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Atom–Rydberg atom processes in the stellar atmospheres: DB white-dwarf atmospheres and solar atmosphere

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Nowadays elementary processes in astrophysical phenomena still attract researchers' attention. This can be attributed to a group of chemi-ionization processes and exitation/deexcitation processes in Rydberg atom collisions with ground state parent atoms. The rate coefficients of the chemi-ionization processes in $H(1s) + H^*(n, l)$ and $He(1s^2) + He^*(n, l)$ collisions, taking into account the influence of the corresponding $(n–n')$-mixing processes, are determined for the temperature range characteristic of the solar and DB white-dwarf atmospheres. The theory and modeling is done on the basis of the method described in Mihajlov et al. (2015, 2016). The direct calculations of the chemi-ionization rate coefficients are carried out for the models of the quiet Sun and DB white-dwarf atmospheres. It is demonstrated that the inclusion of $(n–n')$-mixing processes in the calculation influences the values of chemi-ionization rate coefficients significantly in all examined cases of stellar atmospheres.

Keywords: Atomic processes – stellar atmospheres, spectra, Rydberg atoms

1 Introduction

Although the study of Rydberg atoms has a long history, the development of new experimental techniques has led to great scientific advances in plasma physics, chemistry and in recent years renewed interest in this research (see e.g. Ryabtsev et al. (2005); Bohr et al. (2012); Lim et al. (2013); Bezuglov et al. (2014); Niederprüm et al. (2015)). In science another very important field of research into Rydberg atoms is astrophysics where Rydberg atoms can play a key role in the phenomena of cool stars (Klyucharev et al. (2007a,b); Gnedin et al. (2006, 2009)). Physical phenomena which are the most interesting are related to the so-called chemi-ionization processes (see

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e.g. Mihajlov et al. (2012) and the references therein). Chemi-ionization processes are very important for the evolution of Universe in the early epoch and its chemistry. The process of hydrogen recombination is very important, and Rydberg states can play a crucial role in this process (Puy et al. (2007); Coppola et al. (2013); Glover (2015)).

In modeling the solar atmosphere, the significant contribution of the chemi-ionization processes is shown in Mihajlov et al. (2011a,b); Barklem (2007); Mashonkina (2009, 2010), while the papers of Mihajlov et al. (2003) and Srećković et al. (2013) are devoted to the effect of these processes on the kinetics of helium-rich star atmospheres. Another important thing is that the presented results (see e.g. Mihajlov et al. (2007)) suggest that these processes, due to their influence on free electron density and excited state populations in the atmospheres of M red dwarfs, should also influence the atomic spectral line shapes.

The main aim of this paper is the consideration of two kinds of atomic collision processes which simultaneously occur in the stellar atmospheres and the influence of one on the other.

Bearing in mind the astrophysical orientation of this work, as a chemi-ionization we will here analyze the processes

$$\mathrm{H}^*(n,l) + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + \mathrm{H}^+ + \vec{e} \tag{1a}$$

$$\mathrm{H}^*(n,l) + \mathrm{H}(1s) \rightarrow \mathrm{H}_2^+ + \vec{e} \tag{1b}$$

in the hydrogen case, and

$$\mathrm{He}^*(n,l) + \mathrm{He}(1s^2) \rightarrow \mathrm{He}(1s^2) + \mathrm{He}^+(1s) + \vec{e} \tag{2a}$$

$$\mathrm{He}^*(n,l) + \mathrm{He}(1s^2) \rightarrow \mathrm{He}_2^+ + \vec{e} \tag{2b}$$

in the helium case, where the principal quantum number $n >> 1$, and the orbital quantum number l changes in the interval from 0 to $n-1$. Also, H_2^+ and He_2^+ denote molecular ions in the corresponding ground state and $\vec{e}$ is the free electron.

Here, we also study the processes of $(n$–$n')$-mixing, i.e. excitation–deexcitation processes

$$\mathrm{H}^*(n,l) + \mathrm{H}(1s) \rightarrow \mathrm{H}(1s) + \mathrm{H}^*(n',l'), \tag{3}$$

in the hydrogen case, and

$$\mathrm{He}^*(n,l) + \mathrm{He}(1s^2) \rightarrow \mathrm{He}(1s^2) + \mathrm{He}^*(n',l'), \tag{4}$$

in the helium case, where the final values of the quantum numbers n', $l' \neq n$, l.

