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Advanced relativistic model potential approach to calculation of radiation transition parameters in spectra of multicharged ions

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Abstract. The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order optimized one-particle approximation are used for calculation of the Li-like ions (Z=11-42,69,70) energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, $2s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12). 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 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. It should be mentioned that the correct data about radiative decay widths, probabilities and oscillator strengths of atomic transitions are needed in astrophysics and laboratory, thermonuclear plasma diagnostics and in fusion research. In this light, a special interest includes studying the spectral characteristics of the He-, Li- *etc.* like ions. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for the Li-like ions and other alkali-like ions (see, for example, [1–16]). Particularly, Martin and Wiese have undertaken a critical evaluation and compilation of the spectral parameters for Li-like ions (Z=3-28) [1,2]. The results of the high-precision non-relativistic calculations of the energies and oscillator strengths of $2s$ - $2p$ for Li-like systems up to Z = 50 are presented in Refs. [9-14]. The Hylleraas-type variational method and the $1/Z$ expansion method have been used. Chen Chao and Wang Zhi-Wen [14] have listed the nonrelativistic dipole-length, -velocity and -acceleration absorption oscillator strengths for the 1s22s–1s22p transitions of the Li I isoelectronic sequence on the basis of calculation within a full core plus correlation method with using multiconfiguration interaction wave functions. Fully variational nonrelativistic Hartree-Fock wave functions have been used by Bièmont in calculation of the 1s2n2L (n <8 =s, p, d or f; 3 < Z<22) states of the Li I isoelectronic sequence [16]. In many papers, the Dirac-Fock method, model potential approach, quantum defect approximation in the different realizations have been used for calculating the energies and oscillator strengths of the Li-like ions (see Refs.[1-17]). The consistent Quantum Electrodynamics (QED) calculations of the energies, ionization potentials, hyperfine structure constants for the Li-like ions are reported in Refs. [18-21]. However, it should be stated that for Li-like ions with higher Z,

particularly for their high-excited (Rydberg) states, there is not enough precise information available in the literature. In our paper the combined relativistic energy approach [22-26] and relativistic many-body perturbation theory with the zeroth order optimized one-particle representation [26] are used for calculation the Li-like ions (Z=11-42,69,70) energies and oscillator strengths of radiative transitions from ground state to low-excited and Rydberg states. The comparison of the calculated oscillator strengths with available theoretical and experimental data is performed.

2. The theoretical method

In the relativistic energy approach [4, 5, 22-25] the imaginary part of electron energy shift of an atom is connected with the radiation decay possibility (transition probability). An approach, based on 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:

$$\Delta E = \mathrm{Re}\Delta E + i\,\Gamma/2 \tag{1}$$

where Γ is interpreted as the level width, and the decay probability P = Γ. For the α-n radiation transition the imaginary part of electron energy in the lowest order of perturbation theory is determined as [4]:

$$\mathrm{Im}\,\Delta E = -\frac{1}{4\pi}\sum_{\substack{\alpha>n>f\\ [\alpha<n\le f]}} V_{\alpha n\alpha n}^{|\omega_{\alpha n}|}, \tag{2}$$

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:

$$V_{ijkl}^{|\omega|} = \iint dr_1 dr_2 \Psi_i^*(r_1)\Psi_j^*(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi_k^*(r_2)\Psi_l^*(r_1) \tag{3}$$

The separated terms of the sum in (3) represent the contributions of different channels and a probability of the dipole transition is:

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V_{\alpha_n\alpha_n}^{|\omega_{\alpha_n}|} \tag{4}$$

The corresponding oscillator strength: $gf=\lambda^2\Gamma_{\alpha n}/6.67\cdot10^{15}$, where g is the degeneracy degree, λ is a wavelength in angstrems (Å). When calculating the matrix elements in Equation (3) one should use the angle symmetry and write the expansion for potentials $\sin|\omega|r_{12}/r_{12}$ in spherical functions as follows [2]:

$$\frac{\mathbf{sin}|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}^{\infty}(\lambda)J_{\lambda+1/2}(|\omega|r_1)J_{\lambda+1/2}(|\omega|r_2)P_\lambda(\mathbf{cos}\,\widehat{\boldsymbol{r}_1\boldsymbol{r}_2}), \tag{5}$$

where J is the Bessel function of first kind and (λ)= 2λ + 1. This expansion is corresponding to usual multipole one for probability of radiative decay. Substitution of the expansion (5) to matrix element of interaction gives as follows [20]:

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

$$Q_\lambda = Q_\lambda^{\mathrm{Qul}} + Q_\lambda^{\mathrm{Br}}, \quad (6)$$

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. [4,20]. The relativistic wave functions are calculated by solution of the Dirac equation with the potential, which includes the "outer electron- ionic core" potential and polarization potential [29]. In order to describe interaction of the outer electron with the He-like core the modified model potential [4] has been used. The calibration of the single model potential parameter has been performed on the basis of the special *ab initio* procedure within relativistic energy approach [24] (see also [5]). In Ref.[18] the lowest order multielectron effects, in particular, the gauge dependent radiative contribution Im δE_{ninv} for the certain class of the photon propagator calibration is treated. This value is considered to be representative for the correlation effects, whose minimization is a reasonable criterion in the searching for the optimal one-electron basis of the many-body perturbation theory. The minimization of the density functional Im δE_{ninv} leads to the integral-differential equation that can be solved using one of the standard numerical codes. It provides the construction of the optimized one-particle representation. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results

We applied the above described approach to calculating the energies and 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 [1,2,8]. As an example, in table 1 we present the oscillator strengths values for the 2s1/2 – 2p1/2,3/2 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 [6] and the "best" compillated (experimental) data [1,2] 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.

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

Method	DF [6]	DF [6]	[2]	[2]	Our	Our
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

In Table 2 we present the oscillator strengths values for the $2s_{1/2} - np_j$ (n=3-18, j=1/2) transitions in spectrum of the Li-like ion Zr^{37+}. The quantum defect approximation (QDA) [6,27], the DF oscillator strengths calculation results by Zilitis [6] and some tabulated (experimental) data by Martin-Weiss [1]

are listed as well. It is self-understood that the QDA oscillator strengths data become more exact with the growth of the principal quantum number. At the same time the accuracy of the DF data may be decreased. The agreement between the Martin-Weiss data and our results is acceptable.

Table 2. Oscillator strengths of the $2s_{1/2} - np_{1/2}$ transitions in Zr^{37+}.

Transition	QDA [6]	DF [6]	Our data
$2s_{1/2}–3p_{1/2}$	13.7	13.3	13.684
$–4p_{1/2}$	-	3.22	3.232
$–6p_{1/2}$	-	-	0.682
$–8p_{1/2}$	0.258	0.257	0.260
$–10p_{1/2}$	0.126	0.124	0.125
$–16p_{1/2}$	0.0291	0.0285	0.0287
$–18p_{1/2}$	-	-	0.0216

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