Processes of atom - atom ($n - n'$)-mixing influence on hydrogen atom Rydberg states populations in stellar atmospheres

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Abstract. The ($n - n'$)-mixing processes in $H^+(n) + H(1s)$ collisions, have been considered from the aspect of their influence on of the $H^+(n >> 1)$ atom states in the weakly ionized layers of stellar atmospheres. These processes have been treated by the mechanism of the resonant energy exchange within the electron component of the considered collision system. It was shown that these processes must have significant influence in comparison with corresponding electron-atom collision processes, on the populations of hydrogen Rydberg atoms in Solar photosphere and lower chromosphere (ionization degree of the order of $10^{-4}$). From obtained results follows that the examined ($n - n'$) mixing processes have to be included in the modelisation of Solar and cooler stars atmospheric plasma.

Key words. Atomic processes: $n - n'$ mixing – Sun: photosphere

1. Introduction

Recently, it has been shown in Mihajlov et al. (1997, 1999, 2003) that the non-elastic processes in slow $H^+(n) + H(1s)$ collisions have a significant influence on the populations of hydrogen atom Rydberg states in Solar photosphere and lower chromosphere and cooler star atmospheres. In these papers have been investigated the processes of chemi-ionization:

$$H + H^+(n) \to e_k + \begin{cases} H^+ + H, \\ H + H^+. \end{cases}$$ (1)

and inverse processes of chemi-recombination:

$$e_k + H^+ + H \to \begin{cases} H + H^+(n), \\ H^+(n) + H. \end{cases}$$ (2)

where $H = H(1s)$, $H^+(n)$ is a hydrogen atom in a state with the principal quantum number $n \geq 4$, and $e_k$ is a free electron with energy $e_k$. The processes (1) and (2) have been treated as the result of the mechanism of the resonant energy exchange within the electronic component of the atom - Rydberg atom collisional system, which is in further named the resonant mechanism. It has been shown that these processes are dominant in weakly ionized layers of considered stellar atmospheres, in comparison with other relevant ionization and recombination processes, namely the electron-impact
Rydberg-atom ionization, electron - electron - ion recombination, and electron - ion photorecombination.

Fig. 1. Schematic illustration of $A^*(n) + A$ collision (the region of $R$ where the outer electron is collectivized is shaded).

In all mentioned papers, the usual assumption that the further destiny of Rydberg atoms $H^*(n)$ is determined by their collisions with free electrons, was accepted. In such a way it has been supposed that the electron - atom collisions determine the Rydberg states population distribution. However, in Mihajlov et al. (2004) has been demonstrated that considering the Rydberg - atom state population distribution it is indispensable to take into account the processes of $(n - n')$-mixing in slow $H^*(n) + H$ collisions, namely the processes of excitation:

$$H^*(n) + H \rightarrow \begin{cases} H''(n' = n + p) + H, \\ H + H'(n' = n + p), \end{cases} \tag{3}$$

where $n \geq 4$ and $p \geq 1$, and inverse processes of deexcitation:

$$H^*(n) + H \rightarrow \begin{cases} H''(n' = n - p) + H, \\ H + H'(n' = n - p), \end{cases} \tag{4}$$

where $n - p \geq 4$. These processes were treated as the result of the same resonant mechanism, introduced in Smirnov & Mihajlov (1971) just in connection with the processes (3) and (4). The obtained results demonstrate that in weakly ionized hydrogen plasma the processes (3) and (4), might dominate in comparison with the corresponding processes in $e_k + H^*(n)$ collisions. This fact imposes to examine the real significance of the processes (3) and (4) in weakly ionized layers of stellar atmospheres and particularly in Solar one, since if the domination of these processes in comparison with electron-atom collisional processes will be confirmed in Solar photosphere, our representations on the relative importance of atom - Rydberg atom and electron - Rydberg atom collisional processes, should be completely modified. Consequently we will investigate in this paper the importance of the $(n - n')$-mixing processes (3) and (4) in Solar photosphere and lower chromosphere. We will calculate excitation and deexcitation fluxes generated in the processes (3) and (4) for different $n$ and $p$ by using the semi-classical method for rate coefficients of processes (3) and (4) determination, developed in Mihajlov et al. (2004). Than, the obtained fluxes will be compared with fluxes generated in the corresponding $e_k + H^*(n)$ processes. Here the rate coefficients $\alpha_{n,n+p}(T_e)$ for processes (11) are taken from Vriens & Smeets (1980).

