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Excitations and Decays of Rubidium Rydberg States Induced by Blackbody Radiation

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The rates of excitations and decays induced by blackbody radiation were calculated in the single-electron Fues' model potential approach for states up to $n = 100$ in rubidium *s*-, *p*- and *d*-series. On the basis of the calculations, general regularities for maxima rates of blackbody radiation induced decays and excitations were ascertained and a simple polynomial-based approximation formula was proposed for blackbody radiation induced decay and excitation rates of Rydberg states. A temperature parameterization for $T = 50$–1500 K was also proposed and respective matrices of coefficients were calculated.

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1. Introduction

Blackbody radiation (BBR) is a ubiquitous and inevitable perturbing factor, which affects neutral atoms unless the ambient temperature $T = 0$ K. It should be taken into account in both laboratory experiments and applied devices engineering. At $T = 50$–1500 K the number of thermal photons reaches the maximum in the mid-infrared and far-infrared. These wavelengths correspond to gaps between the Rydberg states, and therefore blackbody radiation affects mainly highly excited states. Thermal photons ionize the Rydberg states [1, 2] and also depopulate them [3] causing the redistribution of electrons by virtue of induced excitations and decays.

Since the pioneer papers [4, 5] interlevel transitions induced by BBR were investigated without separation to BBR-induced decays and BBR-induced excitations. Only the problem of superradiance in the ensembles of the Rydberg atoms requires the account of the decays stimulated by thermal photons; BBR-induced excitations are also the key part of the correct qualitative and quantitative explanation of the selective field ionization processes [2].

This paper provides a systematic investigation of BBR-induced decays and BBR-induced excitations separately in rubidium *s*-, *p*- and *d*-series with an account of fine structure of the states. The proposed approximation formulae for BBR-induced decay and excitation rates ($P^{\rm d}_{nlj}$ and $P^{\rm e}_{nlj}$, respectively) are supplied with a numerical data.

2. Directly calculated decay and excitation rates

In one-electron dipole approximation (it is valid because rubidium has a large energy gap between one-electron and two-electron excitations; BBR intensity is low at $T = 50$–1500 K), BBR-induced decay and excitation rates for $|nlj\rangle$-state may be calculated in the following way (atomic units are used unless otherwise stated explicitly):

$$P^{\rm d}_{nlj} = \frac{4\alpha^3}{3} \sum_{n',j'}^{E_{n'l'j'}<E_{nlj}} l_>(2j'+1) \begin{Bmatrix} l & 1/2 & j \\ j' & 1 & l' \end{Bmatrix}^2 \times M^2_{nlj\to n'l'j'} \frac{\omega^3_{nn'}}{\exp[\hbar\omega_{nn'}/(kT)]-1}, \quad (1)$$

$$P^{\rm e}_{nlj} = \frac{4\alpha^3}{3} \sum_{n',j'}^{E_{n'l'j'}>E_{nlj}} l_>(2j'+1) \begin{Bmatrix} l & 1/2 & j \\ j' & 1 & l' \end{Bmatrix}^2 \times M^2_{nlj\to n'l'j'} \frac{\omega^3_{nn'}}{\exp[\hbar\omega_{nn'}/(kT)]-1}, \quad (2)$$

where α is the fine structure constant, T is the temperature of BBR, k — Boltzmann constant, $\omega_{nn'} = |E_{nlj} - E_{n'l'j'}|/\hbar$:

$$M_{nlj\to n'l'j'} = \int_0^\infty R_{n'l'j'}(r) r R_{nlj}(r) r^2 \,{\rm d}r \quad (3)$$

is a radial matrix element of $|nlj\rangle \to |n'l'j'\rangle$ transition with radial wave functions $R_{nlj}(r)$ and $R_{n'l'j'}(r)$, respectively. In this paper, the Fues' model potential radial wavefunctions for the valence electrons in neutral atom [1] were used for the calculations of matrix elements (3):

$$R_{nlj}(r) = \frac{2}{\nu^2}\sqrt{\frac{(2\lambda+2)_{n_{\rm r}}}{n_{\rm r}!\Gamma(2\lambda+2)}}\,{\rm e}^{-r/\nu}\left(\frac{2r}{\nu}\right)^{\lambda} \times {}_1F_1\left(-n_{\rm r}; 2\lambda+2; \frac{2r}{\nu}\right), \quad (4)$$

where ν is the effective principal quantum number ($E_{nlj} = -1/(2\nu^2)$); ${}_1F_1(a,c,x)$ is the confluent hypergeometric function, $(a)_n = a\cdot(a+1)\cdot\ldots\cdot(a+n-1)$ is the

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Pochhammer symbol, and n_r — the number of nodes in the radial wavefunction. For s-states $n_r = n - n_0 + 1$; for p- and d-states $n_r = n - n_0$, where n_0 is the principal quantum number of the lowest state for the valence electron in series ($5s$, $5p$, $4d$ in rubidium). The effective orbital quantum number λ is determined from the equation $\nu = \lambda + n_r + 1$. Thus, it is necessary to know only one experimental parameter E_{nlj} to construct a radial wavefunction (4). Vast data for E_{nlj} in the Rb states may be found, for example, in NIST database [6].

