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RELATIVISTIC CALCULATION OF RYDBERG AUTOIONIZATION STATES PARAMETERS IN SPECTRUM OF BARIUM

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham one-particle approximation are used for estimating the energies the in Rydberg autoionization 4f5/2,7/2n'f J=6,5,4 states, excited from the initial state 5d3/215f J=5 in spectrum of the barium atom. The comparison with available theoretical and experimental (compillated) data is performed. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth order that significantly provides a physically reasonable agreement between theory and precise experiment.

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. The knowledge of the Rydberg autoionization states parameters for many of atomic systems is of a great importance note for many applications in atomic and molecular physics, plasma chemistry and physics, laser physics and quantum electronics etc. [1-62]. 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, autoionization states energies and widths for the barium and even Ba-like ions (see, for example, [1–3] and refs. therein), however, an accuracy of these data call for further serious analysis and calculation. In many papers the Dirac-Fock method, model potential approach, quantum defect (QD) approximation (different versions such as QD, MCQD etc) 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 MCQD calculations of the transitions energies and oscillator strengths for some chosen transitions between the Rydberg states are performed in Refs. [1,63,64]. However, it should be stated that for majority of the barium Rydberg states and 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 one-particle approximation are used for estimating the energies the in Rydberg autoionization $4f_{5/2,7/2}n'f$ J=6,5,4 states, excited from the initial state $5d_{3/2}15f$ J=5 in spectrum of the barium atom.

2. The theoretical method

In refs. [8-170] the fundamentals of the relativistic many-body PT formalism have been in details presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In refs. [3-65, 17-20] it is realized a field procedure for calculating the energy shifts DE of degenerate states, which is connected with the secular matrix M diagonalization. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the M. The complex secular matrix M is represented in the form [9,10]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \qquad (1)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. The optimized 1-QP representation is the best one to determine the zeroth approximation. 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:

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

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]:

$$\mathrm{Im}\,\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V_{\alpha n \alpha n}^{|\omega_{\alpha n}|}, \qquad (3)$$

where (a>n>f) for electron and (a<n<f) for vacancy. 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 as follows [4]:

$$\frac{\sin|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0}^{\infty} (\lambda) J_{\lambda+1/2}(|\omega| r_1) J_{\lambda+1/2}(|\omega| r_2) P_\lambda(\cos r_1 r_2). \qquad (4)$$

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

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]:

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \times$$

$$\times \quad j \quad j \quad j \quad j \quad m \quad m \times$$

$$\mathrm{x} \sum_{a\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & \mu \end{pmatrix} \times$$

$$\times \qquad ,$$

$$\times \sum_{a\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & -\mu \end{pmatrix} \qquad (5)$$

$$Q_a(n_1 j_1 l_1 n_2 j_2 l_2; n_4 j_4 l_4 n_3 j_3 l_3)$$

$$= Q_a^{\mathrm{Qul}} + Q_a^{\mathrm{B}}. \qquad (6)$$

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. 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 calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_a(akgb)$, where one of the functions describes electron in the continuum state. When calculating this integral, the correct normalization of the wave functions is very important, namely, they should have the following asymptotic at r®0:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} sin(kr+\delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} cos(kr+\delta). \end{cases} \quad (7)$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-Sham density functional [8-17] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (3) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $Im\mathrm{D}E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels.

According to [6,8], "in the fourth order of QED PT (the second order of the atomic PT) there appear the diagrams, whose contribution to the ImdE_{ninv} accounts for correlation effects and this contribution is determined by the electromagnetic potential gauge (the gauge dependent contribution)". The accurate procedure for minimization of the functional ImdE_{ninv} leads to the Dirac-Kohn-Sham-like equations for the electron density that are numerically solved by the Runge-Cutta standard method It is very important to known that the regular realization of the total scheme allow to get an optimal set of the 1QP functions and more correct results in comparison with so called simplified one, which has been used in Refs. [6-8] and reduced to the functional minimization using the variation of the correlation potential parameter *b*. Other details can be found in refs.[8-17, 22-40]. All calculations are performed on the basis of the modified numeral code Superatom (version 93).

3. Results and conclusion

As an important application of the theory we study the Rydberg autoionization states, which are corresponding to transitions into 4fnf, states, in particular, $4f_{5/2,7/2}$n'f J=6,5,4 states, excited from the initial state $5d_{3/2}$15f J=5 (Figure 1).

In Table 1 we present the values of Energies (cm^{-1}) of autoionization states 4fnf, n = 15: Exp.- experiment; Теорія: (1)-data, obtained within the quantum defect method MCQD with empirical fitting by de Graaf et al; (2) –our theory).

Physically reasonable agreement between theory and precise experiment can be reached under condition of an accurate accouting of the complex exchange-correlation effects and using the optimized relativistic orbitals basis sets (the optimal one-quasiparticle representation).

Table 1.

