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RELATIVISTIC THEORY OF EXCITATION AND IONIZATION OF HEAVY ALKALI RYDBERG ATOMS IN A BLACK-BODY RADIATION FIELD: NEW DATA

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth Dirac-Fock potential approximation are used for computing the thermal Blackbody radiation ionization characteristics of the alkali Rydberg atoms, in particular, the rubidium and caesium in Rydberg states with principal quantum number n=20-100. Preliminary application of theory to computing ionization rate for the Rydberg sodium atom in the have demonstrated physically reasonable agreement between the theoretical and experimental data. 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 Refs. [1,2] it has been proposed a combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth model potential approximation for determination the thermal Blackbody radiation ionization characteristics of the Rydberg atoms. As example, there have been computed the ionization parameters of the sodium in Rydberg states with n=17,18,40-70.

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, quasiclassical 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 [11-16] and relativistic perturbation theory (PT) with the Dirac-Fock zeroth approximation [16-20] to computing the thermal BBR ionization characteristics of the heavy alkali Rydberg atoms, in particular, the rubidium, caesium. It is self-understood that the other alkali elements are also of a great actuality and importance.

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:

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

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:

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

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

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

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: DE = ReDE + i G/2, where G is interpreted as the level width, and a decay probability P = G. 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 (a>n>f) for electron and (a<n<f) for vacancy. The matrix element is determined as follows:

$$V^{|\omega|}_{ijkl}=\int dr_1dr_2\Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1)$$

$$V^{|\omega|}_{ijkl}=\int dr_1dr_2\Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \qquad (7)$$

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 Dirac-Fock consistent field potential and additionally polarization potential [20]. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

In Ref.[1] there were presented the results of computing the ionization rate calculation for the Rydberg sodium atom in the states (17,18D, 18P) at temperatures of 300 K and 500 K and obtained physically reasonable agreement between the theoretical and experimental (by Kleppner etal and Burkhardt etal [4,5]) data. Besides, there are listed new results for for the Rydberg sodium atom ionization rate (s^{-1}) with n=20-70 induced by BBR radiation (T = 300 K) . Here (Table 1) we present new data on the ionization rate (s^{-1}) for different alkali atoms Rydberg states (with n=20-70) induced by BBR radiation (T = 300 K) .

Table 1.

Ionization rate (s^{-1}) for the heavy alkali atoms in the Rydberg states (with n = 20-100), induced by BBR radiation (T = 300 K; our data).

Atom	20	30	40
K S	80.5	103	84.5
K P	201	210	159
K D	736	584	391
Rb S	118	170	130
Rb P	159	172	125
Rb D	718	621	432
Cs S	108	181	150
Cs P	471	597	451
Cs D	465	495	368
Atom	50	70	100
K S	66.4	37	17
K P	113	61	27
K D	264	128	57
Rb S	105	60	28
Rb P	89	45	18
Rb D	298	151	68
Cs S	114	66	29
Cs P	329	1671	78
Cs D	261	140	67

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.

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Abstract

The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth Dirac-Fock potential approximation are used for computing the thermal Blackbody radiation ionization characteristics of the alkali Rydberg atoms, in particular, the rubidium and caesium in Rydberg states with principal quantum number n=20-100. Preliminary application of theory to computing ionization rate for the Rydberg sodium atom in the have demonstrated physically reasonable agreement between the theoretical and experimental data. The accuracy of the theoretical data is provided by a correctness of the corresponding relativistic wave functions and accounting for the exchange-correlation effects.

Key words: Rydberg alkali atoms, relativistic theory, radiation field.

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РЕЛЯТИВИСТСКАЯ ТЕОРИЯ ВОЗБУЖДЕНИЯ И ИОНИЗАЦИИ ТЯЖЕЛЫХ ЩЕЛОЧНЫХ РИДБЕРГОВСКИХ АТОМОВ В ПОЛЕ ИЗЛУЧЕНИЯ ЧЕРНОГО ТЕЛА: НОВЫЕ ДАННЫЕ

Резюме

Комбинированный релятивистский энергитический подход и релятивистская теория возмущений многих тел с оптимизированныи дирак-фоковским нулевым приближением используются для вычисления ионизационных характеристик щелочных ридберговских атомов в поле теплового излучения черного тела, в частности, атомов рубидия и цезия в ридберговских состояниях с главным квантовым числом n=20-100. Предварительное применение теории к вычислению скорости ионизации атома натрия ридберговских состояниях продемонстрировало физически разумное согласие между теоретическими и экспериментальными данными. Точность теоретических данных обеспечивается корректностью вычисления соответствующих релятивистских волновых функций и полнотой учета обменно-корреляционных эффектов.

Ключевые слова: ридберговские щелочные атомы, релятивистская теория, тепловое излучение.

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РЕЛЯТИВІСТСЬКА ТЕОРІЯ ЗБУРЕННЯ ТА ІОНІЗАЦІЇ ВАЖКИХ ЛУЖНИХ РІДБЕРГІВСЬКИХ АТОМІВ У ПОЛІ ВИПРОМІНЮВАННЯ ЧОРНОГО ТІЛА: НОВІ ДАНІ

Резюме

Комбінований релятивістський енергетичний підхід і релятивістська теорія збурень багатьох тіл з з оптимізованим дірак-фоківським нульовим наближенням використовуються для обчислення іонізаційних характеристик лужних рідбергівських атомів в полі теплового випромінювання абсолютно чорного тіла, зокрема, атомів рубідію і цезію в рідбергівських станах з головним квантовим числом n = 20-100. Попереднє застосування теорії до обчислення швидкості іонізації атома натрію ридберговских станах продемонструвало фізично розумну згоду між теоретичними і експериментальними даними. Точність теоретичних даних забезпечується коректністю обчислення відповідних релятивістських хвильових функцій і повнотою урахування обмінно-кореляційних ефектів.

Ключові слова: рідбергівські лужні атоми, релятивістська теорія, теплове випромінювання.