The Fues model potential wave functions (4) not only provide a good representation of the Rydberg states [7], but also result in an analytical form of matrix element (3):

$$M_{nlj\to n'l'j'} = \frac{1}{4}\frac{\Gamma(\lambda+\lambda'+4)}{\sqrt{\Gamma(2\lambda+2)\Gamma(2\lambda'+2)}} \times\sqrt{\frac{(2\lambda+2)_{n_r}}{n_r!}\frac{(2\lambda'+2)_{n'_r}}{n'_r!}}\left(\frac{2\nu'}{\nu+\nu'}\right)^{\lambda+2} \times\left(\frac{2\nu}{\nu+\nu'}\right)^{\lambda'+2} F_2(\lambda+\lambda'+4,-n_r,-n'_r;$$

$$2\lambda+2, 2\lambda'+2; 2\nu'/(\nu+\nu'), 2\nu'(\nu+\nu')), \qquad (5)$$

where $F_2(a, b_1, b_2; c_1, c_2; x_1, x_2)$ is a generalized hypergeometric function with five parameters and two arguments.

Matrix elements (5) were calculated for necessary transitions with n up to 200 and stored for quick implementation in (1) and (2) at different temperatures. The total depopulation rates at $T = 300$ K are in good agreement with previous results [4]. The calculations demonstrated that photoexcitation and photodecay rates have distinct maxima. The state with the maximal rate in a series changes with temperature, because the maximum of the spectral radiant energy density $u_\omega(T)$ is shifted with changing temperature ($\approx 2.82kT$). That is, the maximum of energy density coincides with different transitions at different temperatures. As the transitions to the nearest states (with energy gaps $\approx 1/\nu^3$) give the main tribute to rates, the state follows the equation:

$$C_m = \frac{100}{\nu T^{1/3}},$$

where C_m is the constant of the maximum for the series, and T is in kelvin. The values for C_m were found in s-, p-, d-series of rubidium for BBR-induced decay, excitation and total depopulation (sum of decay and excitation) rates. The maximum constants are presented in the table, which demonstrates a quantitative difference between two qualitatively different photoinduced processes.

TABLE

The constants of the maximum in Rb (rubidium).

Series	s	p	d
decay	1.8	1.65	1.7
excitation	1.9	2.05	2.0
total	1.85	1.8	1.8

3. Approximation

The number of the Rydberg states in each investigated series of rubidium is infinitely large; therefore it is not efficient to represent direct calculation results for BBR-induced decay and excitation rates in the form of vast tables. The more proper and practical approach is to construct a simple approximation.

The transitions to the closest in energy states ($|n - n'| \sim 1$) provide a main tribute to the rates of both photoinduced decay and photoinduced excitation processes. Therefore the first step in an approximation construction is to replace $\omega_{nn'}$ with interlevel energy gap asymptotic $1/\nu^3$ and matrix elements with ν^2 asymptotic. The second step of the approximation is the account of other transitions ($|n - n'| > 1$) by means of introducing the inverse powers of ν in a polynomial form in the terms of the dimensionless parameter $x = 100/(\nu T^{1/3})$:

$$P^{d(e)}_{nlj} = \frac{a^{d(e)}_0(1 + a^{d(e)}_1 x + a^{d(e)}_2 x^2 + a^{d(e)}_3 x^3)}{\tilde{\nu}^5\,[\exp(0.315792x^3) - 1]} \qquad (6)$$

with $\tilde{\nu} = \frac{\nu}{100}$. Equation (6) requires the temperature of BBR in kelvin and provides decay and excitation rates in inverse seconds (1/s). $a^{d(e)}_0$ — coefficients fix correct asymptotic behavior for high-n Rydberg states in the series and do not depend on the temperature. The terms with the coefficients $a^{d(e)}_1$, $a^{d(e)}_2$, $a^{d(e)}_3$ reflect the behavior of the approximation near the maximum and on the shallow slope. The coefficients $a^{d(e)}_1$, $a^{d(e)}_2$, $a^{d(e)}_3$ slightly depend on the temperature and may be parameterized in the following way

$$a^{d(e)}_i = \sum_{k=0}^{2} b^{d(e)}_{ik}\left(\frac{T}{100}\right)^{-k}, \quad i = 0, 1, 2, 3. \qquad (7)$$

So, the knowledge of $a^{d(e)}_0$ — coefficient and $b^{d(e)}_{ik}$ — matrix provides enough information on BBR-induced decay (excitation) rates in a given series.

