**Astronomy
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Processes of (n − n′)-mixing in collisions of Rydberg H*(n) atoms with H(1s) in the Solar atmosphere

A. A. Mihajlov[1,2], Lj. M. Ignjatović[1,2], and M. S. Dimitrijević[2,3]

[1] Institute of Physics, PO Box 57, 11001 Belgrade, Serbia and Montenegro
e-mail: mihajlov@phy.bg.ac.yu
[2] Institute Isaac Newton of Chile, Yugoslavia Branch, and Universidad Diego Portales, Chile
[3] Astronomical Observatory, Volgina 7, 11160 Belgrade 74, Serbia and Montenegro

Abstract. The significance of $(n - n')$-mixing processes in $H^*(n) + H(1s)$ collisions, for the principal quantum number $n \geq 4$, in the Solar photosphere and lower chromosphere has been investigated. These processes have been treated by the mechanism of resonant energy exchange within the electron component of the considered collision system. These processes must have significant influence in comparison with corresponding electron-atom collision processes on the populations of hydrogen Rydberg atoms in weakly ionized layers of the Solar atmosphere (ionization degree of the order of 10^{-4}). From the results obtained it follows that the examined $(n - n')$-mixing processes have to be included in any modelling and investigation of Solar plasma, especially in the region of the temperature minimum in the Solar photosphere.

Key words. atomic processes – molecular processes – Sun: atmosphere

1. Introduction

Mihajlov et al. (1997, 1999, 2003) drew attention to the importance of inelastic processes in slow collisions of Rydberg state atoms with ground state H atoms in solar and stellar atmospheres. These papers were devoted to an investigation of the processes of chemi-ionization

$$H + H^*(n) \rightarrow e + \begin{cases} H^+ + H \\ H + H^+, \end{cases} \quad (1)$$

and the inverse process of chemi-recombination

$$e + H^+ + H \rightarrow \begin{cases} H + H^*(n), \\ H^*(n) + H, \end{cases} \quad (2)$$

where H designates a ground state $H(1s)$ atom, $H^*(n)$ a Rydberg state hydrogen atom with principal quantum number $n \geq 4$ and e is a free electron. The processes (1) and (2) were treated using the resonant energy exchange mechanism (Smirnov & Mihajlov 1971; Janev & Mihajlov 1979) between the electrons of the $H + H^*(n)$ system, to which we subsequently refer to as the resonant mechanism. It was shown that the processes (1) and (2) can be of great importance in weakly ionized layers of many stellar atmospheres, in comparison with other possible ionization and recombination processes involving electrons or photons, namely direct ionization by electron impact

$$e + H^*(n) \rightarrow H^+ + e + e, \quad (3)$$

the inverse 3-body electron recombination

$$e + e + H^+ \rightarrow e + H^*(n), \quad (4)$$

and the radiative recombination

$$e + H^+ \rightarrow H^*(n) + \epsilon_{ph}, \quad (5)$$

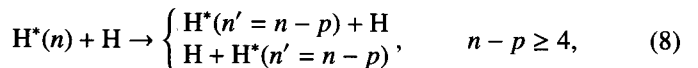where ϵ_{ph} is the energy of the emitted photon.

However, Mihajlov et al. (1997, 1999, 2003) adopted the usual assumption that the distribution of Rydberg states was determined by electron collisions

$$e + H^*(n) \rightarrow e + H^*(n'). \quad (6)$$

More recently, Mihajlov et al. (2004) showed that the Rydberg state distribution in a weakly ionized hydrogen plasma could also be strongly influenced by $(n - n')$-mixing processes in $H^*(n) + H$ collisions. These conclusions were based on the results of an investigation of the excitation processes

$$H^*(n) + H \rightarrow \begin{cases} H^*(n' = n + p) + H \\ H + H^*(n' = n + p) \end{cases}, \quad n \geq 4, \quad p \geq 1, \quad (7)$$
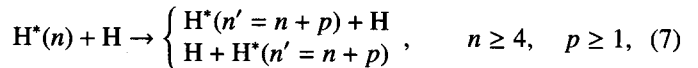
and the inverse de-excitation process

