Relativistic theory of excitation and ionization of Rydberg atomic systems in a Black-body radiation field

2017 J. Phys.: Conf. Ser. 810 012047

(http://iopscience.iop.org/1742-6596/810/1/012047)

Relativistic theory of excitation and ionization of Rydberg atomic systems in a Black-body radiation field

V V Buyadzhi, P A Zaichko, M Y Gurskaya, A A Kuznetsova, E L Ponomarenko, and V B Ternovsky

Odessa State Environmental University, L'vovskaya str.15, Odessa-16, 65016, Ukraine

E-mail: vbuyad@mail.ru

Abstract. The combined relativistic energy approach and relativistic many-body perturbation theory with the zeroth model density functional approximation are used for computing the thermal Blackbody radiation ionization characteristics of the Rydberg atoms, in particular, the sodium and caesium in Rydberg states with n=40-100. The comparison of the calculated ionization rate values with available theoretical and experimental data is carried out.

1. Introduction

This work goes on our research on the thermal Blackbody radiation (BBR) ionization characteristics of the Rydberg atoms. 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]. 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 BBR field [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), quasiclassical methods. It should be mentioned the simple Simons-Fues MP approximation to compute the thermal ionization rate for Rydberg atoms [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 ones, should be used in order to determine a thermal ionization characteristics of neutral and Rydberg atoms [2]. A correct treating the heavy Rydberg atoms parameters in an external electromagnetic field requires using strictly relativistic models. Here we apply an energy approach [11-15] and relativistic perturbation theory (PT) with the model density functional Dirac-Kohn-Sham zeroth approximation [16-21] to computing the thermal BBR ionization characteristics of the Rydberg atoms, in particular, sodium (as a test) and caesium.

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:

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

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 the bound state nl results in the integral over the Blackbody radiation frequencies:

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

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:

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

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 wavefunction $R_{El}(r)$ normalized to the delta function of energy. The corresponding radial matrix element looks as: $M_{nl\to El'} \sim \int_0^{\infty} R_{El'}(r) r^3 R_{nl}(r) dr$. We apply a generalized energy approach [11-15] to computing the Rydberg atoms ionization parameters. The radiation decay probability (cross-section) is connected with the imaginary part of electron energy shift. The latter is presented as: $\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\,\Gamma/2$, where Γ is a level width, and decay probability $P = \Gamma$. The imaginary part of the shift ΔE is defined in the PT second order as (in atomic units)**:**

$$\mathrm{Im}\Delta E = (1/4\pi) \sum_{\alpha>n>f} V^{|\omega_{\alpha n}|}_{\alpha n \alpha n}, \quad (4)$$

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

$$V^{|\omega|}_{ijkl} = \iint dr_1 dr_2 \Psi^*_i(r_1)\Psi^*_j(r_2)\frac{\sin|\omega|r_{12}}{r_{12}}(1-\alpha_1\alpha_2)\Psi^*_k(r_2)\Psi^*_l(r_1) \quad (5)$$

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 relativistic Dirac equation with the model Dirac-Kohn-Sham zeroth approximation plus correlation potential [16-21]. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results

In Table 1 we list the data of the ionization rate computing 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 [3], Th1- theory (nonrelativistic Simons-Fues MP) by Glukhov-Ovsyannikova [9], Th2- theory of Lehman [8], Th3- quasiclassical model by Dyachkov-Pankratov [10], Th4- theory by Beterov et al [1] and E1 – experimental data [4,5]. In whole there is physically reasonable agreement between the theoretical and experimental data. The accuracy of theoretical data is provided by a correctness of the corresponding relativistic wave functions and accounting for the exchange-correlation effects. In Table 2 we firstly list our data of ionization rate (s^{-1}) for the Cs Rydberg states 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	$1.08 \cdot 10^3$	$0.95 \cdot 10^3$	$0.9 \cdot 10^3$	$1.147 \cdot 10^3$	$1.02 \cdot 10^3$
500	18P	-	$4.18 \cdot 10^3$	-	-	-	$5.54 \cdot 10^3$
500	18D	-	$4.07 \cdot 10^3$	-	-	-	$5.46 \cdot 10^3$

Table 2. Ionization rate (s^{-1}) for Cs Rydberg states (n= 40-100), induced by BBR (our data; see text)

Atom	40	50	70	100
Cs S	151	114	67.9	31.5
Cs P	452	330	170	81.1
Cs D	369	261	142	67.9