4. Results

Direct calculations of BBR-induced decays (1) and excitations (2) in each series for n up to 100 gave a basis for fitting $a^{d(e)}_i$ — coefficients in Eq. (6) as the first step. Then the sets of $a^{d(e)}_i$ — coefficients at different temperatures were used for fitting $b^{d(e)}_{ik}$ — coefficients. The obtained data demonstrates a good approximation of direct calculations (see Fig. 1).

4.1. s-states

$$a^d_0 = 1.104, \quad b^d_{ik} = \begin{pmatrix} -0.2391 & 0.0595 & 0.0314 \\ -0.1705 & 0.1821 & -0.0844 \\ 0.1262 & -0.0332 & 0.0225 \end{pmatrix},$$

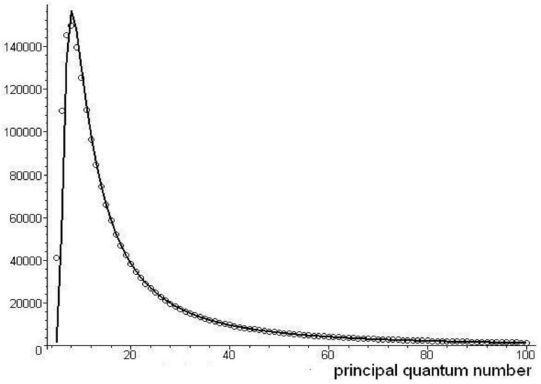

Fig. 1. Excitation rates (1/s) of Rydberg states in $d_{3/2}$-series at 600 K; circles — direct calculations, full line — approximation.

$$a_0^{\rm e} = 0.9342, \quad b_{ik}^{\rm e} = \begin{pmatrix} 0.1310 & 0.1185 & -0.0443 \\ -0.7012 & 0.0028 & 0.0193 \\ 0.4646 & -0.0751 & 0.0127 \end{pmatrix}.$$

4.2. $p_{1/2}$-states

$$a_0^{\rm d} = 1.4885, \quad b_{ik}^{\rm d} = \begin{pmatrix} -0.5184 & 0.1206 & -0.0406 \\ 0.0644 & -0.0680 & 0.0218 \\ 0.0666 & 0.0134 & 0.0037 \end{pmatrix},$$

$$a_0^{\rm e} = 0.5732, \quad b_{ik}^{\rm e} = \begin{pmatrix} 0.1968 & 0.1727 & -0.0608 \\ -0.6840 & -0.1673 & 0.0676 \\ 0.4136 & 0.0714 & -0.0306 \end{pmatrix}.$$

4.3. $p_{3/2}$-states

$$a_0^{\rm d} = 1.5414, \quad b_{ik}^{\rm d} = \begin{pmatrix} -0.5260 & 0.0325 & -0.0047 \\ 0.0690 & 0.0160 & -0.0076 \\ 0.0681 & -0.0194 & 0.0061 \end{pmatrix},$$

$$a_0^{\rm e} = 0.5505, \quad b_{ik}^{\rm e} = \begin{pmatrix} 0.0485 & 0.2301 & -0.0706 \\ -0.4515 & -0.4157 & 0.1581 \\ 0.3336 & 0.1956 & -0.0786 \end{pmatrix}.$$

4.4. $d_{3/2}$-states

$$a_0^{\rm d} = 1.1936, \quad b_{ik}^{\rm d} = \begin{pmatrix} -0.9873 & 0.6452 & -0.2224 \\ 0.4247 & -0.5073 & 0.1756 \\ -0.0397 & 0.1441 & -0.0486 \end{pmatrix},$$

$$a_0^{\rm e} = 0.8134, \quad b_{ik}^{\rm e} = \begin{pmatrix} -0.1647 & 0.3949 & -0.1385 \\ -0.0770 & -0.6981 & 0.2396 \\ 0.1398 & 0.2623 & -0.0916 \end{pmatrix}.$$

4.5. $d_{5/2}$-states

$$a_0^{\rm d} = 1.1858, \quad b_{ik}^{\rm d} = \begin{pmatrix} -1.0085 & 0.6949 & 0.2437 \\ 0.4394 & -0.5832 & 0.2116 \\ -0.0436 & 0.1777 & -0.0656 \end{pmatrix},$$

$$a_0^{\rm e} = 0.8215, \quad b_{ik}^{\rm e} = \begin{pmatrix} -0.0865 & 0.2614 & -0.0519 \\ -0.2152 & -0.4875 & 0.1002 \\ 0.1931 & 0.1732 & -0.0357 \end{pmatrix}.$$

5. Conclusion

The Fues model potential was successfully employed for the calculation of BBR-induced decay and excitation rates in Rb *s*-, *p*- and *d*- Rydberg states. The obtained results were approximated with a simple analytical formula (6) and a temperature parameterization (7). They provide a correct reflection of maximal rates, and deviations in high-n asymptotic area not more than 2%.

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