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OPTIMIZED QUANTUM DEFECT METHOD IN RELATIVISTIC THEORY OF SPECTRA OF LI-LIKE MULTICHARGED IONS

The relativistic theory of radiative transitions using the general relativistic quantum defect approximation (GDA) was also used to study the wavelengths and oscillator strengths for the $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) transitions in Li-like multicharged ions with a nuclear charge Z= 14-70. and. The obtained results were compared with available theoretical and experimental (summarized) data. An important point is related to the accurate accounting of the complex contributions of the exchange-correlation (polarization) effect and the use of an efficient single-quasi-particle representation based on the general relativistic approximation of the quantum defect, which significantly ensures a physically reasonable agreement between the theory and the experiment.

1. Introduction

In the last two decades, the sought-after interest grew even more, when the fundamentally important role of multi-electron Rydberg atoms (RA; i.e., atoms in highly excited states) and multi-charged ions, photon emission and absorption processes with their participation in a wide class of physical applications became apparent. We are talking, first of all, about the problems of astrospectroscopy, astrophysics (radiation processes in nebulae and fragments of Nadnova; according to the idea of Ginzburg et al., radiation transitions between the components of the fine, ultrafine structure of H-, Li-, Be-like ions, N, Fe provide diagnostics of the sought-after radiation), physics of the Sun and auroras (radiation of Ne, Ca, Fe ions, etc.), diagnostics of laboratory, astrophysical, thermonuclear plasma, topical problems of laser physics and quantum electronics, including creation of short-wavelength lasers (razers, grazers etc) [1-30].

There have been sufficiently many papers, devoted to calculations and compilation of energies and oscillator strengths for the Li-like ions and other alkali-like ions (see, for example, [1–14]). Particularly, Martin and Wiese have undertaken a critical evaluation and compilation of the spectral parameters for Li-like ions (Z=3-28) [1,2]. Khetselius [3] has studied the radiative transitions wavelengths and oscillator strengths for some Li-like multicharged ions within the relativistic many-body perturbation theory with the optimized Dirac-Kohn-Sham zeroth approximation and an effective taking the relativistic, exchange-correlation, nuclear, radiative effects into account. The method includes the generalized Glushkov-Ivanov-Ivanova procedure (relativistic energy approach) for generation of the optimal basis set of relativistic electron wave functions with fulfilment of the gauge invariance principle [17-22]. The results of the non-relativistic calculations of the energies and oscillator strengths of $1s22s_j1s22p$ for Li-like systems up to Z = 50 are presented in Ref. [12]. The Hylleraas-type variational method and the $1/Z$ expansion method have been used. In ref. [13] there are listed the nonrelativistic dipole-length, -velocity, -acceleration oscillator strengths for 1s22s–1s22p transitions of LiI isoelectronic sequence calculated within a full core plus correlation method with using multiconfiguration interaction wave functions. Fully variational nonrelativistic Hartree-Fock wave functions were used by Bièmont in calculating 1s2n2L (n<8=s,p,d,f; 3<Z<22) Li-like

states [14]. In many papers the Dirac-Fock (DF) method, model potential, quantum defect approximation in the different realizations have been used for calculating the energies and oscillator strengths of the Li-like and similar ions (see Refs.[3-18]).

In our paper the relativistic theory of radiative transitions using the general relativistic quantum defect approximation (GDA) is used to study the wavelengths and oscillator strengths for $1s^22s(^2S_{1/2}) \rightarrow 1s^23p\ (^2P_{1/2})$ transitions in Li-like multicharged ions with a nuclear charge Z= 14-70. and. The model [15,16] has received the further development. The obtained results were compared with available theoretical and experimental (summarized) data. An important point is related to the effective accounting of the contributions of the exchange-correlation (polarization) effect and the use of an efficient 1-quasi-particle representation based on the general relativistic approximation of the quantum defect, which significantly ensures a physically reasonable agreement between the theory and the experiment.

2. The theoretical method

In atomic spectroscopy there is well known a nonrelativistic and relativistic quantum defect approximation (QDA). Usually, the most exact version of the QDA is provided by using the empirical data in order to determine the quantum defect values for different state. IN [15,16] it was presented ab initio optimized QDA scheme, satisfying a principle of minimization for the gauge dependent radiative contributions to Im δE_{ninv} for the certain class of the photon propagator calibration according to ideas of Refs. [19-22,25,26]. A relativistic quantum defect is usually defined as (see, for example, [15,16]:

$$\mu_\chi(E_n) = n - \nu_n + \gamma - |\chi|, \qquad (1)$$

where χ is he Dirac quantum number, and

$$\gamma = \sqrt{\chi^2 - (\alpha z)^2},$$
$$\nu_n = \frac{z\varepsilon}{\lambda},$$
$$\lambda = \sqrt{-E_n(1+\varepsilon)}, \varepsilon = 1 + \alpha^2 E_n. \qquad (2)$$

In the non-relativistic limit (i.e. the fine structure constant $\alpha \rightarrow 0$) expression (1) transfers to the well known non-relativistic expression for quantum defect:

$$\mu_{l^{NR}}(E_n) = n - n * n - \frac{z}{\sqrt{-2E_n}}, \qquad (3)$$

where n is the principal quantum number, n^* is an effective quantum number, E_n is an electron energy and z is a charge of a core (ion).