$$H^*(n) + H \rightarrow \begin{cases} H^*(n' = n - p) + H \\ H + H^*(n' = n - p) \end{cases}, \quad n - p \geq 4, \quad (8)$$

which were caused by the same resonant mechanism as the processes of chemi-ionization and chemi-recombination. The results obtained impose the necessity of an investigation of

the processes (7) and (8) in weakly ionized layers of stellar atmospheres and particularly in the Solar atmosphere. The confirmation of the importance of these processes in the Solar photosphere would support the necessity of including of the whole group of non-elastic processes in H*(n) + H collisions, i.e. Eqs. (1), (2), (7) and (8), in models of weakly ionized layers of Solar and stellar atmospheres. That should be confirmed by one of the known and widely used non-LTE models of the Solar atmosphere.

For the reason mentioned we shall examine here in more detail the significance of $(n - n')$-mixing processes (7) and (8) in the Solar photosphere and lower chromosphere. For this purpose we shall calculate the rate coefficients of these processes for different n and p using a semiclassical method developed by Mihajlov et al. (2004). The rate coefficients obtained will be compared with the rate coefficients of electron-atom mixing processes (6) for electron and hydrogen atom densities and temperatures from the model C of the Solar photosphere and the lower chromosphere of Vernazza et al. (1981).

2. Theoretical comments

The resonant mechanism. Since the resonant mechanism for processes (1)–(8) has been discussed in several previous papers, and especially has been described in detail in Mihajlov et al. (2004), only the basic facts will be given here. On the basis of the resonant mechanism the H*(n) + H collision system is treated within the domain

$$R \ll r_n, \tag{9}$$

where R is the internuclear distance and $r_n \sim n^2$ is the average radius of the Rydberg atom H*(n). 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 using the adiabatic electronic ground state $|1s\sigma_g; R\rangle$, or of the first excited state $|2p\sigma_u; R\rangle$ of the molecular ion H$_2^+$. The relative internuclear motion is described in the approximation of two classical trajectories: the first one, which corresponds to the adiabatic $1s\sigma_g$-term, and the other, which corresponds to the $2p\sigma_u$-term. It is assumed that each of these trajectories is realized with the same probability p_{in} which is equal to $1/2$.

The processes (7) and (8) of $(n - n')$-mixing, as well as the processes of chemi-ionization/recombination (1) and (2), are treated as a result of the resonant energy exchange between the outer electron e and the electronic component of the H$^+$ + H subsystem. This means that the transition of the outer electron from the initial energetic state to the upper ones occurs simultaneously with the transition of the H$^+$ + H subsystem from the electronic excited state $|2p\sigma_u; R\rangle$ to the ground state $|1s\sigma_g; R\rangle$, 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 $|1s\sigma_g; R\rangle$ to the excited state $|2p\sigma_u; R\rangle$ as illustrated in Fig. 1. Within the considered mechanism one assumes that all mentioned transitions are caused by the interaction of the outer electron with the dipole momentum of the H$^+$ + H subsystem.
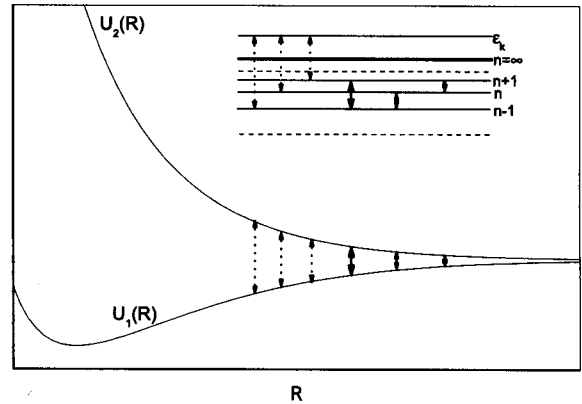

Fig. 1. The resonant mechanism in chemi-ionization/recombination channels (dashed arrows), and $(n - n')$-mixing channels (full arrows).