References

[1] Beterov I I, Tretyakov D V, Ryabtsev I I, Entin V M, Ekers A, Bezuglov N N 2009 *New J. Phys.* **11** 013052
[2] Li W, Noel M W, Robinson M P, Tanner P J, Gallagher T F 2004 *Phys. Rev. A.* **70** 042713
[3] Svinarenko A A, Khetselius O Yu, Buyadzhi V V, Florko T A, Zaichko P A, Ponomarenko E L 2014 *J. of Phys.: Conf. Ser*. **548** 012048
[4] Spencer W P, Vaidyanathan A, Kleppner D, Ducas T 1982 *Phys.Rev.A.* **26** 1490.
[5] Burkhardt C, Corey R, Garver W, Leventhal J, Allergini M, Moi L 1986 *Phys. Rev. A*. **34** 80.
[6] Malinovskaya S V, Glushkov A V, Khetselius O Yu, Loboda A V, Lopatkin Yu, Nikola L, Svinarenko A A, Perelygina T 2011 *Int.Journ.Quant.Chem.* **111** 288
[7] Khetselius O Yu, Florko T A, Svinarenko A A, Tkach T B 2013 *Phys. Scr.* **T153** 014037
[8] Lehman G W 1983 *J. Phys. B: At. Mol. Phys*. **16** 2145.
[9] Glukhov I and Ovsiannikov V 2009 *J.Phys.B:At.Mol.Phys*. **42** 075001.
[10] D'yachkov L G and Pankratov P M 1994 *J. Phys. B: At. Mol. Opt. Phys*. **27** 461.
[11] Glushkov A V and Ivanov L N 1992 *Phys. Lett. A* **170** 33; 1993 *J. of Phys. B* **26** L379
[12] Glushkov A V, Ambrosov S V, Ignatenko A V, Korchevsky D A 2004 *Int. Journ. Quant. Chem.* **99** 936; Glushkov A V 1988 *Sov. Journ. Struct. Chem.* **29**(4) 3
[13] Glushkov A V 2012 *Advances in the Theory of Quantum Systems in Chemistry and Physics*. *Ser. Progress in Theor. Chemistry and Physics*, vol. 28, ed. by K Nishikawa, J Maruani, E Brandas, G Delgado-Barrio, P Piecuch (Berlin: Springer) p 131
[14] Glushkov A V 2012 *J.of Phys.: Conf. Ser*. **397** 012011; 2014 *J.of Phys.: Conf. Ser.* **548** 012020
[15] Glushkov A V, Malinovskaya S V, Chernyakova Y G, Svinarenko A A 2004 *Int. Journ. Quant. Chem.* **99** 889; Khetselius O 2012 *J. of Phys.: Conf. Ser.* **397** 012012
[16] Glushkov A V, Khetselius O Yu, Svinarenko A A 2013 *Phys. Scr.* **T153** 014029
[17] Malinovskaya S V, Glushkov A V, Khetselius O Yu, Svinarenko A A, Mischenko E V, Florko T A 2009 *Int.Journ.Quant.Chem.* **109** 3325; Glushkov A V, Malinovskaya S V, Khetselius O Yu, Loboda A V, Sukharev D E, Lovett L 2009 *Int.Journ.Quant.Chem.* **109** 1717
[18] Khetselius O Yu 2009 *Phys.Scr.* **T135** 014023; 2009 *Int. J. Quant. Chem*. **109** 3330
[19] Glushkov A V, Malinovskaya S V, Gurnitskaya E P, Khetselius O Yu, Dubrovskaya Yu V 2006 *J. of Phys.: Conf. Ser.* **35** 425; Glushkov A V, Khetselius O Yu, Lopatkin Y M, Florko T A, Kovalenko O A, Mansarliysky V F 2014 *J. of Phys.: Conf. Ser.* **548** 012026
[20] Serga I N, Dubrovskaya Yu V, Kvasikova A S, Shakhman A N, Sukharev D E 2012 *J. of Phys.: Conf. Ser.* **397** 012013; Malinovskaya S V, Dubrovskaya Yu V, Vitavetskaya L A 2005 *AIP Conf. Proc.* **796** 201; Svinarenko A A 2014 *J.of Phys.: Conf. Ser*. **548** 012039
[21] Glushkov A V, Malinovskaya S 1988 *Rus.J.Phys.Chem.* **62**(1) 100; Glushkov A V, Khetselius O Yu, Malinovskaya S V 2008 *Europ.Phys.Journ.ST* **160** 195; 2008 *Mol.Phys.* **106** 1257