2. The resonant mechanism and $(n - n')$-mixing rate coefficients

Since the mentioned resonant mechanism for processes (1)-(4) has been discussed in several previous papers, and especially has been described in detail in Mihajlov et al. (2004), only basic facts will be given here. For the same reason, only final expressions for the (3) and (4) processes rate coefficients will be presented here.

On the basis of the resonant mechanism the $H^*(n) + H$ collisional system is treated within the domain

$$R \ll r_n, \tag{5}$$

where $R$ is the internuclear distance, and $r_n \sim n^2$ is the average radius of the Rydberg atom
A diagram showing the resonant mechanism in chemi-ionization/recombination channels (dashed arrows), and \((n - n')\)-mixing channels (full arrows).

**Fig. 2.** A diagram showing the resonant mechanism in chemi-ionization/recombination channels (dashed arrows), and \((n - n')\)-mixing channels (full arrows).

**Fig. 3.** A diagram showing the partial “smearing” of discrete Coulomb spectrum into continuum.

\(H^+(n)\), as it is illustrated by Fig 2. Within this domain the \(H^+(n) + H\) system is treated in the form: \(e + (H^+ + H)\), where \(e\) is the outer electron of the \(H^+(n)\) Rydberg atom. The electronic states of the subsystem \(H^+ + H\) are described as a superposition of the ground \([1, R]\) and first excited \([2, R]\) adiabatic electronic states of the molecular ion \(H_2^+\). The processes (3) and (4) of \((n - n')\)-mixing, as well as the processes of the chemi-ionization/recombination (1) and (2), are treated as the result of the resonant energy exchange between the outer electron \(e\) and the electronic component of the \(H^+ + H\) subsystem. This means that the outer electron \(e\) transition from the initial state to the upper energetic ones occurs simultaneously with the transition of the \(H^+ + H\) subsystem from the electronic excited state \([2, R]\) to the ground state \([1, R]\), and the transition of the outer electron to the lower energetic state occurs simultaneously with the transition of the \(H^+ + H\) subsystem from the ground electronic state \([1, R]\) to the excited state \([2, R]\) as illustrated in Fig. 1. Within the considered mechanism one assumes that all mentioned transitions are caused by the outer electron e interaction with the dipole momentum of the \(H^+ + H\) subsystem.

The rate coefficients of processes (3) and (4) for fixed \(n\) and \(n' = n ± p\), are determined semi-classically, describing the internuclear motion by using the trajectories determined in the potential corresponding to the excited electronic state \([2, R]\) of the \(H^+ + H\) subsystem. For the considered rate coefficient calculations one uses the approximation where a block of Rydberg states with the principal quantum numbers from \(n + p_1\) to \(n + p_2\), where \(p_2 \geq p_1 \geq 1\), is “smeared” in the continuum within the effective principal quantum number range from \(n + p_1 - \Delta p\) to \(n + p_2 + 1 - \Delta p\), where \(0 < \Delta p < 1\). Such “smearing” (see Fig. 3) is produced under the conditions described in Mihajlov et al. (2004). The rate coefficients \(K_{n,n+p}(T)\) for the excitation processes (3), for the given \(n\), \(p\) and the temperature \(T\), are obtained in the form

\[
K_{n,n+p}(T) = \frac{2\pi}{3\sqrt{3}} \frac{(e\alpha_0)^2}{\hbar} \cdot n^{-5} \cdot g_{n,n+p} \times
\]

\[
\times \int_{R_{\text{min}}}^{R_{\text{max}}} X(R) \cdot \exp \left[ -\frac{U_2(R)}{kT} \right] \frac{R^4}{\alpha_0^3} dR,
\]

where \(g_{n,n+p}\) is the Gaunt factor defined in Johnson (1972), \(R_{\text{min}}(n, n + p)\) and \(R_{\text{max}}(n, n + p)\) are roots of equations

\[
\epsilon(R_{\text{min}}) = \epsilon_{n+p+1} - \epsilon_n, \epsilon(R_{\text{max}}) = \epsilon_{n+p-\Delta p} - \epsilon_n
\]