These processes have always been considered separately, although both processes are caused by the same mechanism (dipole resonant mechanism (Mihajlov et al., 2008, 2012; Srećković et al., 2013)). Because of that, the inclusion of $(n$–$n')$-mixing processes in the procedure of calculation of rate coefficients of the chemi-ionization processes is the main task of this paper. Thus, this paper will consider the chemi-ionization processes (1a–1b) and (2a–2b) in the presence of $(n$–$n')$-mixing channel ((3) and (4)) from the astrophysical aspect and analyze their real influence for the cases of different DB white-dwarf atmospheres and solar atmosphere.

The schematic of Fig. 1 illustrates the simultaneous resonant transitions of the outer electron from the initial bound to the final state and the sub-system $A^+ + A$

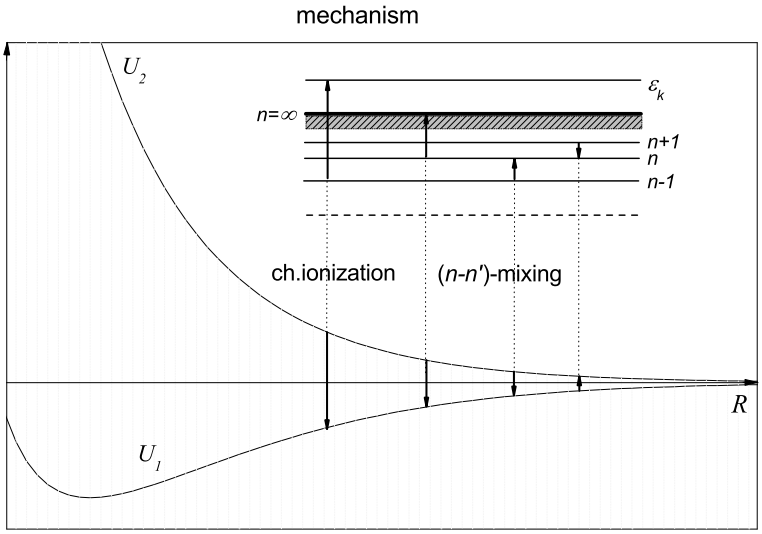


Figure 1 Illustrative presentation of the resonant transitions which cause the processes (1a–2b) and (3–4).

(where A, A^+ are atoms and their positive ions) from the initial state excited to the final ground electronic state. If the outer electron becomes free $\varepsilon_k > 0$ the chemi-ionization processes occur, while if the outer electron remains in the bound state $\varepsilon_{n'} < 0$ the $(n–n')$-mixing processes occur.

The above mentioned processes are characterized by the partial rate coefficients which are function of quantum numbers n and l as well as function of plasma temperature T. In this work these rate coefficients are calculated in both cases of hydrogen and of helium, for $3 \leq n \leq 15$. Bearing in mind the application of the results obtained here to the photosphere of the Sun and to some of DB white dwarfs the averaged rate coefficients are determined in the corresponding temperature ranges. Temperatures and atom and electron densities necessary for calculations have been taken from DB white dwarf models (Koester 2015, private communication) and in the case of solar photosphere from Vernazza et al. (1981).

2 Theory

Here $K^a_{1,2}(n,l;T)$ and $K^b_{1,2}(n,l;T)$ are the rate coefficients of processes (1a), (1b) or (2a), (2b) separately determined for given n, l and T, and $K^{ab}_{1,2}(n,l;T)$ is the total rate coefficient of processes (1a,1b) or (2a,2b) together, namely

$$K^{ab}_{1,2}(n,l;T) = K^a_{1,2}(n,l;T) + K^b_{1,2}(n,l;T). \tag{5}$$

Then because of further applications, we will determine the average total rate coefficient

$$K_{1,2}(n,T) = \frac{1}{n^2} \cdot \sum_{l=0}^{n-1} (2l+1) \cdot K^{ab}_{1,2}(n,l;T). \tag{6}$$

Also, we will determine the average rate coefficient of the associative ionization $K^b_{1,2}(n,T)$ given by

$$K^b_{1,2}(n,T) = \frac{1}{n^2} \cdot \sum_{l=0}^{n-1} (2l+1) \cdot K^b_{1,2}(n,l;T), \tag{7}$$

which is caused by the fact that just associative ionization is the subject of intensive investigations (see for e.g. Barbier & Cheret (1987); Ryabtsev et al. (2005); Golubkov & Devdariani (2011); O'Keeffe et al. (2012)). Let us note that following our previous papers we will characterize the efficiency of associative ionization over the corresponding branch coefficients

$$X^b_{1,2}(n;T) = \frac{K^b_{1,2}(n;T)}{K_{1,2}(n,T)}. \tag{8}$$

Partial rate coefficients $K^{ab}_{1,2}(n,l;T)$ and $K^b_{1,2}(n,l;T)$ are determined on the basis of standard expressions