At present, there are detailed tables of QD values for states with different l for a number of one-quasiparticle atomic systems, in particular, neutral atoms of alkaline elements (see, e.g. [16] and refs therein). At the same time, it should be noted that for most ions of the isoelectronic series of alkali and other atoms and ions, detailed data, as a rule, are not available, since the standard method for determining the QD is a fitting from the experimental values of the energy levels, which for a huge number of multiply charged ions are currently generally, are missing. In the corresponding review of Section 1, we presented the usual Ritz-type variational formula for the series expansion for QD. Calculation of CD is carried out according to the standard formula of the form:

$$\mu_L(n) = a + b/(n-a)^2 + c/(n-a)^4 + d/(n-a)^6 + e/(n-a)^8, \qquad (4)$$

where *a, b, c, d, e* are the Rydberg-Ritz coefficients. The corresponding orbitals of the relativistic QDA without the use of exchange-correlation potentials are determined by the analytical solution of the Dirac-type relativistic equation with a model Hamiltonian containing QD.

In our generalized QDA the "shell-external particle" interaction potential is improved by means of adding the model potentials of the following type:

$$V^{\text{GMMP}}(r) = V_C^D(r) + V_X^{\text{Sl}}(r) + V_C[r \vee b] \quad .(5)$$

where V_C^D- QDA potential of atomic core, V_{XC}^{Sl} is an exchange -correlation potential of the Kohn-Sham type and Gunnarsson-Lundqvist type. The datils regarding the last potentials

can be found in Refs. [15,16]. Further, the key element of our approach is the use of an iterative procedure for building an optimized one-electron representation for relativistic bi-spinors of the QDA model and, accordingly, a new ab initio scheme for determining the QD parameters, based on the fundamental principle of minimizing gauge-non-invariant contributions to the radiation widths of atomic levels ΔE_{ninv}, which is related with the exchange of longitudinal photons. Accordingly, the procedure for minimizing ΔE_{ninv} is further reduced to a chain of variations (in fact, we are talking about a system of equations of the Dirac-QDA type).

In the usual versions of the QD theory it is mandatory to have reliable experimental information in fact for the corresponding fitting of the CD. The expression for the normalized relativistic wave functions (Dirac spinors) of the discrete spectrum $E_n < 0$) for $r > r_0$ has the standard form is as:

$$\left.\begin{matrix} G_{n\chi}(r) \\ F_{n\chi}(r) \end{matrix}\right\} = \pm\left[\frac{(1\pm\varepsilon)(z-\lambda\chi)}{4zr\zeta(E_n)\Gamma(\nu_n+\gamma+1)\Gamma(\nu_n-\gamma+1)}\right]^{1/2}$$

$$\left\{W_{\nu_n+1/2,\gamma}(2\lambda r)\pm(\eta_n+\chi)W_{\nu_n-1/2,\gamma}(2\lambda r)\right\}, \quad (6a)$$

where

$$\zeta(E)=1+\frac{\lambda^3}{z}\frac{d\mu_\chi(E)}{\mathrm{dE}}, \eta_n=\frac{z}{\lambda}. \quad (6b)$$

Here $W_{k,m}(x)$ is the Whittaker's type function, a γ, λ, υ_n , ε are determined on the basis of standard formulas.

For a continuous spectrum ($E\geq 0$), the wave functions can be represented as a linear combination of two linearly independent relativistic Coulomb functions. The coefficients in this linear combination are determined so that at $r\to\infty$:

$$\left.\begin{matrix} G_\chi(E,r) \\ F_\chi(E,r) \end{matrix}\right\} \approx \sqrt{\frac{\varepsilon\pm1}{\pi p}}\begin{matrix}\sin \\ \cos\end{matrix}[pr+$$

$$y\ln 2pr+\xi-arg\Gamma(\gamma+1+iy)-\frac{\pi\gamma}{2}+\delta_\chi(E) \quad (7a)$$

where

$$p=\sqrt{E(1+\varepsilon)},$$
$$\varepsilon=1+\alpha^2E,$$
$$y=\frac{z\varepsilon}{p},$$

$$\xi=\frac{1}{2}\arg\frac{\chi-i\frac{z}{p}}{\gamma-\mathrm{iy}} \quad (7b)$$

Within an anergy approach [18-22] the probability of the E dipole transition is:

$$\Gamma_{\alpha_n}=\frac{1}{4\pi}\cdot V_{\alpha_n\alpha_n}^{|\omega_{\alpha_n}|} \quad (9)$$

where the matrix element is determined as follows:

$$V_{ijkl}^{|\omega|}=\iint dr_1dr_2\Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \quad (10)$$

