CHEMI-IONIZATION/RECOMBINATION PROCESSES AS FACTORS OF THE INFLUENCE ON THE SPECTRAL LINES SHAPES IN STELLAR ATMOSPHERES

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INTRODUCTION

- 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 excited-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.

We investigate this in the following papers:

Mihajlov, A.A., Dimitrijevic, M.S., & Djuric, Z. 1996, Physica Scripta, 53, 159

Mihajlov, A.A., Djuric, Z., Dimitrijevic, M.S., & Ljepojevic, N.N. 1997b, Physica Scripta, 56, 631

Mihajlov, A.A., Ignjatovic, L.M., Vasilijevic, M.M., & Dimitrijevic, M.S. 1997a, A&A, 324, 1206

Mihajlov, A.A., Ignjatovic, L.M., Dimitrijevic, M.S.,& Djuric, Z. 2003a, ApJS, 147, 369

Mihajlov, A.A., Jevremovic, D., Hauschildt, P., Dimitrijevic, M. S., Ignjatovic, Lj. & Alard, N. 2003b, A&A, 403, 787

Mihajlov, A.A., Jevremovic, D., Hauschildt, P., Dimitrijevic, M. S., Ignjatovic, Lj. & Alard, N. 2007b, A&A, 471, 671

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- 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 modeling of the solar atmospheres should be investigated further.

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

$$A^{*}(n)+X \Rightarrow AX^{+}+e \qquad (1)$$

as well as the processes of **Penning ionization**

$$A^{*}(n)+X \Rightarrow A+X^{+}+e \qquad (2)$$

where A, X and X^{+} are atoms and the atom ion in their ground states, $A^{*}(n)$ atom in a highly excited (Rydberg) state with the principal quantum number n >>1 and AX^{+} is the corresponding molecular ion in its ground electronic state.

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$$A^{*}(n)+X \Rightarrow A+X^{+}+e \qquad (2)$$

- 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 from all the processes, 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), namely as it is illustrated in **figure 1**.

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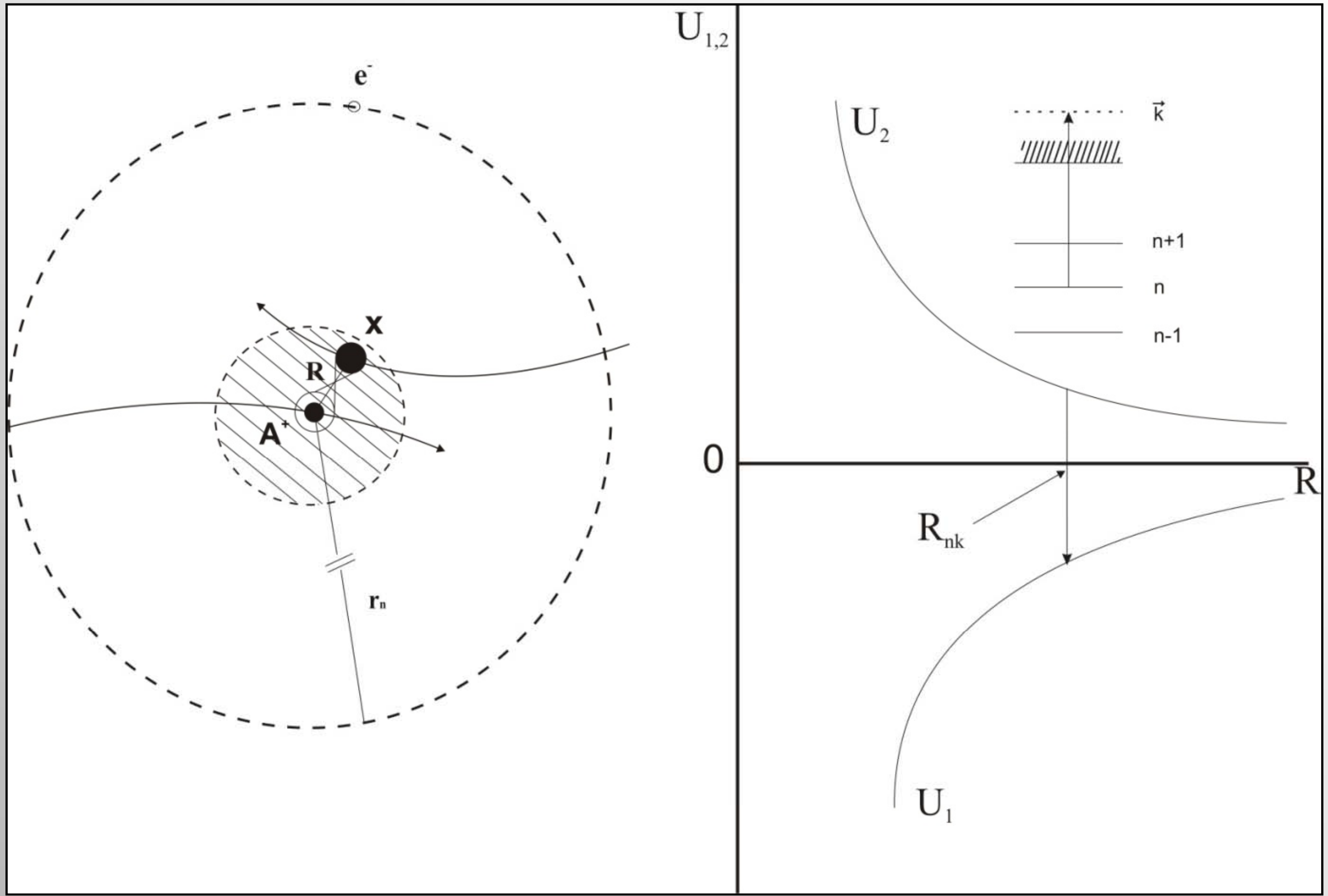

