THE INFLUENCE OF CHEMI-IONIZATION AND RECOMBINATION PROCESSES ON SPECTRAL LINE SHAPES IN STELLAR ATMOSPHERES

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Abstract. In this work, the chemi-ionization processes in atom–Rydberg atom collisions, as well as the corresponding chemi-recombination processes are considered as factors of influence on the atom exited-state populations in weakly ionized layers of stellar atmospheres. The presented results are related to the photospheres of the Sun and some M red dwarfs as well as weakly ionized layers of DB white dwarfs atmospheres. It has been found that the mentioned chemi ionization/recombination processes dominate over the relevant concurrent electron-atom and electron-ion ionization and recombination process in all parts of considered stellar atmospheres. The obtained results demonstrate the fact that the considered chemi ionization/recombination processes must have a very significant influence on the optical properties of the stellar atmospheres. Thus, it is shown that these processes and their importance for non-local thermodynamic equilibrium (non-LTE) modeling of the solar atmospheres should be investigated further.

Key words: ISM: extinction – stars: atomic processes

1. INTRODUCTION

Chemi-ionization processes in principle include the processes of associative ionization

\[ A^*(n) + X \rightarrow AX^+ + e, \]  

(1)
as well as the processes of Penning ionization

\[ A^*(n) + X \rightarrow A + X^+ + e, \]  

(2)

where \( A, X \) and \( X^+ \) are atoms and the atomic ions in their ground states, \( A^*(n) \)-atom in a highly excited (Rydb erg) state with the principal quantum number
\( n \gg 1 \), and \( AX^+ \) is the corresponding molecular ion in its ground electronic state. It is customary that in the case \( A = X \) chemi-ionization processes are treated as symmetric, and in the case \( A \neq X \) as non-symmetric. Concerning Penning-ionization processes let us draw attention to the fact that for all the processes which can be described by the scheme (2), only those are treated as chemi-ionization which go on in a similar way as the associative-ionization processes (1). Here, all chemi-ionization processes are treated on the basis of dipole resonant mechanism, which was introduced in the considerations in Smirnov & Mihajlov (1971) and was described in details in Ignjatovic & Mihajlov (2005) and Ignjatovic et al. (2008).

The symmetric \( A = X \) chemi-ionization processes

\[
A^+(n) + A \Rightarrow A^+_2 + e, \quad (3)
\]
\[
A^+(n) + A \Rightarrow A + A^+ + e, \quad (4)
\]

and the corresponding inverse recombination processes,

\[
A^+_2 + e \Rightarrow A^+(n) + A, \quad (5)
\]
\[
A + A^+ + e \Rightarrow A^+(n) + A, \quad (6)
\]

where \( A = H(1s) \) or \( He(1s^2) \), were theoretically considered in Refs. Mihajlov et al. (1997b) and Mihajlov et al. (1996) as factors of influence on the populations of excited atoms in the weakly ionized hydrogen and helium plasmas. It means that the efficiency of these processes had to be compared with the efficiency of the processes

\[
A^+(n) + e \Rightarrow A^+ + 2e, \quad (7)
\]
\[
A^+ + 2e \Rightarrow A^+(n) + e, \quad (8)
\]
\[
A^+ + e \Rightarrow A^+(n) + \varepsilon_\lambda, \quad (9)
\]

where \( A = H(1s) \) or \( He(1s^2) \) and \( \varepsilon_\lambda \) is the energy of a photon with wavelength \( \lambda \).

For the considered conditions in Refs. Mihajlov et al. (1997b) and Mihajlov et al. (1996) the rate coefficients for all chemi-ionization and chemi-recombination processes (3)-(6) were determined. It was found that under the mentioned conditions these processes in the region \( n \leq 10 \) are dominant or at least comparable with the concurrent electron-atom and electron-ion processes (from the aspect of their influence on excited-atom populations) when the ionization degree of the considered plasma is \( \leq 10^{-3} \).

It was just these results, as well as the experience gained earlier with radiation ion-atom processes (Mihajlov & Dimitrijevic (1986, 1992), etc.), that suggested the idea that the chemi-ionization processes (3), (4) and the chemi-recombination processes (5), (6) should be of considerable interest from the aspect of their influence on excited-atom populations for the weakly ionized layers of stellar atmospheres. This was proven at a qualitative level for the hydrogen case (solar photosphere) in Mihajlov et al. (1997a), and for the helium case (atmospheres of DB white dwarfs with \( T_{eff} = 12000 \div 18000K \)) in Mihajlov et al. (2003a).