In Janev & Mihajlov (1979, 1980) the resonant mechanism described was applied in the range $n > 4$ where there are no crossings of the terms of H*(n) + H(1s) systems with the term of H$^+$ + H$^-$ system. However, following our later papers, we will take $n = 4$ as a lower boundary of the considered principal quantum number region. In accordance with Sidis et al. (1983) the corresponding crossing point is placed at such a large internuclear distance that it does not influence the considered processes.

The resonant mechanism was also treated within the framework of theories related to a wider class of collision atomic systems $A^*(n) + B$, where in the general case A and B denote different atoms (Flannery 1980; Lebedev 1991b; Lebedev & Fabrikant 1996). However, in the symmetrical case these theories give the same results as the theory presented in Janev & Mihajlov (1979, 1980) and Mihajlov & Janev (1981). Besides, the processes of $(n - n')$-mixing in the Li*(n) + Li collisions were experimentally studied in Dubreuil (1983). The experimental results obtained were compared with the results from Janev & Mihajlov (1979). It was demonstrated that the agreement of these results is good enough to confirm the validity of the described resonant mechanism.

The processes (1)–(8), caused by the resonant mechanism, should not be confused with the processes in H*(n) + A collisions caused by the direct interaction of the electron of atom H* with atom A whose electronic state does not change during the collision (Matsuzawa 1974; Gerstein 1976; Olson 1977; Percival 1978; Lebedev 1991a; Lebedev & Fabrikant 1996). The influence of such processes can be neglected in comparison with the influence of processes (7) and (8) at thermal collision energies ($\lesssim 1$ eV), as was discussed in Janev & Mihajlov (1979).

The rate coefficients of processes (7) and (8) for fixed n and $n' = n \pm p$ have been determined semi-classically, describing the internuclear motion by using the trajectories determined in the potential corresponding to the excited electronic state $|2p\sigma_u; R\rangle$ of the H$^+$ + H subsystem. For the calculations of the considered rate coefficient an approximation was used 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" to a continuum within the effective principal quantum number range
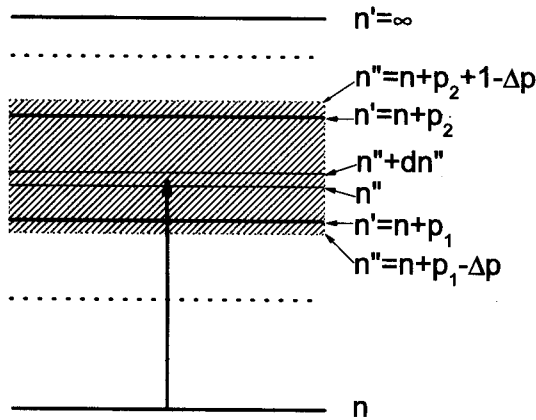
Fig. 2. The partial "smearing" of the discrete Coulomb spectrum to a continuum.

from $n + p_1 - \Delta p$ to $n + p_2 + 1 - \Delta p$, where $0 < \Delta p < 1$, as is shown in Fig. 2. Such "smearing" is performed under the conditions described in Mihajlov et al. (2004).

The described procedure for determination of the rate coefficients of the examined $(n - n')$-mixing processes means that the hydrogen (nl)-states with fixed n are populated according to their statistical weights. This assumption is based on the properties of the existing models of the photosphere and lower chromosphere of the Sun and similar stars, of some cooler stars (as for example M and K type stars), and of some other stars (like some of DB white dwarfs for example). It is well known that these models assume only limited deviations from the LTE. For example in Vernazza's model C of the Solar atmosphere used here it is assumed that the distribution of the total populations of the atomic shells with different principal quantum number n can deviate from the corresponding Boltzman distribution, but that there are no such deviations within particular shells. There are physical reasons for such an approach. Namely, it is well known that the processes of $(l - l')$-mixing for fixed n are practically resonant and are very effective over the distances proportional to an average Rydberg atom radius (Olson 1977; Percival 1978; Lebedev 1991a). Consequently such processes are much faster that the $(n - n')$-mixing processes, especially within the region where the $(n - n')$ transition energy is of the order of kT. A similar assumption for the population distribution of (nl) – states with fixed n was used and discussed in many previous articles, including Janev & Mihajlov (1979, 1980).

