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OPTIMIZED RELATIVISTIC MODEL POTENTIAL METHOD AND QUANTUM DEFECT APPROXIMATION IN THEORY OF RADIATIVE TRANSITIONS IN SPECTRA OF MULTICHARGED IONS

The combined relativistic model potential approach and relativistic many-body perturbation theory with the zeroth order optimized one-particle approximation are used for calculation of the Li-like ions energies and oscillator strengths of radiative transitions from ground state to low-excited and Rydberg states. New element in our scheme is an implementation of optimized relativistic model potential and quantum defect approximation) approach to energy approach frames. Comparison of 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 on 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, [1–19]). 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 $1s22s_j 1s22p$ for Li-like systems up to $Z = 50$ are presented in Refs. [9-17]. The Hylleraas-type variational method and the $1/Z$ expansion method have been used. Chen Chao and Wang Zhi-Wen [14] 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 [16]. 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.[3-6,16-30]). The consistent QED calculations of the energies, ionization potentials, hyperfine structure constants for the Li-like ions are performed in Refs. [18,19]. However, for Li-like ions with higher Z, particularly, for their high-excited (Rydberg) states, there are not enough precise data available in literatures. In our paper the optimized relativistic model potential (ORMP) [26-29] combined with the relativistic energy approach [3-5] and many-body perturbation theory (PT) [19,29] with zeroth order optimized 1-particle representation [4,21-24] 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 key feature of the presented basis theory is an implementation of the relativistic model potential

(quantum defect approach) to the frames of energy approach for studying spectral parameters of Rydberg multi-electron ions. The comparison of calculated oscillator strengths with available theoretical and experimental (compillated) data is performed.

2. The theoretical method

In the relativistic energy approach [3,4,22-24] the imaginary part of electron energy shift of an atom is directly connected with the radiation transition probability. An approach, using the Gell-Mann and Low formula is used in treating the relativistic atom. The total energy shift of the state is usually presented as (see, for example, [3,4,24] and also [21]):

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

where Γ is interpreted as the level width and decay possibility $P = \Gamma$. The imaginary part of electron energy of the system, which is defined in the lowest PT order as [3]:

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

where $\sum_{\alpha>n>f}$ for electron and $\sum_{\alpha<n\le f}$ for vacancy. The matrix element is determined as follows:

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

$$(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1)$$

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, λ 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 $\sin|\omega|r_{12}/r_{12}$ on spherical functions as follows [3,4]:

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

where J is the Bessel function of first kind and $(\lambda)= 2\lambda + 1$. This expansion corresponds to usual multipole one for radiative probability. Substitution of expansion (5) to matrix element of interaction gives [3,4]:

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

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

where j_i is the total single electron momentum, m_i – the projections; Q^{Qul}_λ is the Coulomb part of interaction, Q^{B}_λ – the Breit part. The Coulomb part Q^{Qul}_λ is expressed in terms of radial integrals R_λ, angular coefficients S_λ:

$$Q^{\mathrm{Qul}}_\lambda = \frac{1}{Z}\{R_l(1243)S_\lambda(1243) + R_\lambda(\tilde{1}243)S_\lambda(\tilde{1}243) + R_\lambda(1\tilde{2}43)S_\lambda(1\tilde{2}43) + R_\lambda(\tilde{1}\tilde{2}43)S_\lambda(\tilde{1}\tilde{2}43)\}. \qquad (7)$$

The different items in (7) include large and small components of the Dirac functions; the sign «~» means that in (7) the large radial component f_i is to be changed by the small g_i one and the moment l_i is to be changed by $\tilde{l}_i = l_i - 1$ for the Dirac number æ> 0 and l_i+1 for æ<0. The Breit interaction part is defined by similar way (see [3-5,21,24]. 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 [21]. In order to describe interaction of the outer electron with the He-like core the simplified Ivanova-Ivanov type model potential [3] is 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 [22] (see also [4,5,21]). In Ref.[22] 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 PT. The minimization of functional Im dE_{ninv} leads to integral-differential equation that can be solved using one of the standard codes. Therefore, it provides the construction of the optimized 1-particle representation and thus ORMP scheme [27-29]. The same procedure is used in generalization of the 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. The above described approach allows to generalize the QDA and get a new ab initio optimized QDA (OQDA) 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. A relativistic quantum defect is usually defined as (see, for example, [30]:

$$\mu_\chi(E_n) = n - \nu_n + \gamma - |\chi|, \tag{8}$$

where χ is he Dirac quantum number, and

$$\gamma = \sqrt{\chi^2 - (\alpha z)^2}\,,\ \nu_n = \frac{z\varepsilon}{\lambda},\ \lambda = \sqrt{-E_n(1+\varepsilon)}\,,\ \varepsilon = 1 + \alpha^2 E_n\,. \tag{9}$$

In the non-relativistic limit (i.e. the fine structure constant $\alpha \to 0$) expression (8) transfers to the well known non-relativistic expression for quantum defect:

$$\mu_l^{\text{R}}(E_n) = n - n^* = n - \frac{z}{\sqrt{-2E_n}}\,, \tag{10}$$

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).

