного уявлення в нульовому наближенні релятивістської багаточастинкової теорії збурень, що визначає певну згоду теорії та експерименту.

Ключові слова: релятивістська теорія, радіаційні переходи, принцип калібрувальної інваріантності, літій-подібні іони