The procedure of "smearing" a discrete spectrum has already been used. For example in Sobel'man (1979) this has been used for description of the electron – ion recombination with transition of the free electron in a block of Rydberg states. In Duman & Shmatov (1980), "smearing" the discrete spectrum of the molecular ion A_2^+ has been used to describe the chemi – ionization processes in $A^*(n) + A$ collisions. In these cases it was used as physically acceptable approximation without special justifications.

In our case however, well-determined physical reasons exist for the approximation of "smearing". Concerning the "smearing" of the hydrogen Rydberg spectrum, some results from Janev & Mihajlov (1979) have been taken into account.

These are the results related to the behavior of the $(n - n')$ transition probability due to $H^*(n) + H(1s)$ collisions as a function of collision parameters for fixed impact energies. On the basis of the results obtained one can consider that the $(n - n')$ transition occurs within some interval of internuclear distances whose center is a point of resonance (where the observed transition may be treated as a result of the strictly resonant energy exchange within the electronic component of the considered system) and that such intervals overlap significantly for n' and $n' \pm 1$. These results are related to the case when the atom – atom impact energy is at least several times greater than energies for the considered $(n - n')$ transitions, which justified the use of the straight line trajectory approximation in the mentioned article.

This allows the considered process to be treated as the continuous decay of the initial electronic state (of the total system), during the internuclear motion within the reaction zone (the internuclear distance range being less or close to the resonant distance for the transition $n \to n + 1$).

The rate coefficients. Since the procedure of obtaining the rate coefficients for the processes (7) and (8) is described in detail in Mihajlov et al. (2004), only the corresponding final expressions are presented here. The rate coefficients $K_{n;n+p}(T)$ for the excitation processes (7), for given n, p and the temperature T, are obtained in the form

$$K_{n;n+p}(T) = \frac{2\pi}{3\sqrt{3}} \frac{(ea_0)^2}{\hbar} \cdot n^{-5} \cdot g_{n;n+p}$$

$$\times p_{in} \cdot 2 \cdot \int_{R_{min}(n,n+p)}^{R_{max}(n,n+p)} X(R) \cdot \exp\left[-\frac{U_2(R)}{kT}\right] \frac{R^4 \cdot dR}{a_0^5}, \tag{10}$$

where e and a_0 are the electron charge and the atomic unit of length, $g_{n;n+p}$ is the Gaunt factor defined in Johnson (1972), $R_{min}(n, n + p)$ and $R_{max}(n, n + p)$ are roots of equations

$$\epsilon(R_{min}) = \epsilon_{n+p+1-\Delta p} - \epsilon_n,$$
$$\epsilon(R_{max}) = \epsilon_{n+p-\Delta p} - \epsilon_n, \tag{11}$$

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 $|1s\sigma_g; R\rangle$ and $|2p\sigma_u; R\rangle$, respectively, and $\epsilon_n = -Ry/n^2$. $X(R)$ denotes the function

$$X(R) = \frac{\Gamma\left(3/2; \frac{|U_1(R)|}{kT}\right)}{\Gamma(3/2)}, \tag{12}$$

where $\Gamma(3/2; x)$ and $\Gamma(3/2)$ are the corresponding values of the incomplete and complete Gamma functions. The factor $p_{in} = 1/2$ in Eq. (10) is the mentioned above probability for the realization of a trajectory which describes the internuclear motion in the potential $U_2(R)$, while the factor 2 reflects the fact that the system $H^*(n) + H$ crosses the transition zone twice: once on entry and once on leaving.

The rate coefficients $K_{n;n-p}(T)$ for de-excitation processes (8) are obtained from the thermodynamic balance principle in the form

