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RELATIVISTIC CALCULATION OF OSCILLATOR STRENGTHS OF THE RADIATION TRANSITIONS BETWEEN BARIUM RYDBERG STATES

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham one-particle approximation are used for preliminary estimating the energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, 6s2 -6snp (n =7-30) transitions, of the barium atom. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed. The important point is linked with non-accounting for the polarization effect contribution into the oscillator strength value that has led to ~40% difference between the empirical (compillated) and theoretical data.

1. Introduction

The research in many fields of modern atomic physics (spectroscopy, spectral lines theory, theory of atomic collisions etc), astrophysics, plasma physics, laser physics and quantum and photo-electronics requires an availability of sets of correct data on the energetic, spectroscopic and structural properties of atoms, especially in the high excited, Rydberg states. Naturally, the correct corresponding data about radiative decay widths, probabilities and oscillator strengths of atomic transitions are needed in building adequate astrophysical models, realizing regular astrophysical, laboratory, thermonuclear plasma diagnostics and in fusion research. Besides, a great interest to studying Rydberg atomic states parameters can be easily explained by a powerful development of such new fields as quantum computing, and quantum cryptography, construction of new type Rydberg atomic lasers etc. Traditionally, considerable attention is devoted to studying the energetic and spectral characteristics of the light atoms (H, He, Li etc) and corresponding multicharged ions. However, studying spectral characteristics of heavy atoms and ions in the Rydberg states has to be more complicated as it requires a necessary accounting the relativistic , exchange-correlations effects and possibly the QED corrections for superheavy atomic systems. There have been sufficiently many reports of calculations and compilation of energies and oscillator strengths for the barium and even Ba-like ions (see, for example, [1–3] and refs. therein), however, an accuracy of theses data call for further serious analysis and calculation. In many papers the Dirac-Fock method, model potential approach, quantum defect approximation in the different realizations have been used for calculating the energy and spectral properties of barium and it has been shown that an account of the polarization interelectron corrections is of a great quantitative importance. The consistent relativistic perturbation theory calculations of the transitions energies and oscillator strengths for some chosen transitions between the Rydberg states are performed in Refs. [4]. However, it should be stated that for majority of the barium Rydberg states and Ba-like ions with high values of a nuclear charge Z, there is not enough precise information available in literatures [1-3]. In our paper the combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham 1-particle approximation are used for preliminary estimating the energies and oscillator strengths of radiative transitions from the ground state to the low-excited and Rydberg states, in particular, $6s^2$ -6snp (n =7-50) transitions, of the barium atom. The comparison of the calculated oscillator strengths with available theoretical and experimental (compillated) data is performed. The important point is linked

with non-accounting for the polarization effect contribution into the oscillator strength value that has led to ~30% difference between the empirical (compillated) and theoretical data

2. The theoretical method

In the relativistic energy approach [4-9], which has received a great applications during solving numerous problems of atomic, molecular and nuclear physics (e.g. , see Refs. [10-59]), 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:

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

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 [4]:

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

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 [5-8]:

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

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

where j_i is the total single electron momentums, m_i – the projections; Q^{Cul} is the Coulomb part of interaction, Q^{Br} - the Breit part. Their detailed definitions are presented in Refs. [4,20]. The detailed expressions for the Coulomb and Breit parts and the corresponding radial R_l and angular S_l integrals can be found in Refs. [22-32].The total probability of a λ - pole transition is usually represented as a sum of the electric P^E_λ and magnetic P^M_λ parts. The electric (or magnetic) λ - pole transition $\gamma \to \delta$ connects two states with parities which by λ (or λ +1) units. In our designations

$$P^E_\lambda(\gamma\to\delta) = 2(2j+1)Q^E_\lambda(\gamma\delta;\gamma\delta)$$
$$P^M_\lambda(\gamma\to\delta) = 2(2j+1)Q^M_\lambda(\gamma\delta;\gamma\delta) \qquad (7)$$

$$Q^E_\lambda = Q^{Cul}_\lambda + Q^{Br}_{\lambda,\lambda-1} + Q^{Br}_{\lambda,\lambda+1}$$
$$Q^M_\lambda = Q^{Br}_{\lambda,\lambda}. \qquad (8)$$

In our work the relativistic wave functions are determined by solution of the Dirac equation with the potential, which includes the modified Kohn-Sham exchange potential [17] insist of the standard Fock one. The important point of

the many-body calculations is in accurate account of the exchange–correlation effects [5-15]. However, in this preliminary studying the energy and spectroscopic parameters of the barium spectra we are limited by non-accounting for the polarization effect contribution and other correlation corrections. Its consistent and accurate accounting will be considered in the next paper. All calculations are performed on the basis of the modified numeral code Superatom (version 93).