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). All calculations are performed on the basis of the numeral code Superatom. 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+} . 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. 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. Letus note that an estimate of the gauge-noninvariant 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%. It means that the results are practically equal within schemes with using the different photon propagator gauges (such as Coulomb, Babushkin, Landau). In table 3 we present the our oscillator strengths values (ORMP and OQDA) for the $2s_{1/2}$ – np_j (n=3-12, j=1/2,3/2) transitions in spectrum of the Li-like Ca^{17+}.

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

	DF	Exp.	Our data: ORMP	Our data: OQDA
Ion	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{1/2}$	$2s_{1/2}$–$2p_{1/2}$
S^{13+}	0.0299	0.030	0.0301	0.0303
Ca^{17+}	0.0234	0.024	0.0236	0.0238
Fe^{23+}	0.0177	0.018	0.0179	0.0181
Zn^{27+}	0.0153	–	0.0156	0.0158
Zr^{37+}	0.0114	–	0.0118	0.0121
Mo^{39+}	–	0.011	0.0110	0.0114
Sn^{47+}	0.0092	–	0.0095	0.0099
Tm^{66+}	–	–	0.0072	0.0076
Yb^{67+}	0.0067	–	0.0069	0.0073

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

	DF	Exp.	Our data: ORMP	Our data: OQDA
Ion	$2s_{1/2}$–$2p_{3/2}$	$2s_{1/2}$–$2p_{3/2}$	$2s_{1/2}$–$2p_{3/2}$	$2s_{1/2}$–$2p_{3/2}$
S^{13+}	0.0643	0.064	0.0641	0.0643
Ca^{17+}	0.0542	0.054	0.0541	0.0544
Fe^{23+}	0.0482	0.048	0.0481	0.0484
Zn^{27+}	0.0477	–	0.0475	0.0479
Zr^{37+}	0.0543	–	0.0540	0.0544
Mo^{39+}	–	0.056	0.0558	0.0562
Sn^{47+}	0.0686	–	0.0684	0.0688
Tm^{66+}	–	–	01140	01145
Yb^{67+}	0.1170	–	0.1167	0.1172

Table 3. Oscillator strengths of the $2s_{1/2} - np_{1/2}$ transitions in Ca^{17+}.

Transition	QDA	DF	Exp.	Our data: ORMP	Our data: OQDA
$2s_{1/2}$–$3p_{1/2}$	–	–	0.123	0.122	0.127
$2s_{1/2}$–$3p_{3/2}$	–	–	0.241	0.243	0.248
$2s_{1/2}$–$4p_{1/2}$	–	–	–	0.029	0.032
$2s_{1/2}$–$8p_{1/2}$	2.54[a]	2.53[a]	–	2.55[a]	2.55[a]
$2s_{1/2}$–$10p_{1/2}$	1.24[a]	1.24[a]	–	1.25[a]	1.25[a]
$2s_{1/2}$–$12p_{1/2}$	0.70[a]	0.698[a]	–	0.71[a]	0.71[a]

Note: [a] ($10^{-3}gf$).

The standard QDA, DF oscillator strengths calculation results by Zilitis and some experimental data by Martin-Weiss [1,2,6,24] are listed in table 3 too. 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 for the transitions between low-lying terms is sufficiently good.

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Abstract. The combined relativistic model potential approach and relativistic many-body perturbation theory with the zeroth order optimized one-particle approximation are used for calculation of the Li-like ions energies and oscillator strengths of radiative transitions from ground state to low-excited and Rydberg states. New element in our scheme is an implementation of optimized relativistic model potential and quantum defect approximation) approach to energy approach frames. Comparison of calculated oscillator strengths with available theoretical and experimental (compillated) data is performed.

Key words: optimized model potential approach, oscillator strengths, radiative transition

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ОПТИМИЗИРОВАННЫЙ РЕЛЯТИВИСТСКИЙ МЕТОД МОДЕЛЬНОГО ПОТЕНЦИАЛА И МЕТОД КВАНТОВОГО ДЕФЕКТА В ТЕОРИИ РАДИА-ЦИОННЫХ ПЕРЕХОДОВ В СПЕКТРАХ МНОГОЗАРЯДНЫХ ИОНОВ

Резюме. Комбинированный релятивистский метод модельного потенциала и метод теории возмущений с оптимизированным 1-частичным нулевым приближением использованы для вычисления энергий и сил осцилляторов радиационных переходов из основного состояния в низколежащие и ридберговские состояния в спектрах Li-подобных ионов. Основная особенность нового подхода заключается в имплементации оптимизированного релятивистского приближения модельного потенциала (квантового дефекта) в рамки энергетического подхода. Выполнен анализ и сравнение полученных данных для сил осцилляторов с имеющимися теоретическими и экспериментальными данными.

Ключевые слова: оптимизированный метод модельного потенциала, силы осцилляторов, радиационные переходы