$$K_{n;n-p}(T) = K_{n-p;n}(T) \cdot \frac{(n-p)^2}{n^2} \cdot \exp\left(\frac{\epsilon_{n-p;n}}{kT}\right), \tag{13}$$
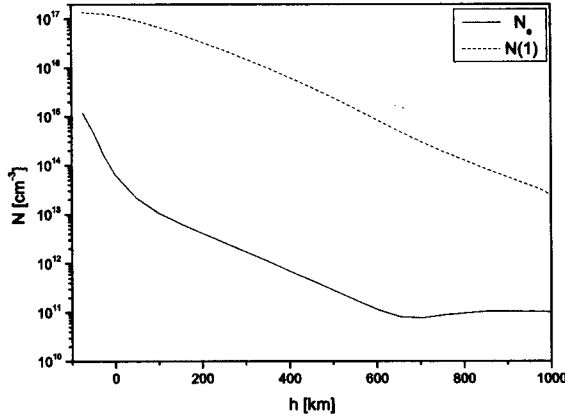
where $\epsilon_{n-p;n} = \epsilon_n - \epsilon_{n-p}$.

Fig. 3. The behavior of N_e and $N(1)$ in [cm^{-3}] as functions of height h within the considered part of the Solar atmosphere from model C of Vernazza et al. (1981)
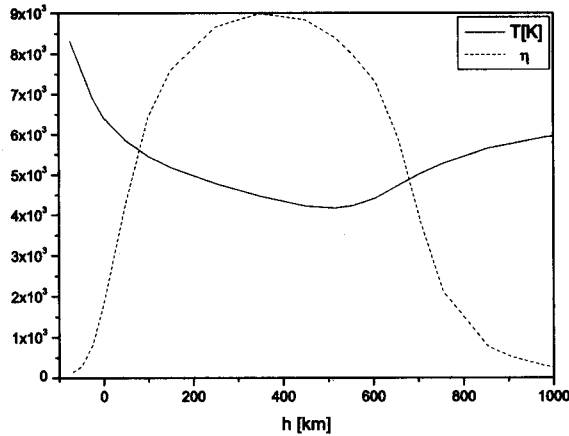

Fig. 4. The behavior of the temperature T and the parameter $\eta = N(1)/N_e$ as functions of height h within the considered part of the Solar atmosphere from model C of Vernazza et al. (1981)

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 to take 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 the Solar atmosphere as a function of height (h) is shown in Fig. 3, while Fig. 4 shows the behavior of T and the parameter η defined by the relation

$$\eta_{ea} = \frac{N(1)}{N_e}. \tag{14}$$

In our case the parameter η is close to the inverse value of the considered plasma's degree of ionization. Also, we will use the data about the hydrogen atom excited state population ($n \geq 2$) from Vernazza et al. (1981). In order to determine the relative influence of processes (7) and (8) in the considered parts of Solar atmosphere, we will compare them with electron-atom collision processes (6). Following the mentioned above papers related to chemi-ionization/recombination processes,
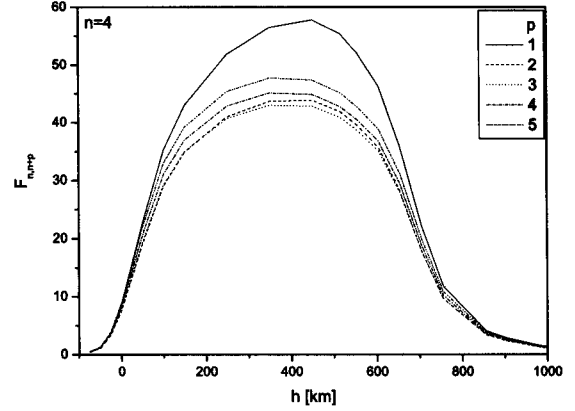
Fig. 5. The behavior of the parameter $F_{n,n+p} = (K_{n,n+p} \cdot \eta)/\alpha_{n,n+p}$, characterizing the relative efficiency of atom-atom and electron-atom $(n - n')$- mixing processes, as a function of height h for $n = 4$ and $p = 1$–5. The atom-atom rate coefficient $K_{n,n+p}$ is given by Eqs. (10)–(12) and the parameter η- by Eq. (14). The electron-atom rate coefficient $\alpha_{n,n+p}$ is taken from Vriens & Smeets (1980).

we compare the studied collision processes only with other relevant collision processes, omitting the radiative decay of hydrogen Rydberg states. The radiative decay, which causes the deviation from LTE in the considered part of the Solar atmosphere, is already included in Vernazza's model, so that the "optical part" of this model does not need to undergo any changes. We show that the "collision part" of Vernazza's model has to be changed by adding atomic collision processes (1)–(8).

