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SPECTROSCOPY OF RYDBERG ATOMS IN A BLACK-BODY RADIATION FIELD: RELATIVISTIC THEORY OF EXCITATION AND IONIZATION

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth model potential approximation are used for computing the thermal Blackbody radiation ionization characteristics of the Rydberg atoms, in particular, the sodium in Rydberg states with n=17,18,40-70. The comparison of the calculated ionization rate values with available theoretical and experimental data is carried out.

1. Introduction

A great progress in experimental laser physics and appearance of the so called tunable lasers allow to get the highly excited Rydberg states of atoms. In fact this is a beginning of a new epoch in the atomic physics with external electromagnetic field. It has stimulated a great number of papers on the ad and dc Stark effect [1-12].

From the other side, the experiments with Rydberg atoms had very soon resulted in the discovery of an important ionization mechanism, provided by unique features of the Rydberg atoms. Relatively new topic of the modern theory is connected with consistent treating the Rydberg atoms in a field of the Blackbody radiation (BBR). It should be noted that the BBR is one of the essential factors affecting the Rydberg states in atoms [1].

The account for the ac Stark shift, fast redistribution of the levels' population and photoionization provided by the environmental BBR became of a great importance for successfully handling atoms in their Rydberg states.

The most popular theoretical approaches to computing ionization parameters of the Rydberg atom in the BBR are based on the different versions of the model potential (MP) method, quasi-classical models. It should be mentioned a simple approximation for the rate of thermal ionization of Rydberg atoms, based on the results of our systematic calculations in the Simons-Fues MP [1].

In fact, using the MP approach is very close to the quantum defect method and other semi-empirical methods, which were also widely used in the past few years for calculating atom–field interaction amplitudes in the lowest orders of the perturbation theory.

The significant advantage of the Simons-Fues MP method in comparison with other models is the possibility of presenting analytically (in terms of the hypergeometric functions) the quantitative characteristics for arbitrarily high orders, related to both bound–bound and bound–free transitions. Naturally, the standard methods of the theoretical atomic physics, including the Hartree-Fock and Dirac-Fock approximations should be used in order to determine the thermal ionization characteristics of neutral and Rydberg atoms [2].

One could note that the correct treating of the heavy Rydberg atoms parameters in an external electromagnetic field, including the BBR field, requires using strictly relativistic models. In a case of multielectron atomic systems it is necessary to account for thee exchange-correlation corrections.

Here we apply an energy approach [11-15] and relativistic perturbation theory (PT) with the MP zeroth approximation [16-20] to computing the thermal BBR ionization characteristics of the Rydberg atoms, in particular, the sodium. It is self-understood that the other alkali elements are also of a great actuality and importance.

2. Ionization of the Rydberg atoms in the Blackbody radiation

Qualitative picture of the BBR Rydberg atoms ionization is in principle easily understandable. Even for temperatures of order T=10^4 K, the frequency of a greater part of the BBR photons ω does not exceed 0.1 a.u. One could use a single- electron approximation for calculating the ionization cross section $\sigma_{nl}(\omega)$. The latter appears in a product with the Planck's distribution for the thermal photon number density:

$$\rho(w,T) = \frac{\omega^2}{\pi^2 c^3 [\exp(\omega / kT) - 1]}, \qquad (1)$$

where k=3.1668×10^{-6} a.u., K^{-1} is the Boltzmann constant, c = 137.036 a.u. is the speed of light.

Ionization rate of a bound state *nl* results in the integral over the Blackbody radiation frequencies:

$$P_{nl}(T) = c \int_{|E_{nl}|}^{\infty} \sigma_{nl}(\omega)\rho(\omega,T)d\omega . \qquad (2)$$

The ionization cross-section from a bound state with a principal quantum number n and orbital quantum number l by photons with frequency ω is as follows:

$$\sigma_{nl}(\omega) = \frac{4\pi^2\omega}{3c(2l+1)}[lM^2_{nl\to El-1} + (l+1)M^2_{nl\to El+1}], \qquad (3)$$

where the radial matrix element of the ionization transition from the bound state with the radial wavefunction $R_{nl}(r)$ to continuum state ith the wavefunction $R_{El}(r)$ normalized to the delta function of energy. The corresponding radial matrix element looks as:

$$M_{nl\to El'} = \int_0^{\infty} R_{El'}(r) r^3 R_{nl}(r) dr . \qquad (4)$$

We apply a generalized energy approach [11-15] and relativistic perturbation theory with the MP zeroth approximation [16-20] to computing the Rydberg atoms ionization parameters. In relativistic theory radiation decay probability (ionization cross-section etc) is connected with the imaginary part of electron energy shift. The total energy shift of the state is usually presented in the form: ΔE = ReΔE + i Γ/2, where Γ is interpreted as the level width, and a decay probability P = Γ. The imaginary part of electron energy shift is defined in the PT lowest order as:

$$\mathrm{Im}\Delta E(B) = -\frac{e^2}{4\pi} \sum_{\substack{\alpha>n>f \\ [\alpha<n\le f]}} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \qquad (6)$$