with \(\epsilon(R) = U_2(R) - U_1(R)\) and \(\Delta p = 0.380\). Here, \(U_1(R)\) and \(U_2(R)\) are adiabatic terms corresponding to the electronic states \([1, R]\) and \([2, R]\), respectively, and \(\epsilon_n = -\Delta \epsilon R)\). With \(X(R)\) is denoted the function

\[
X(R) = \Gamma(3/2; x)/\Gamma(3/2),
\]
where $\Gamma(3/2, x)$ and $\Gamma(3/2)$ are the corresponding values of the incomplete and complete Gamma functions.

The rate coefficients $K_{n_n-p_n}(T)$ for de-excitation processes (4) are obtained from the thermodynamic balance principle in the form

$$K_{n_n-p_n}(T) = K_{n_n-p_n}(T) \cdot \frac{(n - p)^2}{\exp\left(\frac{\epsilon_{n-p,n}}{kT}\right)}.$$  \hspace{1cm} (9)

where $\epsilon_{n-p,n} = \epsilon_n - \epsilon_{n-p}$.

Fig. 4. $N_e$ and $N(1)$ in $[cm^{-3}]$ for Solar atmosphere model C of [Vernazza et al. (1981)].

Fig. 5. $T(h)$ and $\eta(h)$ for Solar atmosphere model C of [Vernazza et al. (1981)].

Fig. 6. $N(4)$, $N(6)$ and $N(8)$ in $[cm^{-3}]$ for Solar atmosphere model C of [Vernazza et al. (1981)].

3. Results and discussion

As in the previous article related to the chemi-ionization/recombination processes (1) and (2), we will treat the Solar photosphere and lower chromosphere using the standard C model of [Vernazza et al. (1981)]. For our calculations we need directly from this model the electron density $N_e$, the density of hydrogen atoms in the ground state ($n=1$), denoted here by $N(1)$, and the temperature $T$. The behavior of $N_e$ and $N(1)$ in Solar atmosphere as a function of height ($h$) is shown in Fig. (3), while the Fig. (4) shows the behavior of $T$ and the parameter $\eta$ defined by relation

$$\eta_{ea} = \frac{N(1)}{N_e}.$$  \hspace{1cm} (10)

One should draw attention that in our case the parameter $\eta$ is close to the inverse value of the considered plasma degree of ionization. Also, we will use from [Vernazza et al. (1981)] model the data about hydrogen atom excited states population ($n \geq 2$), illustrated by Fig. 6.

In order to determine the relative influence of processes (3) and (4) in considered parts of Solar atmosphere, we will compare them with electron-atom collisional processes:

$$e_k + H^*(n) \rightarrow e_{k'} + H^*(n'),$$  \hspace{1cm} (11)

where $n' = n \pm p$. The rate coefficients of these processes, denoted here with $\alpha_{n,p}(T_e)$, will be taken from
Vriens & Smeets (1980). The relative efficiency of processes (3) and (4) in comparison with processes (11) is characterized by the parameter $F_{n,n+p}(T)$:

$$F_{n,n+p}(T) = \frac{K_{n,n+p}(T)N(n)N(n)}{\alpha_{n,n+p}(T)N(n)N_e} = \frac{K_{n,n+p}(T)\eta_{ea}}{\alpha_{n,n+p}(T)},$$

where $N(n)$ is the excited atom states population for given $n$, and the parameter $\eta_{ea}$ is defined by (10).

Fig. 7. The parameter $F_{n,n+p}$ for $n = 4$ and $p = 1 - 5$.

Fig. 8. The parameter $F_{n,n+p}$ for $n = 5$ and $p = 1 - 5$.

Fig. 9. The parameter $F_{n,n+p}$ for $n = 6$ and $p = 1 - 5$.

Fig. 10. The parameter $F_{n,n+p}$ for $n = 7$ and $p = 1 - 5$.