The relative efficiency of processes (7) and (8) in comparison to process (6) is characterized by the parameter $F_{n;n\pm p}(T)$

$$F_{n;n\pm p}(T) = \frac{K_{n;n\pm p}(T)N(n)N(1)}{\alpha_{n;n\pm p}(T)N(n)N_e} = \frac{K_{n;n\pm p}(T)\eta_{ea}}{\alpha_{n;n\pm p}(T)}, \tag{15}$$

where $N(n)$ is the excited atom states population for given n, the parameter η_{ea} is defined by Eq. (14), and $\alpha_{n;n\pm p}(T_e)$ is the rate coefficient for the electron-atom process (6) taken from Vriens & Smeets (1980).

We have calculated the values of the parameter $F_{n;n\pm p}$ for $n \geq 4$ and $p \geq 1$, within the range of h corresponding to the Vernazza et al. (1981) model C of the Solar photosphere. Our results are illustrated in Figs. 5–7. In these figures the behavior of the parameter $F_{n;n+p}$ is shown, for $4 \leq n \leq 8$ and $1 \leq p \leq 5$, as a function of h within the range -50 km $\leq h \leq 1000$ km. In the largest part of the photosphere the $(n-n')$-mixing processes (7) and (8) are totally dominant in comparison to the electron-atom processes (6) for $n = 4$, 5, 6 and practically any $p \geq 1$, and have similar intensities for $n = 7$, 8. Comparing Figs. 5–7 with Fig. 4 one can see that the region of the maximal $F_{n;n\pm p}$ values corresponds to an h region near the temperature minimum, where the parameter η, defined by Eq. (14), is also maximal.

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

$$N^{(V)}\left(n = n_{\min}^{(V)}\right) = \min_{n \geq 1} N^{(V)}(n), \tag{16}$$
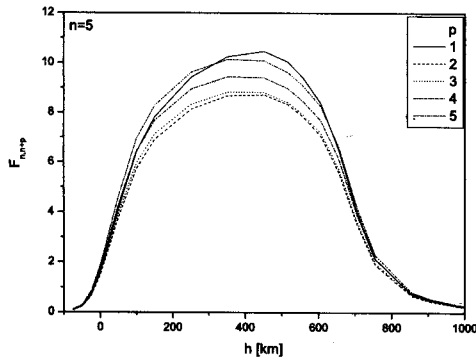
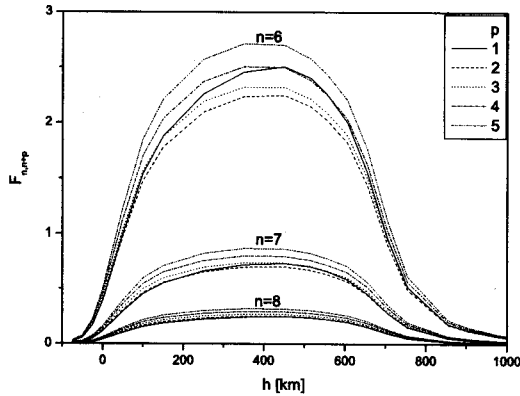**Fig. 6.** The same as in Fig. 5, but for $n = 5$.

Fig. 7. The same as in Fig. 5, but for $n = 6, 7, 8$.

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

	$h\,(km)$								
	−50	0	100	250	350	555	755	980	1065
$n_{min}^{(eq)}$	4	4	5	5	5	6	5	5	5
$n_{min}^{(V)}$	5	5	5	6	6	6	6	6	5

where $N^{(V)}(n)$ are excited atom populations from model C for a given h, and the second one is the value of n defined by the condition:

$$N^{(eq)}(n = n_{min}^{(eq)}; T) = \min_{n \geq 1} N^{(eq)}(n; T) \tag{17}$$

where $N^{(eq)}(n; T)$ are equilibrium (Boltzmanian) excited atom populations for T from model C for the same h as in the previous case. It could be shown that in the considered temperature range, $n_{(min)}^{(eq)}$ is close to the value of $(Ry/kT)^{(1/2)}$. In Table 1 the values of $n = n_{min}^{(V)}$ and $n = n_{min}^{(eq)}$ are presented for a series of h values in −50 km to 1065 km range. Within the considered domain of h the values of $n = n_{min}^{(V)}$ and $n = n_{min}^{(eq)}$ are 4, 5 and 6 for which domination of the processes (7) and (8) in comparison with the processes (6) is demonstrated.