$$K^{ab}_{1,2}(n,l;T) = \int_{E_{n;i}}^{\infty} \sigma^{ab}_{1,2}(n,l;E) \sqrt{\frac{2E}{m_{\rm red}}} f_T(E) dE, \tag{9}$$

$$K^b_{1,2}(n,l;T) = \int_{E_{n;i}}^{\infty} \sigma^b_{1,2}(n,l;E) \sqrt{\frac{2E}{m_{\rm red}}} f_T(E) dE, \tag{10}$$

where E is impact energy, $\sigma^{a,b}_{1,2}(n,l;E)$ and $\sigma^b_{1,2}(n,l;E)$ are the corresponding cross sections, $m_{\rm red}$ is the reduced mass of the subsystem H(1s)+H^+ or He($1s^2$)+He^+(1s), and $f_T(E)$ is the Maxwell distribution function: $f_T(E) = \exp(-E/kT)\sqrt{E}$. Parameter $E_{n;i}$ is given here with the relation $E_{n;i} = U_2(R_{n;i})$ where $R_{n;i}$ is the upper limit of the chemi-ionization zone, defined as the root of the equation $U_{12}(R) \equiv U_2(R) - U_1(R) = 1/2n^2$.

The above mentioned cross sections are determined here within the semi-classical approximation, with the help of the standard expressions

$$\begin{aligned} \sigma^{ab}_{1,2}(n,l;E) &= 2\pi \int_0^{\rho^{ab}_{\rm max;1,2}} P^{ab}_{1,2}(n,l;\rho;E) \rho d\rho, \\ \sigma^b_{1,2}(n,l;E) &= 2\pi \int_0^{\rho^b_{\rm max;1,2}} P^b_{1,2}(n,l;\rho;E) \rho d\rho, \end{aligned} \tag{11}$$

where ρ is the impact parameter, $\rho^{ab}_{\rm max;1,2}$ and $\rho^b_{\rm max;1,2}$ are the corresponding maximal values of this parameter, and $P^{ab}_{1,2}(n,l;\rho;E)$ and $P^b_{1,2}(n,l;\rho;E)$ are the total probability of chemi-ionization and the probability of associative ionization, respectively, determined for the given values of n, l, ρ and E in the presence of (n–n')-mixing processes. The expressions for these probabilities are described in detail in Mihajlov et al. (2015, 2016).

We draw attention to the fact that at this point there is already a difference from the previous works of Mihajlov et al. (2003, 2011a,b) concerning the chemi-ionization processes in stellar atmospheres. As a difference from this previous article,

chemi-ionization rate coefficients are here calculated without the simplification of the expression for Gaunt factor, connected with the photo-ionization cross sections for the transitions of Rydberg electron. Also, here, as a difference from Mihajlov et al. (2011a,b), the average chemi-ionization rate coefficient for a given n is obtained as a result of the corresponding averaging of partial chemi-ionization rate coefficients for every l where $0 \leq l \leq n-1$.

3 Results and discussion

In accordance with the aim of this work we consider here model C of solar atmosphere from Vernazza et al. (1981) and Fontenla et al. (2007) and model for DB white dwarfs from Koester 2015 (private communication).

In order to show the importance of the investigated chemi-ionization processes we compared their efficiencies with the efficiencies of the relevant concurrent processes, i.e. electron–Rydberg atom impact ionization

$$\mathrm{H}^*(n) + e \rightarrow \mathrm{H}^+ + e + e, \tag{12}$$

in the hydrogen case and

$$\mathrm{He}^*(n) + e \rightarrow \mathrm{He}^+ + e + e, \tag{13}$$

in the helium case, which are treated in the same range of the principal quantum numbers.

Because it is not the main objective of this paper to present the rate coefficients of the considered processes here we will demonstrate the impact of these processes on the modeling of stellar atmospheres by analysing fluxes caused by atom–Rydberg atom and electron–excited atom impact ionization. Here, fluxes generated in atom–Rydberg atom and electron–excited atom impact ionization are denoted by $I^{aa}_{1,2}(T; A^*)$ and $I^{ea}_{1,2}(T; A^*)$ and given by the expressions

$$I^{aa}_{1,2}(T; A^*) = K_{1,2}(n, T; A^*) \cdot N(\mathrm{A}^*) \cdot N(\mathrm{A}), \tag{14}$$

$$I^{ea}_{1,2}(T; A^*) = \alpha^{ea}_{1,2}(n, T; A^*) \cdot N(\mathrm{A}^*) \cdot N(e), \tag{15}$$

where $A^* = \mathrm{H}^*(n)$ or $\mathrm{He}^*(n)$, the rate coefficient $K_{1,2}(n, T; A^*)$ is given by Eq. (6) and the ionization rate coefficient $\alpha^{ea}_{1,2}(n, T; A^*)$ is determined based on the semiempirical expressions from Vriens & Smeets (1980).