Fig. 1 Schematic illustration of chemi-ionization processes in $A^*(n)+X$ collision: $r_n \sim n^2$ is the mean radius of the Rydberg atom $A^*(n)$; R -internuclear distance; R_{nk} – the resonant distance for the transition $|2,n> \rightarrow |1,k>$; $U_1(R)$ and $U_2(R)$ are the potential curves of the molecular ion AX^+ in the ground and the first excited electronic states $|1>$ and $|2>$, respectively; the region of R where the subsystem $A^+(n)+X$ can be treated as the quasi-molecular complex is shaded.

- here, all chemi-ionization processes are treated on the basis of **dipole resonant mechanism**, which was introduced in the considerations in Smirnov, V.M. & Mihajlov, A.A. 1971, Opt. Spektrosk., 30, 984 and was described in details in Ignjatovic, L.M. & Mihajlov, A.A. 2005, Phys. Rev. A.,72, 022715.
- It means that such processes are considered as a result of the resonant energy conversion within the electronic component of the system $A^*(n)+X$, which is realized inside the region of the intenuclear distances

$$R \ll r_n, \qquad (3)$$

where $r_n \sim n^2$ is the mean radius of the Rydberg atom, and which is caused by the dipole part of the interaction of the outer electron with the inner subsystem $[A^+ + X]$.

- some of the mentioned processes were described already in Hornbeck, J.A., & Molnar, J.P.1951, Physical Review,84,621,

- their intensive experimental research began some later, when the development of the **laser technique** made possible the precise transition of the atoms in chosen Rydberg states (Boulmer, J., Bonanno, R., & Weiner, J. 1983, J.Phys.B Atomic Molecular Physics, 16, 3015 ; Weiner, J., & Boulmer, J. 1986, Journal of Physics B Atomic Molecular Physics, 19, 599; Klyucharev, A.N., & Lazarenko, A.V. 1980, Optics and Spectroscopy, 48, 229).

- since it was easiest when the ionization potential of atom A is small, chemi-ionization processes were studied particulary wide in the cases of **alkali metal** atoms (Li, Na, etc.). They remain the subject of experimental research until now (Johnson, B.C., Wang, M.-X., & Weiner, J. 1988, J.Phys.B Atomic Molecular Physics, 21, 2599; Wang, M.-X., & Weiner, J. 1987, 35, 4424).