Than, the influence of the chemi-ionization processes (3), (4) and the chemi-recombination processes (5), (6) with \( A = H \) on the excited hydrogen atom populations was examined in much more detail in Mihajlov et al. (2003b), where these processes were included ab initio in a non-LTE modeling of an M red dwarf
atmosphere with the effective temperature $T_{\text{eff}} = 3800$ K, using PHOENIX code (see Baron & Hauschildt (1998)). A fact was established that including even the chemi-ionization/recombination only for $4 \leq n \leq 8$, generates significant changes (by up to 50 percent), at least in the populations of hydrogen-atom excited states with $2 \leq n \leq 20$.

Later, again using the PHOENIX code for the case of the atmosphere of the same red dwarf, the influence was examined of the processes (3-6) with $n \leq 10$ on the free electron density and the profiles of hydrogen atom spectral lines. It was established that if all these processes (with $n \geq 2$) are included, a significant change (somewhere up to 2 - 3 times) for the free electron density $N_e$, is also generated and, as one of further consequences, significant changes in hydrogen line profiles.

In this paper one of our main aims is to draw attention to the importance of all processes (1) - (4) with $A = H$ for non-LTE modeling of the solar atmosphere. For this purpose, it should be demonstrated that in the solar photosphere the efficiency of these processes is greater than, or at least comparable to, the efficiency of processes (7) - (9) with $A = H$ within those ranges of values of $n \geq 2$ and temperature $T$ which are relevant to the chosen solar atmosphere model. However, until now only, for chemi-recombination processes (3) and (4) was qualitatively shown that for $4 \leq n \leq 8$ their efficiency is comparable to the efficiency of the concurrent processes (8) and (9) in a part of the solar photosphere (see Mihajlov et al. (1997a)).

Besides all mentioned, the fact that the processes (1) - (4) can be important for the solar photosphere is supported by the results obtained in Mihajlov et al. (2003a, 2007) in connection with an M red dwarf atmosphere ($T_{\text{eff}} = 3800$ K).

2. THE RATE COEFFICIENTS OF THE CHEMI-IONIZATION/RECOMBINATION PROCESSES

The corresponding partial rate coefficients of the chemi-ionization processes (3) and (4) are denoted here with $K_{ci}^{(a,b)}(n; T)$, where $T$ is the temperature of the considered plasma, and the partial rate coefficients of the inverse chemi-recombination processes (5) and (6) - with $K_{cr}^{(a,b)}(n; T)$. Under the conditions which exist in the solar atmosphere, we can determine the rate coefficients $K_{ci}^{(a,b)}(n; T)$ over the rate coefficients $K_{ci}^{(a,b)}(n; T)$ from the principle of the thermodynamical balance for processes (3), (4), (5) and (6) in the form

$$K_{ci}^{(a,b)} \cdot N_n N_1 = K_{cr}^{(a,b)}(n; T) \cdot N_1 N_{ai} N_e,$$

where $N_1$ and $N_n$ denote the densities of ground- and excited-state hydrogen atoms respectively. Using these partial rate coefficients we will determine the total ones, namely,

$$K_{ci,cr}(n, T) = K_{ci}^{(a)}(n, T) + K_{ci}^{(b)}(n, T),$$

which characterizes the efficiency of the considered chemi-ionization and chemi-recombination processes together.

Here we will consider processes (3) - (6) with $A = H$ within the regions $n \geq 5$ and $2 \leq n \leq 4$ separately. The reason for it is the behavior of the adiabatic potential curves of atom-atom systems $H^*(n) + H(1s)$. Namely, in the first region the atom-atom curves lie above the adiabatic curve of the ion-ion system $H^+ +$
\( H^- (1s^2) \) for any \( R \), and the dipole resonant mechanism can be applied for \( n \geq 5 \) without any exceptions. Consequently, for \( n \geq 5 \) we will determine the rate coefficients of these processes following the previous papers (Mihajlov et al. 1997a, 2003a, b, 2007).

However, in the region \( n \leq 4 \) there are points where the atom-atom curves cross the ion-ion one and application of this mechanism generates some errors (see Janev & Mihajlov (1979)).

Due to this fact and the mentioned errors, we use here semi-empirical rate coefficients \( K_{cr,ci}(n=3,T) \) and \( K_{cr,ci}(n=4,T) \), which are obtained on the bases of the data from Janev et al. (1987). For relatively minor chemi-ionization/recombination processes with \( n = 2 \) we use here rate coefficients \( K_{cr}(n=2,T) \) and \( K_{ci}(n=2,T) \), which are 10 - 30 percent greater than the corresponding coefficients obtained using the data from Janev et al. (1987), in accordance with the calculated results from Urbain et al. (1991) and Rawlings et al. (1993). It gives a possibility to compensate the decrease of the rate coefficients \( K_{ci}(n \geq 5,T) \) and \( K_{cr}(n \geq 5,T) \) in comparison with the corresponding ones obtained using Janev et al. (1987), due to the fact that here, unlike Janev et al. (1987), the decay of the considered system’s initial electronic state has been taken into account.