For plasmas similar to the considered photospheric one, the exchange rate between both hydrogen basic components, atoms $H(1s)$ and ions H^+, is limited by the group of excited atom states with n close to the $n_{min}^{(V)}$ or $n_{min}^{(eq)}$. However, one can see that the processes (7) and (8) play the dominant role in this group of excited states. This means that the exchange between the excited state atom populations within the lower part

of the Rydberg region of n is determined by the processes (7) and (8). If we add to this the fact that the exchange 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), (7) and (8), closely connected by the resonant mechanism, completely dominate for the excited states with n close to $n_{min}^{(V)}$ or $n_{min}^{(eq)}$.

We gave here all relevant results demonstrating the significance of the processes (7) and (8) for a large part of the Solar photosphere and lower chromosphere, particularly in the neighborhood of the temperature minimum. On the basis of presented results we can conclude that the influence of the $(n - n')$-mixing processes (7) and (8), as well as the chemi-ionization/recombination processes (1) and (2), must be taken into account for any modelling of the Solar photosphere and lower chromosphere. Our findings are also related to similar stellar atmospheres as well as to stellar atmospheres with lower effective temperatures but where the atomic component is still dominant over the molecular one.

References

Dubreuil, B. 1983, Phys. Rev. A, 27, 2479
Duman, E. L., & Shmatov, I. P. 1980, JETP, 51, 1061
Gerstein, J. I. 1976, Phys. Rev. A, 14, 1354
Flannery, M. R. 1980, Phys. Rev. A, 22, 2408
Johnson, L. C. 1972, ApJ, 174, 227
Janev, R. K., & Mihajlov, A. A. 1979, Phys. Rev., 20, 1890
Janev, R. K., & Mihajlov, A. A. 1980, Phys. Rev., 21, 819
Lebedev, V. S. 1991a, J. Phys. B: At. Mol. Opt. Phys., 24, 1977
Lebedev, V. S. 1991b, J. Phys. B: At. Mol. Opt. Phys., 24, 1993
Lebedev, V. S., & Fabrikant, I. I. 1996, Phys. Rev. A, 54, 2888
Matsuzawa, M. 1974, J. Electron Spectrosc. Relat. Phen., 4, 1
Mihajlov, A. A., & Janev, R. K. 1981, J. Phys. B: At. Mol. Opt. Phys., 14, 1639
Mihajlov, A. A., Ignjatović Lj, M., Vasilijević, M. M., & Dimitrijević, M. S. 1997, A&A, 324, 1206
Mihajlov, A. A., Dimitrijević, M. S., Ignjatović, Lj. M., & Vasilijević, M. M. 1999, A&ATr, 18, 145
Mihajlov, A. A., Jevremović, D., Hauschildt, P., et al. 2003, A&A, 403, 787
Mihajlov, A. A., Ignjatović, Lj. M., Djurić, Z., & Ljepojević, N. N. 2004, J. Phys. B, 37, 4493
Olson, R. E. 1977, Phys. Rev. A, 15, 631
Percival, I. C. 1978, in Electronic and Atomic Collisions: Invited Papers, ed. G. Watel, North-Holland, 569
Sidis, V., Kubach, C., & Fussen, D. 1983, Phys. Rev. A, 27, 2431
Smirnov, V. A., & Mihajlov, A. A. 1971, Opt. Spektrosk., 30, 984 (Opt. Spectrosc., USSR 5, 525)
Sobel'man, I. I. 1979, it Atomic Spectra and Radiative Transitions (Berlin: Springer)
Vernazza, J. E., Avrett, E. H., & Loser, R. 1981, ApJS, 45, 635
Vriens, L., & Smeets, A. 1980, Phys. Rev. A, 22, 940