The relative importance of the chemi-ionization processes in comparison with electron–excited atom impact ionization can be characterized by parameters $F_{1,2}(n, T)$ defined as:

$$F_{1,2}(n, T) = I^{aa}_{1,2}(T; A^*)/I^{ea}_{1,2}(T; A^*). \tag{16}$$

According to (16), (14) and (15) we have that

$$F_{1,2}(n, T; A^*) = \frac{K_{1,2}(n, T; A^*)}{\alpha^{ea}_{1,2}(n, T; A^*)} \frac{N(A)}{N(e)}. \tag{17}$$

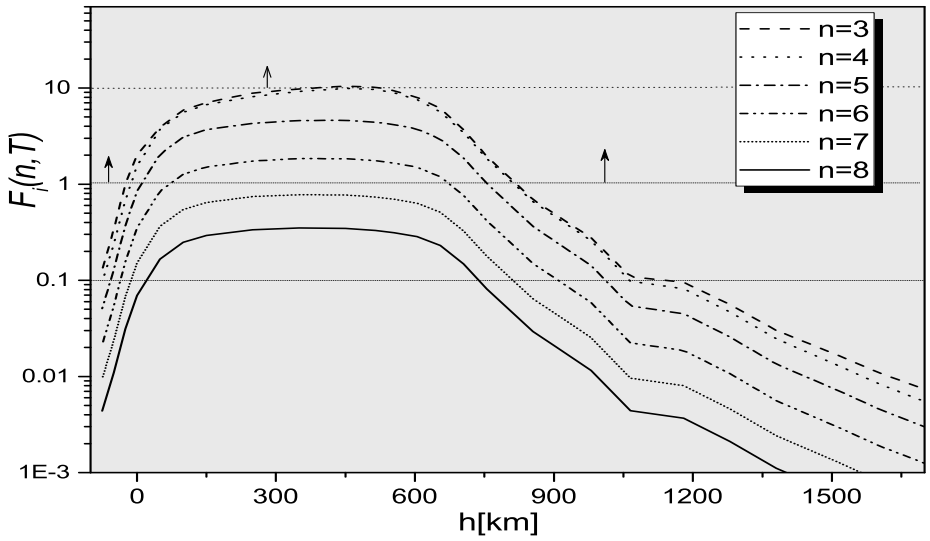


Figure 2 Parameter $F_i(n, T; \mathrm{H}^*(n))$ as a function of height h, for principal quantum numbers $n = 3$–8, for model of solar photosphere (Vernazza et al., 1981).

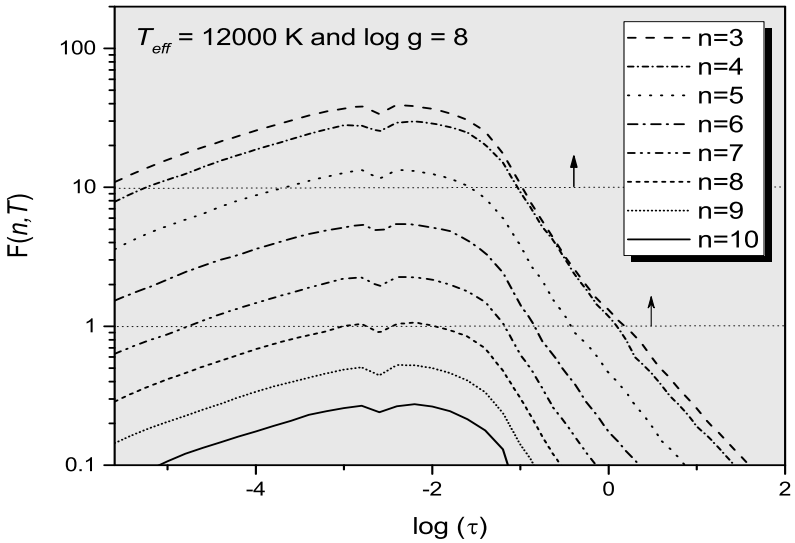


Figure 3 Parameter $F_i(n, T; \mathrm{He}^*(n))$ as a function of the logarithm of Rosseland optical depth $\log(\tau)$, for principal quantum numbers $n = 3$–10, for model of DB white dwarf atmosphere with $T_{\mathrm{eff}} = 12000$ K and $\log g = 8$ (Koester 2015).