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). Namely, this is a non-LTE model which is still actual (see Stix (2002)), and it is only for this model that all the quantities necessary for our calculations are available in tabular form as functions of height \( h \) in Solar photosphere.

Let \( I_{ci}(n,T), I_{cr}(n,T) \) be the total chemi-ionization and chemi-recombination fluxes caused by the processes (3,4) and (5,6), i.e.,

\[
I_{ci}(n,T) = K_{ci}(n,T) \cdot N_1 N_e, \quad I_{cr}(n,T) = K_{cr}(n,T) \cdot N_1 N_i N_e,
\]

(12)

and \( I_{i,ea}(n,T), I_{r,eea}(n,T) \) and \( I_{r,ph}(n,T) \) be the fluxes caused by ionization and recombination processes (7), (8) and (9), i.e.

\[
I_{i,ea}(n,T) = K_{i,ea}(n,T) \cdot N_n N_e, \quad I_{r,eea}(n,T) = K_{r,eea}(n,T) \cdot N_i N_e N_e, \quad I_{r,ph}(n,T) = K_{r,ph}(n,T) \cdot N_i N_e.
\]

(13)

where \( N_1, N_n, N_i, \) and \( N_e \) are, respectively, the densities of the ground and excited states of a hydrogen atom, of ion \( H^+ \), and of free electron in the considered plasma with given \( T \).

Using these expressions, we will first calculate quantities \( F_{i,ea}(n,T) \) given by

\[
F_{i,ea}(n,T) = \frac{I_{i,ea}(n,T)}{I_{rea}(n,T)} = \frac{K_{i,ea}(n,T)}{K_{rea}(n,T)} \cdot N_1 N_e,
\]

(14)

which characterize the relative efficiency of partial chemi-ionization processes (3) and (4) together and the impact electron-atom ionization (7) in the considered plasma. The impact ionization rate coefficients \( K_{ea}(n,T) \) are taken from Vriens & Smeets (1980). In Figure 1 the behavior of the quantities \( F_{i,ea}(n,T) \) for \( 2 \leq n \leq 8 \) as functions of height \( h \) is shown. One can see that the efficiency of the considered
chemi-ionization processes in comparison with the electron-atom impact ionization is dominant for \(2 \leq n \leq 6\) and becomes comparable for \(n = 7\) and \(8\).

Thus, in order to compare the relative influence of the chemi-ionization processes (3) and (4) together to that of the impact electron-atom ionization process (7) on the whole block of the excited hydrogen atom states with \(2 \leq n \leq 8\), we will calculate quantity \(F_{i,ea;2-8}(T)\), given by

\[
F_{i,ea;2-8}(T) = \frac{\sum_{n=2}^{8} I_{ci}(n, T) \cdot N_n}{\sum_{n=2}^{8} I_{i,ea}(n, T) \cdot N_n} \times N_1 N_e,
\]

which can reflect the influence of the existing populations of excited hydrogen atom states within a non-LTE model of solar atmosphere. In Figure 2, the behavior of the quantity \(F_{i,ea;2-8}(T)\) as functions of height \(h\) is shown. As one can see, the real influence of the chemi-ionization processes on the total populations of states with \(2 \leq n \leq 8\) remains dominant with respect to the concurrent electron-atom impact ionization processes almost in the whole photosphere (50 km \(\leq h \leq 750\) km).

Finally, we compared the relative influence of the chemi-recombination processes (5) and (6) together and total influence of the electron - electron - \(H^+\) recombination process (8) and photo-recombination electron - \(H^+\) process (9) on the same block of excited hydrogen atom states with \(2 \leq n \leq 8\). It was confirmed a domination of the chemi-recombination processes with \(2 \leq n \leq 8\) over the mentioned concurrent processes in a significant part of the photosphere (-50 km \(\leq h \leq 600\) km).

Figure 1: Behavior of the quantity \(F_{i,ea}(n)\) given by Eq. (14), as a function of height \(h\).

Figure 2: Behavior of the quantity \(F_{i,ea;2;8}(T)\) given by Eq. (15), as a function of height \(h\).

The obtained results demonstrate the fact that the considered chemi-ionization/recombination processes must have a very significant influence on the optical properties of the solar photosphere in comparison to the concurrent electron-atom impact ionization and electron-ion recombination processes. Thus it is shown that the importance of these processes for non-LTE modeling of solar atmosphere should be necessarily investigated.
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