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QUANTUM DEFECT APPROXIMATION IN THEORY OF RADIATIVE TRANSITIONS IN SPECTRUM OF Li-like CALCIUM

The combined relativistic quantum defect approximation and relativistic many-body perturbation theory with the zeroth order optimized approximation are applied to studying the Li-like calcium oscillator strengths of radiative transitions from ground state to the Rydberg states. New element in our scheme is an implementation of optimized relativistic quantum defect approximation to an energy approach frames. Comparison of calculated oscillator strengths with available theoretical and experimental (compillated) data is performed and a number of oscillator strengths are presented firstly.

1. Introduction

This paper goes on our work on studying radiative transitions characteristics in the multicharged ions on the basis of the combined relativistic quantum defect approximation [1,2] and relativistic many-body perturbation theory with the zeroth order optimized approximation [3].

Let us remind (look, for example, [1,2]) that the spectral data for highly ionized atoms has a fundamental importance in many fields of atomic physics (spectroscopy, spectral lines theory), plasma physics and chemistry, laser physics and quantum electronics, astrophysics and laboratory, thermonuclear plasma diagnostics and in fusion research.

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, [1–23]). Particularly, Martin and Wiese have undertaken a critical evaluation and compilation of the spectral parameters for Li-like ions (Z=3-28) [4,5]. 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. [12-20]. The Hylleraas-type variational method and the $1/Z$ expansion method have been used. Chen Chao and Wang Zhi-Wen [15] 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 [18].

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.[4-9,19-30]). 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 this paper the combined relativistic quantum defect approximation (QDA) and relativistic many-body perturbation theory with the zeroth order optimized approximation are applied to studying

the Li-like calcium oscillator strengths of radiative transitions from ground state to the Rydberg states. New element in our scheme is an implementation of optimized relativistic quantum defect approximation to an energy approach frames. Comparison of calculated oscillator strengths with available theoretical and experimental (compillated) data is performed and a number of oscillator strengths are presented firstly.

2. Relativistic energy approach to atom in a strong laser field: Multiphoton resonances

As the detailed presentation of our version of the relativistic quantum defect approximation is in , for example, Ref. [1,2], here we present only the key elements. The relativistic energy approach in gauge-invariant form is presented in many books, articles (look [5-7,3]). Within an energy approach the imaginary part of electron energy shift of an atom is directly connected with the radiation transition probability. The total energy shift of the state is usually presented as (see, for example, [5,6] and also [3]):

$$\mathrm{DE} = \mathrm{ReDE} + \mathrm{i}\, G/2 \qquad (1)$$

where G is interpreted as the level width and decay possibility $P = G$. 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:

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

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: $gf = \lambda_g^2 \cdot \Gamma_{\alpha n} / 6.67 \cdot 10^{15}$, 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 $\sin|w|r_{12}/r_{12}$ on spherical functions and this expansion corresponds to usual multipole one for radiative probability. Substitution of expansion (5) to matrix element of interaction gives [5,6]:

$$V^{\omega}_{1234} = [(j_1)(j_2)(j_3)(j_4)]^{1/2} \times \times \sum_{\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & \lambda \\ m_1 & -m_3 & \mu \end{pmatrix} \times \mathrm{Im}[Q^{Qul}_{\lambda} + Q^{B}_{\lambda}] \qquad (5)$$

where j_i is the total single electron momentum, m_i – the projections; Q^{Qul}_{λ} is the Coulomb part of interaction, Q^{Br}_{λ} - the Breit part. The Coulomb part Q^{Qul}_{λ} is expressed in terms of radial integrals R_l, angular coefficients S_l. The Breit interaction part is defined by similar way (see [3]). 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 [3]. The calibration of the single model potential parameter has been performed on the basis of the special ab initio procedure within relativistic energy approach (see also [5-7]). In Ref.[6] 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 optimized relativistic model potential ORMP

scheme [6]. The same procedure is used in generalization of the relativistic 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 scheme, satisfying a principle of minimization for the gauge dependent radiative contributions to Im dE_{ninv} for the certain class of the photon propagator calibration. A relativistic quantum defect is usually defined as (see, for example, [3]:

$$\mu_\chi(E_n) = n - \nu_n + \gamma - |\chi|, \qquad (6)$$

where χ is he Dirac quantum number, and

$$\gamma = \sqrt{\chi^2 - (\alpha z)^2}\,,$$

$$\nu_n = \frac{z\varepsilon}{\lambda},$$

$$\lambda = \sqrt{-E_n(1+\varepsilon)}\,,$$

$$\varepsilon = 1 + \alpha^2 E_n\,. \qquad (7)$$

In the non-relativistic limit (i.e. the fine structure constant $\alpha \to 0$) expression (7) transfers to the well known non-relativistic expression for quantum defect:

$$\mu_l^{NR}(E_n) = n - n^* = n - \frac{z}{\sqrt{-2E_n}}\,, \qquad (8)$$

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 and conclusions

We applied the above described approach to calculating the energies and oscillator strengths of transitions in spectra of the Li-like calcium (Z=12). All calculation is performed on the basis of the numeral code Superatom. There are considered the radiative transitions from ground state to the Rydberg states, particularly, $2s_{1/2} - np_{1/2,3/2}$ (n=3-12). ASome preliminary data were listed in [1]. As usually, to test the obtained results, we compare our data on the oscillator strengths values for some Li-like ions with the known theoretical and compillated data [8-18]. In table 1 we present the our oscillator strengths values (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 values (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+}

Transition	Exp	QDA	DF
$2s_{1/2}$–$3p_{1/2}$	0.123	–	–
$2s_{1/2}$–$3p_{3/2}$	0.241	–	–
$2s_{1/2}$–$4p_{1/2}$	–	–	–
$2s_{1/2}$–$8p_{1/2}$	–	2.54[a]	2.53[a]
$2s_{1/2}$–$9p_{1/2}$	–	1.74[a]	1.73[a]
$2s_{1/2}$–$10p_{1/2}$	–	1.24[a]	1.24[a]
$2s_{1/2}$–$11p_{1/2}$	–	0.919[a]	0.916[a]
$2s_{1/2}$–$12p_{1/2}$	–	0.70[a]	0.698[a]
$2s_{1/2}$–$13p_{1/2}$	–	0.546[a]	0.54[a]
Transition	MBP	Our1	Our2
$2s_{1/2}$–$3p_{1/2}$	0.126	0.120	0.121
$2s_{1/2}$–$3p_{3/2}$	0.246	0.237	0.238
$2s_{1/2}$–$4p_{1/2}$	–	0.028	0.029
$2s_{1/2}$–$8p_{1/2}$	–	2.52	2.52
$2s_{1/2}$–$9p_{1/2}$	–	1.75	1.75
$2s_{1/2}$–$10p_{1/2}$	–	1.24	1.24
$2s_{1/2}$–$11p_{1/2}$	–	0.91	0.91
$2s_{1/2}$–$12p_{1/2}$	–	0.70	0.70
$2s_{1/2}$–$13p_{1/2}$	–	0.55	0.55

In Table 1 we list also the corresponding results on oscillator strengths obtained by computing within the standard QDA, Dirac-Fock (DF) by Zilitis and some experimental data by Martin-Weiss [1,4,8]. 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 (our 1 and Our 2 are corresponding to two different gauges of a photon propagator or at usual amplitude approach language length and velocity forms of transition operator) is physically reasonable. The closeness of oscillator strength values proves a gauge invariance principle conservation in the radiative transition probabilities scheme.

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Abstract.

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Key words: quantum defect approximation, oscillator strengths, radiative transition, Li-like calcium

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ПРИБЛИЖЕНИЕ КВАНТОВОГО ДЕФЕКТА В ТЕОРИИ РАДИАЦИОННЫХ ПЕРЕХОДОВ В СПЕКТРЕ Li-ПОДОБНОГО КАЛЬЦИЯ

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: квантового дефекта приближение, силы осцилляторов, радиационные переходы, Li-подобный кальций

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НАБЛИЖЕННЯ КВАНТОВОГО ДЕФЕКТУ В ТЕОРІЇ РАДІАЦІЙНИХ ПЕРЕХОДІВ У СПЕКТРІ Li-ПОДІБНОГО КАЛЬЦІЮ

Резюме.

Комбінований релятивістське наближення квантового дефекту і релятивістська теорія збурень з оптимізованим одночастинковим нульовим наближенням використані для вивчення сил осциляторів радіаційних переходів з основного стану у рідбергівські стани у спектрі Li-подібного кальцію. Основна особливість нового підходу пов'язана з імплементацією оптимізованого релятивістського наближення квантового дефекту у межи енергетичного підходу. Виконано аналіз та порівняння отриманих результатів по силам осциляторів з наявними теоретичними та експериментальними даними і ряд значень сил осциляторів представлені, по-перше.

Ключові слова: квантового дефекту наближення, сили осциляторів, радіаційні переходи, Li-подібний кальцій