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

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1 - \alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (7)$$

Their detailed description of the matrix elements and procedure for their computing is presented in Refs. [12,13,15]. The relativistic wave functions are calculated by solution of the Dirac equation with the potential, which includes the "outer electron- ionic core" potential (in the Miller-Green form [21]) and exchange-polarization potential [20]. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results

In Table 1 we present results of the ionization rate calculation for the Rydberg sodium atom in the states (17,18D, 18P) at temperatures of 300 K and 500 K: Th5 – our (relativistic MP theory) data, E1 – experimental data by Kleppner etal and Burkhardt etal [4], Th1- theory (nonrelativistic Simons-Fues MP) by Glukhov-Ovsyannikova [9], Th2- theory of Lehman [8], Th3- quasiclassical model by Dyachkov-Pankratov [10] and Th4- theory by Beterov et al. [1].

In whole there is physically reasonable agreement between the theoretical and experimental data. Obviously, the accuracy of the theoretical data is provided by a correctness of the corresponding relativistic wave functions and accounting for the exchange-correlation effects.

In Table 2 we list our results of ionization rate (s^{-1}) for sodium Rydberg states (with n=40-70) induced by BBR radiation (T = 300 K) .

Table 1

Theoretical and experimental values of the ionization rate (10^3 s^{-1}) of sodium Rydberg states: E1- Kleppner et al Burkhardt etal; Th1 – theory by Glukhov-Ovsyannikova; Th2- theory by Lehman, Th3- theory by Dyachkov-Pankratov; Th4- theory by Beterov et al; Th5 – this work.

T	*nL*	E1	Th1	Th2	Th3	Th4	Th5
300	17D	10^3	1.08×10^3	0.95×10^3	0.9×10^3	1.147×10^3	1.02×10^3
500	18P	-	4.18×10^3	-	-	-	5.54×10^3
500	18D	-	4.07×10^3	-	-	-	5.46×10^3

Table 2

Ionization rate (s^{-1}) for the sodium Rydberg states (with n = 40-70), induced by BBR radiation (T = 300 K; our data).

Atom	40	50	60	70
Na S	142	106	61.4	29.5
Na P	804	576	311	141
Na D	707	496	268	122

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Abstract
The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth model potential approximation are used for computing the thermal Blackbody radiation ionization characteristics of the Rydberg atoms, in particular, the sodium in Rydberg states with n=17,18,40-70. The comparison of the calculated ionization rate values with available theoretical and experimental data is carried out.
Key words: Rydberg atoms, relativistic theory, radiation field.

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А. А. Свинаренко, О. Ю. Хецелиус, В. В. Буяджи, А. С. Квасикова, П. А. Заичко

СПЕКТРОСКОПИЯ РИДБЕРГОВСКИХ АТОМОВ В ПОЛЕ ИЗЛУЧЕНИЯ ЧЕРНОГО ТЕЛА: РЕЛЯТИВИСТСКАЯ ТЕОРИЯ ВОЗБУЖДЕНИЯ И ИОНИЗАЦИИ

Резюме
Комбинированный релятивистский энергитический подход и релятивистская теория возмущений многих тел с нулевым потенциалом модели приближения используются для вычисления ионизационных характеристик ридберговских атомов в поле теплового излучения черного тела, в частности, натрия в ридберговских состояниях с n=17,18,40-70. Сравнение расчетных значений скорости ионизации с имеющимися теоретическими и экспериментальными данными проводится.
Ключевые слова: ридберговские атомы, релятивистская теория, поля излучения.

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СПЕКТРОСКОПІЯ РІДБЕРГІВСЬКИХ АТОМІВ У ПОЛІ ВИПРОМІНЮВАННЯ ЧОРНОГО ТІЛА: РЕЛЯТИВІСТСЬКА ТЕОРІЯ ЗБУРЕННЯ ТА ІОНІЗАЦІЇ

Резюме
Комбінований релятивістський енергетичний підхід і релятивістська теорія збурень багатьох тіл з нульовим потенціалом моделі наближення використовуються для обчислення іонізаційних характеристик рідбергівських атомів у полі теплового випромінювання чорного тіла, зокрема, натрия в рідбергівських станах з n=17,18,40-70. Порівняння розрахованих значень швидкості іонізації з наявними теоретичними та експериментальними даними проводиться.
Ключові слова: рідбергівські атоми, релятивістська теорія, поля випромінювання.