The corresponding oscillator strength: $gf=\lambda_g^2\cdot\Gamma_{\alpha n}/6.67\cdot10^{15}$, where g is the degeneracy degree, λ is a wavelength in angstrems (Å). The relativistic QDA wave functions are substituted into matrix element (10). To increase an accuracy of computing oscillator strengths we add the two-quasiparticle polarization potential [19] into the radiation transition matrix element. 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 calculating the energies and oscillator strengths of transitions in spectra of the Li-like ions with Z-13-70. Below we list the corresponding data for some chosen ions, namely S13+ Ca17+ Fe23+ Zn^{27+} Zr^{37+} Mo^{39+} Sn^{47+} Tm^{66+} Yb^{67+}. 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 data on the oscillator strengths values for some Li-like ions with the known theoretical and compillated data [1,2,6-17,25].

As example, in table 1,2 we list our oscillator strengths values (ORMP and OQDA) for $2s_{1/2}$–$2p_{1/2,3/2}$ transitions in Li-like ions

S^{13+},Ca^{17+},Fe^{23+},Zn^{27+},Zr^{37+}, Mo^{39+}, Sn^{47+}, Tm^{66+}, Yb^{67+}.

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

	DF	Our data	Exp.
Ion	$2s_{1/2}–2p_{1/2}$	$2s_{1/2}–2p_{1/2}$	$2s_{1/2}–2p_{1/2}$
S^{13+}	0.0299	0.0304	0.030
Ca^{17+}	0.0234	0.0239	0.024
Fe^{23+}	0.0177	0.0183	0.018
Zn^{27+}	0.0153	0.0159	–
Zr^{37+}	0.0114	0.0123	–
Mo^{39+}	–	0.0116	0.011
Sn^{47+}	0.0092	0.0099	–
Tm^{66+}	–	0.0078	–
Yb^{67+}	0.0067	0.0075	–

The DF calculation data by Zilitis [6] and the "best" compillated (experimental) data [1,2] for the some low-Z Li-like ions are listed in tables 1,2 for comparison too. It should be reminded that the experimental data on the oscillator strengths for many (especially, high-Z) Li-like ions are absent.

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

	DF	Exp.	Our data
Ion	$2s_{1/2}–2p_{3/2}$	$2s_{1/2}–2p_{3/2}$	$2s_{1/2}–2p_{3/2}$
S^{13+}	0.0643	0.064	0.0645
Ca^{17+}	0.0542	0.054	0.0546
Fe^{23+}	0.0482	0.048	0.0486
Zn^{27+}	0.0477	–	0.0480
Zr^{37+}	0.0543	–	0.0545
Mo^{39+}	–	0.056	0.0564
Sn^{47+}	0.0686	–	0.0689
Tm^{66+}	–	–	01146
Yb^{67+}	0.1170	–	0.1173

Let us note 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 2.5%. It means that the results are very closed within schemes with using the different photon propagator gauges.

In is worth to underline that the QDA oscillator strengths data become more exact with the growth of the principal quantum number. The most optimal variant is consideration of essentially Rydberg atomic starts. At the same time the accuracy of the DF data may be decreased. The agreement between the Martin-Weiss data and our results for the transitions between low-lying terms is sufficiently good. An important point is related to the accurate accounting of the complex contributions of the exchange-correlation (polarization) effect and the use of an efficient single-quasi-particle representation based on the general relativistic approximation of the quantum defect, which significantly ensures a physically reasonable agreement between the theory and the experiment.

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Key words: relativistic theory, quantum defect method, radiative transitions, lithium-like ions

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ОПТИМІЗОВАНИЙ МЕТОД КВАНТОВОГО ДЕФЕКТУ В РЕЛЯТИВІСТСЬКІЙ ТЕОРІЇ СПЕКТРІВ ЛІТІЙ-ПОДІБНИХ БАГАТОЗАРЯДНИХ ІОНІВ

Резюме. Релятивістська теорія радіаційних переходів з використанням узагальненого релятивістського наближення квантового дефекту (GDA) використана і з для дослідження довжин хвиль та сил осциляторів для переходів $1s^22s$ ($^2S_{1/2}$) → $1s^23p$ ($^2P_{1/2}$) та інших у Li-подібних багатозарядних іонах із зарядом ядра Z=14-70. Проведено порівняння отриманих результатів з наявними теоретичними та експериментальними (зведеними) даними. Важливий момент розробленої моделі пов'язаний з додатковим ефективним урахуванням обмінно-кореляційного (поляризаційного) ефекту та використанням ефективногго одноквазічастинкового представлення на основі узагальненого релятивістського наближення квантового дефекту, що суттєво забезпечує фізично розумну узгодженість між теорією та експериментом.

Ключові слова: релятивістська теорія, метод квантового дефекта, радіаційні переходи, літій-подібні іони

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