3. Results and conclusion

Table 1, 2 shows the energies and oscillators strengths of the transitions between the terms of the configurations $6s^2$ -6snp (n~50). Taking into account a great size of the obtained data we are limited below only by some data. As it has been underlined above, here during this preliminary studying the energy and spectroscopic parameters of the barium spectra we were limited by non-accounting for the polarization effect contribution and other correlation corrections. By the way, it is well-known that the similar complicated atomic systems, spectra and corresponding computing the radiative parameters require very accurate accounting for the different groups of the many-body exchange-correlation effects (see, for example, refs. [5-25]). Moreover, only such a way is able to provide spectral data with sufficient accuracy for modern spectroscopic applications. Such calculations are now in progress and more full information will be presented in the next papers special Preprint.

Table 1

The energy (cm^{-1}) and the oscillators strengths of $6s^2$ -6snp transitions (see text)

Transition	Terms	E (cm^{-1}) [2]	gf [2]	gf (our)
$6s^2$ -6s13p	^1S-$^1P^o$	40763	2.1-4	1.3-4
$6s^2$ -6s15p	^1S-$^1P^o$	41183	1.4-3	0.8-3
$6s^2$ -6s16p	^1S-$^1P^o$	41306	6.0-4	3.8-4

Table 2

The energy (cm^{-1}) and the oscillators strengths of the $6s^2$ -6snp transitions (n = 16-30; our data)

Transition	Terms	E (cm^{-1})	gf
$6s^2$ -6s16p	^1S-$^1P^o$	41306	3.7-4
$6s^2$ -6s20p	^1S-$^1P^o$	41615	0.6-4
$6s^2$ -6s21p	^1S-$^1P^o$	41662	1.8-5
$6s^2$ -6s30p	^1S-$^1P^o$	41871	2.2-5

We are planning to pay especial attention on the accurate accounting for the different groups of the many-body exchange-correlation effects and consider a problem of using the optimized one-particle representation and account for the polarization effect. It is obvious that a possible 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) will be of order 40%, i.e. results, obtained with using different photon propagator gauges (Coulomb, Landau etc) differ significantly (see [6, 60-62]).

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Key words: relativistic theory, oscillator strengths, radiative transitions

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РЕЛЯТИВИСТСКИЙ РАСЧЕТ СИЛ ОСЦИЛЛЯТОРОВ РАДИАЦИОННЫХ ПЕРЕХОДОВ МЕЖДУ РИДБЕРГОВСКИМИ СОСТОЯНИЯМИ БАРИЯ

Резюме

Комбинированный релятивистский энергитический подход и релятивистская теория возмущений многих тел с дирак-кон-шэмовским одночастичным приближением нулевого порядка используются для предварительной оценки энергий и сил осцилляторов радиационных переходов из основного состояния в низкие возбужденные и ридберговские состояния, в частности, $6s^2$ -6snp (n =7-50) переходоваирма бария. Выполнено сравнение расчетных сил осцилляторов с имеющимися теоретическими и экспериментальными данными. Важнейшая особенность связана с неучетом вклада в величину силы осцилятора, обусловленного эффектом поляризации остова и некоторіми другими корреляционными поправками, что приводит к ~40% отличию между экспериментальными (компиллированными) и теоретическими данными.

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

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РЕЛЯТИВІСТСЬКИЙ РОЗРАХУНОК СИЛ ОСЦИЛЯТОРІВ РАДІАЦІЙНИХ ПЕРЕХОДІВ МІЖ РІДБЕРГІВСЬКИМИ СТАНАМИ БАРІЯ

Резюме

Комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з дірак-кон-шемівським одночастинковим наближенням нульового порядку використовуються для попередньої оцінки енергій і сил осциляторів радіаційних переходів з основного стану в низько збуджені і рідбергівські стани, зокрема, 6s2 -6snp (n = 7 -50) переходів атома барія. Виконано порівняння розрахункових сил осциляторів з наявними теоретичними і експериментальними даними. Найважливіша особливість даного розрахунку пов'язана з неврахуванням вкладу в величину сили осцилятора, обумовленого ефектом поляризації остова та декотрими іншими кореляційними поправками, що призводить до ~ 40% відмінності між експериментальними (компіллірованними) і теоретичними даними.

Ключові слова: релятивістська теорія, сили осцилляторів, радіаційнні переходи, рідбергівські стани.