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ADVANCED RELATIVISTIC MODEL POTENTIAL APPROACH TO CALCULATION OF RADIATION TRANSITION PARAMETERS IN SPECTRA OF MULTICHARGED IONS

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). The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) 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, an special interest attracts 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 $1s22s_j1s22p$ 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 LiI 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 wavefunctions have been used by Biémont in calculation of the 1s2n2L (n <8 =s, p, d or f; 3 < Z<22) states of the LiI 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 QED calculations of the energies, ionization potentials, hyperfine structure constants for the Li-like ions are performed 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 literatures. 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 Ry-

dberg states.. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) 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 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:

$$DE = ReDE + i\ G/2 \qquad (1)$$

where G is interpreted as the level width, and the decay possibility P = G. The imaginary part of electron energy of the system, which is defined in the lowest order of perturbation theory as [4]:

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

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

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1 - \alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (3)$$

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

$$\Gamma_{\alpha_n} = \frac{1}{4\pi}\cdot V^{|\omega_{\alpha_n}|}_{\alpha_n\alpha_n} \qquad (4)$$

The corresponding oscillator strength : $gf = \lambda^2_g \cdot \Gamma_{\alpha_n} / 6.67\cdot 10^{15}$, where g is the degeneracy degree, l is a wavelength in angstrems (Å). Under calculating the matrix elements (3) one should use the angle symmetry of the task and write the expansion for potential sin|w|r12/r12 on spherical functions as follows [2]:

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

where J is the Bessel function of first kind and (l)= 2l + 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]:

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

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

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 Ivanova-Ivanov 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 dE_{ninv} for the certain class of the photon propagator calibration is treated. This value is considered to be the typical representative of the electron correlation effects, whose minimization is a reasonable criterion in the searching for the optimal one-electron basis of the relativistic many-body perturbation theory. The minimization of the density functional Im dE_{ninv} leads to the integral-differential equation that can be solved using one of the standard numerical codes. Therefore, it provides the construction of the op-

timized 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 data on the oscillator strengths values for some Li-like ions with the known theoretical and compillated 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.

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

It should be reminded that the experimental data on the oscillator strengths for many (especially, high-Z) Li-like ions are absent. In a whole, there is a physically reasonable agreement between the listed data. The important features of the approach used are using the optimized one-particle representation and account for the polarization effect. 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 using the different photon propagator gauges (Coulomb, Babushkon, Landau) are practically equal.

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 compillated (experimental) data by Martin-Weiss [1] are listed too.

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 is sufficiently good.

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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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). The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed.

Key words: relativistic theory, oscillator strengths, radiative transitions

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РАСШИРЕННАЯ РЕЛЯТИВИСТСКАЯ МОДЕЛЬ ПОТЕНЦИАЛЬНОГО ПОДХОД К РАСЧЕТУ ПЕРЕХОДНЫХ ПАРАМЕТРОВ ИЗЛУЧЕНИЯ В СПЕКТРАХ МНОГОЗАРЯДНЫХ ИОНОВ

Резюме

Комбинированный релятивистский энергитический подход и релятивистская теория возмущений многих тел с оптимизированным одночастичным приближением нулевого порядка используются для расчета Li-подобных ионов (Z = 11-42,69,70) энергии и силы осцилляторов радиационных переходов из основного состояния в низкие возбужденные и ридберговские состояния, в частности, $2s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12). Сравнение расчетных сил осцилляторов с имеющимися теоретическими и экспериментальными данными выполнено.

Ключевые слова: релятивистская теория, силы осцилляторов, радиационные переходы.

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РОЗШИРЕНА РЕЛЯТИВІСТСЬКА МОДЕЛЬ ПОТЕНЦІАЛЬНОГО ПІДХОДУ ДО РОЗРАХУНКУ ПЕРЕХІДНИХ ПАРАМЕТРІВ ВИПРОМІНЮВАННЯ В СПЕКТРАХ БАГАТОЗАРЯДНИХ ІОНОВ

Резюме

Комбінований релятивістський енергетичний підхід і релятивістська теорія збурень багатьох тіл з оптимізованим одночастковим наближенням нульового порядку використовується для розрахунку Li-подібних іонів (Z = 11-42,69,70) енергії і сили осциляторів радіаційних переходів із основного стану в низькі збуджені та рідбергівські стани, зокрема, $2s_{1/2} - np_{1/2,3/2}$, $np_{1/2,3/2}$-$nd_{3/2,5/2}$ (n=2-12). Порівняння розрахованих сил осциляторів з наявними теоретичними та експериментальними даними виконане.

Ключові слова: релятивістська теорія, сили осциляторів, радіаційнні переходи.