Illustrative calculations were carried out for the photosphere of the Sun, for the hydrogen case, and some DB white dwarfs with $\log g = 8$ and the temperatures $T_{\mathrm{eff}} = 12000$ K and $T_{\mathrm{eff}} = 14000$ K for the case of helium.

Figures 2, 3 and 4 show the results of these calculations. These parameters are shown as functions of height h for the case of the solar photosphere, and $\log(\tau)$ for DB white dwarfs, where τ is the Rosseland optical depth. Temperatures and atom and electron densities necessary to determine $F_A(n, T; A^*(n))$ have been taken from DB white dwarf models (Koester 2015, private communication) and in the case of solar photosphere from Vernazza et al. (1981).

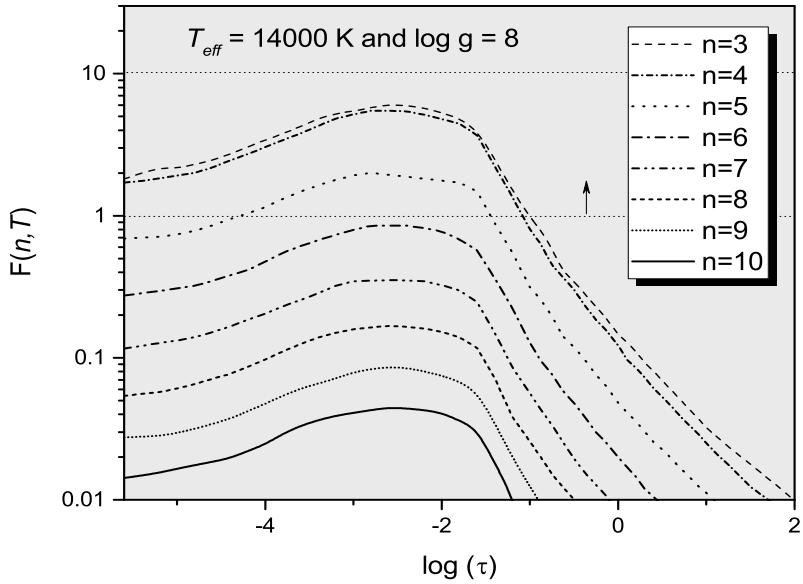


Figure 4 Parameter $F_i(n, T; \mathrm{He}^*(n))$ as a function of the logarithm of Rosseland optical depth $\log(\tau)$, for principal quantum numbers n = 3–10, for model of DB white dwarf atmosphere with $T_{\mathrm{eff}} = 14000$ K and $\log g = 8$ (Koester 2015).

Our results show that for the lower temperatures the chemi-ionization processes are still dominant over electron–excited atom ionization processes, for n = 3, 4, and 5 almost in the whole observed atmosphere which is illustrated by Figs 2, 3 and 4. For n = 6, 7 and 8 and in the whole observed atmosphere, chemi-ionization processes are comparable with electron–excited atom ionization processes. This is illustratively shown by dashed lines and arrows in Figs 3 and 4 for DB white dwarf atmospheres with $T_{\mathrm{eff}} = 12000$ K and $T_{\mathrm{eff}} = 14000$ K and $\log g = 8$ (helium case) and in Fig. 2 for the solar photosphere (the hydrogen case). It can be noticed that if effective temperature T_{eff} is increasing the influence of chemi-ionization processes begins to weaken. The behavior of the curves in these figures indicates the range where it is particularly important to take into account the studied processes.

Our analyses show that the influence of processes (3) decreases with increase of n, and for $n > 10$ it practically does not exist.

4 Conclusions

The presented material shows that the processes of $(n–n')$-mixing considerably influence the rates of chemi-ionization processes. Direct calculations, which demonstrate this influence on the quantitative level, have been performed. The obtained results show that the efficiency of the chemi-ionization processes in spite of the influence of $(n–n')$-mixing processes with $n' > n$ in most parts of the photosphere of the Sun and most parts of white dwarfs atmospheres remains dominant or at least comparable to the efficiency of the concurrent processes (12) and (13). It is shown that the importance of these processes for non-LTE modeling of considered atmospheres should be necessarily investigated. The results presented in this paper highly recommend the method of calculating the rate coefficients of the investigated chemi-ionization processes and $(n–n')$-mixing processes both for theoretical research in the field of weakly ionized plasmas and for interpretation of corresponding experimental data.

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