Energies (cm^{-1}) of autoionization states $4f_{5/2,7/2}$n'f J=6,5,4, n = 15: Exp.- experiment; Theory: (1)-quantum defect method MCQD with empirical fitting; (2) –our theory

AC	J	Exp.	(1)	(2)
$4f_{5/2}15f_{7/2}$	6	89 758.4±0.5	89759.1	89758.8
$4f_{7/2}15f_{5/2}$	6	89 993.6±0.5	89992.4	89993.6
$4f_{7/2}15f_{7/2}$	6	89 926.6±5.0	89937.1	89926.8
$4f_{5/2}15f_{7/2}$	5	89 726.3±1.0	89718.7	89726.9
$4f_{7/2}15f_{7/2}$	5	89 951.0±0.5	89952.9	89951.6
$4f_{7/2}15f_{5/2}$	5	-	89943.6	89942.3
$4f_{5/2}15f_{5/2}$	4	89 705.6±0.5	89706.8	89705.4
$4f_{5/2}15f_{5/2}$	4	-	89720.0	89718.5
$4f_{5/2}15f_{7/2}$	4	-	89937.2	89937.6
$4f_{7/2}15f_{5/2}$	3	-	-	89953.4
$4f_{5/2}15f_{7/22}$	2	-	-	89767.8

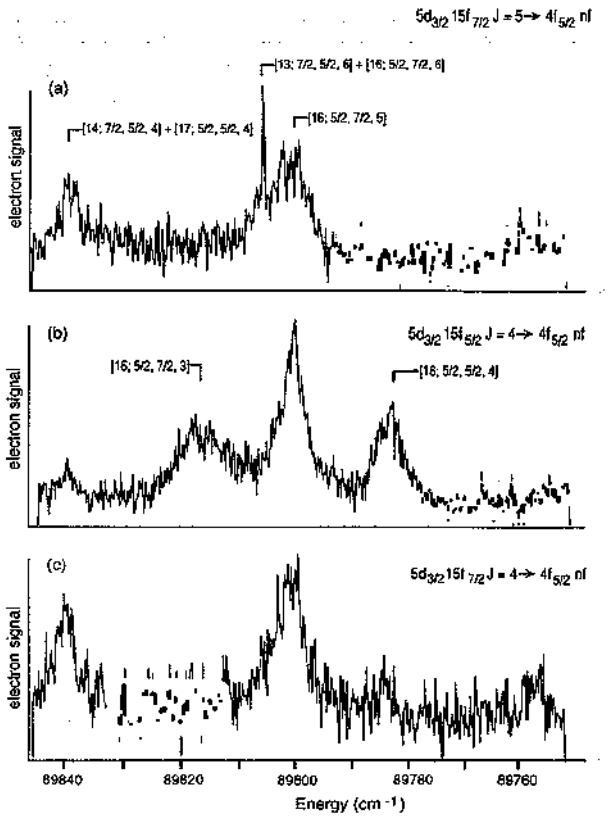

Figure 1. The experimental spectrum of the Ba $4f_{5/2}$n'f J=6,5,4 autoionization states, excited from initial state: $5d_{3/2}$15f, J=5

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RELATIVISTIC CALCULATION OF RYDBERG AUTOIONIZATION STATES PARAMETERS IN SPECTRUM OF BARIUM

Summary

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth order Dirac-Kohn-Sham one-particle approximation are used for estimating the energies the in Rydberg autoionization $4f_{5/2,7/2}n'f$ J=6,5,4 states, excited from the initial state $5d_{3/2}15f$ J=5 in spectrum of the barium atom. The comparison with available theoretical and experimental (compillated) data is performed. The important point is linked with an accurate accounting for the complex exchange-correlation (polarization) effect contributions and using the optimized one-quasiparticle representation in the relativistic many-body perturbation theory zeroth order that significantly provides a physically reasonable agreement between theory and precise experiment.

Key words: relativistic theory, Rydberg autoionization states, barium

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РЕЛЯТИВИСТСКИЙ РАСЧЕТ ПАРАМЕТРОВ РИДБЕРГОВСКИХ АВТОИОНИЗАЦИОННЫХ СОСТОЯНИЙ В СПЕКТРЕ БАРИЯ

Резюме

Комбинированный релятивистский энергетический подход и релятивистская многочастичная теория возмущений с дирак-кон-шэмовским одночастичным нулевым приближением используются для вычисления энергий ридберговских автоионизационных состояний $4f_{5/2,7/2}n'f$ J=6,5,4, возбуждаемых из начального состояния $5d_{3/2}15f$, J=5 в спектре атома бария. Проведено сравнение с имеющимися теоретическими и экспериментальными (скопированными) данными. Важный момент связан с аккуратным учетом вкладов сложных многочастичных обменных корреляционных (поляризационных) эффектов и с использованием оптимизированного одноквазичастичного представления в нулевом приближении релятивистской многочастичной теории возмущений, что существенно определяет физически разумное согласие между теорией и точным экспериментом.

Ключевые слова: релятивистская теория, ридберговские автоионизационные состояния, барий

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РЕЛЯТИВІСТСЬКИЙ РОЗРАХУНОК ПАРАМЕТРІВ РІДБЕРГІВСЬКИХ АВТОІОНІЗАЦІЙНИХ СТАНІВ В СПЕКТРІ БАРІЯ

Резюме

Комбінований релятивістський енергетичний підхід і релятивістська багаточастинкова теорія збурень з дірак-кон-шемівським одночастинковим наближенням нульового порядку використовуються для енергій рідбергівських автоіонізаційних станів $4f_{5/2,7/2}n'f$ J=6,5,4, збуджених з початкового стану $5d_{3/2}15f$, J=5 в спектрі атома барію. Проведено порівняння з наявними теоретичними і експериментальними (скопійованими) даними. Важливий момент пов'язаний з акуратним урахуванням вкладів складних багаточасткових обмінних кореляційних (поляризаційних) ефектів з використанням оптимізованого одноквазічастічного уявлення в нульовому наближенні релятивістської багаточастинкової теорії збурень, що істотно визначає фізично розумне згоду між теорією і точним експериментом..

Ключові слова: релятивістська теорія, рідбергівські автоіонізаційні стани, барій