Fig. 11. The parameter $F_{n,n+p}$ for $n = 8$ and $p = 1 - 5$. 
We have calculated here values of the parameter $F_{e+n}$ for $n \geq 4$ and $p \geq 1$, within the range of $h$ corresponding to the Vernazza et al. (1981) model C of Solar photosphere. Our results are illustrated in Figures [7][11]. In these figures is shown the behavior of the parameter $F_{e+n}$, for $4 \leq n \leq 8$ and $1 \leq p \leq 5$, as a function of $h$ within the range $-50 \text{ km} \leq h \leq 1000 \text{ km}$. One can see that in the largest part of the photosphere the $n, n'$ mixing processes (3) and (4) are totally dominant in comparison with the electron-atom processes (11) for $n=4,5,6$ and practically any $p \geq 1$, and have similar intensities for $n=7,8$. Comparing Figs. (3) - (5) with the Fig. (2) one can see that the region of the maximal $F_{e+n}$ values correspond to the $h$ region near the temperature minimum, where also the parameter $\eta$ defined by (10) is maximal.

In order to demonstrate the significance of the obtained results we will introduce the quantities $n = n_{\text{min}}^{(\text{eq})}$ and $n = n_{\text{min}}^{(V)}$, dependent on $h$. The first of them is the $n$ value defined by the condition:

$$N^{(V)}(n_{\text{min}}^{(V)}) = \min_{n \geq 1} N^{(V)}(n)$$  \hspace{1cm} (13)

where $N^{(V)}(n)$ are excited state atom populations from Vernazza et al. (1981) model C for given $h$, and the second one is the $n$ value defined by the condition:

$$N^{(\text{eq})}(n_{\text{min}}^{(\text{eq})}; T) = \min_{n \geq 1} N^{(\text{eq})}(n; T)$$  \hspace{1cm} (14)

where $N^{(\text{eq})}(n; T)$ are equilibrium (Boltzmannian) excited state atom populations for $T$ from Vernazza et al. (1981) model C for the same $h$ as in previous case. It could be shown that in the considered temperature range $n_{\text{min}}^{(\text{eq})}$ is close to the value of $(\text{Ry}/kT)^{1/2}$. In Table 1 are presented the values of $n = n_{\text{min}}^{(V)}$ and $n = n_{\text{min}}^{(\text{eq})}$ for a series of $h$ values from the -50 km to 1065 km range. From this Table one can see that within the considered $h$ domain the values of $n = n_{\text{min}}^{(V)}$ and $n = n_{\text{min}}^{(\text{eq})}$ have just values 4, 5 and 6 for which is demonstrated domination of the processes (3) and (4) in comparison with the processes (11).

### Table 1. The values of $n_{\text{max}}^{(eq)}$ and $n_{\text{min}}^{(V)}$ for $h$ and $T$ from Vernazza et al. (1981) model C.

<table>
<thead>
<tr>
<th>$h$ [km]</th>
<th>-50</th>
<th>0</th>
<th>100</th>
<th>350</th>
<th>555</th>
<th>755</th>
<th>980</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{\text{min}}^{(eq)}$</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>$n_{\text{min}}^{(V)}$</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>6</td>
</tr>
</tbody>
</table>

One should take into account that for plasmas similar to the considered photospheric plasma, the exchange rate between the both basic pools, atoms in the ground state and the ionized atoms, is limited by the group of excited atom states with $n$ close just to the $n_{\min}^{(V)}$ or $n_{\min}^{(\text{eq})}$. However one can see that for this group of states the dominant role have the processes (3) and (4). This means that the redistribution of the population within the lower part of the Rydberg region of $n$ is determined by the processes (3) and (4). If we add to this the fact that the exchange rate between the mentioned group of Rydberg states and the continuum is determined by the chemi-ionization/recombination processes (1) and (2), one can conclude that the processes (1), (2), (3) and (4) closely connected by the resonant mechanism completely dominate for the group of Rydberg states with $n$ close to $n_{\min}^{(V)}$ or $n_{\min}^{(eq)}$.

On the basis of presented facts we can conclude that the influence of the $n, n'$ mixing processes (3) and (4), as well as the chemi-ionization/recombination processes (1) and (2) must be taken into account for any modelling of Solar photosphere and lower chromosphere. In connection with this one should have in view that all mentioned is related also to the stellar atmospheres of similar type as well as to stellar atmospheres with lower effective temperatures but where the atomic component is still dominant over molecular one.

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References