- the large atom ionization potentials were not an insurmountable obstacle and processes (1) and (2) with atoms of some **rare gases** (He, Ne, etc.) also were experimentally researched during several years (see e.g. Hitachi, A., Davies, C., King, T.A., Kubota, S., & Doke, T. 1980, 22, 856; Runge, S., Pesnelle, A., Perdrix, M., Watel, G., & Cohen, J.S. 1985, 32, 1412; Harth, K., & Hotop, H. in *Highly Excited States of Atoms and Molecules* S.S. Kato and M. Matsuzawa, Editors, Invited Papers of the Oji International Seminar, Fuji-Yoshida, Japan (1986), p. 117.

- in the above papers the chemi-ionization processes were studied mostly under the conditions of **single- and cross-beams**, in the symmetric (A=X) as well as in the non-symmetric (A ≠X) case. However, later the symmetric **chemi-ionization processes**

$$A^{*}(n) + A \Rightarrow A_2^{+} + e \qquad (4)$$

$$A^{*}(n) + A \Rightarrow A + A^{+} + e \qquad (5)$$

and the corresponding **inverse recombination processes**,

$$A_2^+ + e \Rightarrow A^*(n) + A \qquad (6)$$

$$A + A^+ + e \Rightarrow A^*(n) + A \qquad (7)$$

where A=H(1s) or He($1s^2$), were theoretically considered in Refs.

Mihajlov, A.A., Ljepojevic, N.N., & Dimitrijevic, M.S.1992, J.Phys.B Atomic Molecular Physics, 25, 5121

Mihajlov, A.A., Djuric, Z., Dimitrijevic, M.S., & Ljepojevic, N.N. 1997b, Physica Scripta, 56, 631

They were considered as factors of influence on the populations of excited atoms in the weakly ionized hydrogen and helium plasmas, by comparison of its efficiency with the efficiency of the processes

$$A^*(n) + e \Rightarrow A^+ + 2e, \qquad (8)$$

$$A^+ + 2e \Rightarrow A^*(n) + e, \qquad (9)$$

$$A^+ + e \Rightarrow A^*(n) + \varepsilon_\lambda, \qquad (10)$$

where A=H(1s) or He($1s^2$) and ε_λ is the energy of a photon with wavelength λ.

For the considered conditions in Refs.Mihajlov et al. (1997b) and Mihajlov, A.A., Dimitrijevic, M.S., & Djuric, Z. 1996, Physica Scripta, 53, 159 the rate coefficients for all chemi-ionization and chemi-recombination processes (4)-(7) were determined. It was founded that under the mentioned conditions these processes in the region n ≤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, A. A. & Dimitrijevic, M.S. 1986, A&A, 155,319; M.S. 1992, A&A, 256, 305.), that suggested the idea that the chemi-ionization processes (4), (5) and the chemi-recombination processes (6), (7) 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, A.A., Ignjatovic, L.M., Vasilijevic, M.M., & Dimitrijevic, M.S. 1997a, A&A, 324, 1206, and for the helium case (**atmospheres of DB white dwarfs** with Teff= 12000 - 18 000 K) in Mihajlov et al. (2003a). In the case of DB white dwarfs with Teff= 12000 K, this is illustrated by the **figure 2**, showing the behavior of the quantity Fir defined by relations

$$F_{ir}^{ab} = \frac{K_i^{ab}(n,T)}{\alpha_i^{ea,eea}} \cdot \eta_e^a = \frac{K_r^{ab}(n,T)}{\alpha_r^{ea,eea}} \cdot \eta_e^a \qquad (11)$$

where $K_{i,r}^{ab}(n, T)$ are rate coefficients of chemi-ionization/recombination processes from Mihajlov et al. (1996), $\alpha_{i,\, r}^{ea,eea}$ are the rate coefficients of concurrent electron-atom and electron-ion processes from Vriens & Smeets (1980), η_e^a=N(He)/N(e), and N(He) and N(e) are the densities of the helium atoms and free electrons.

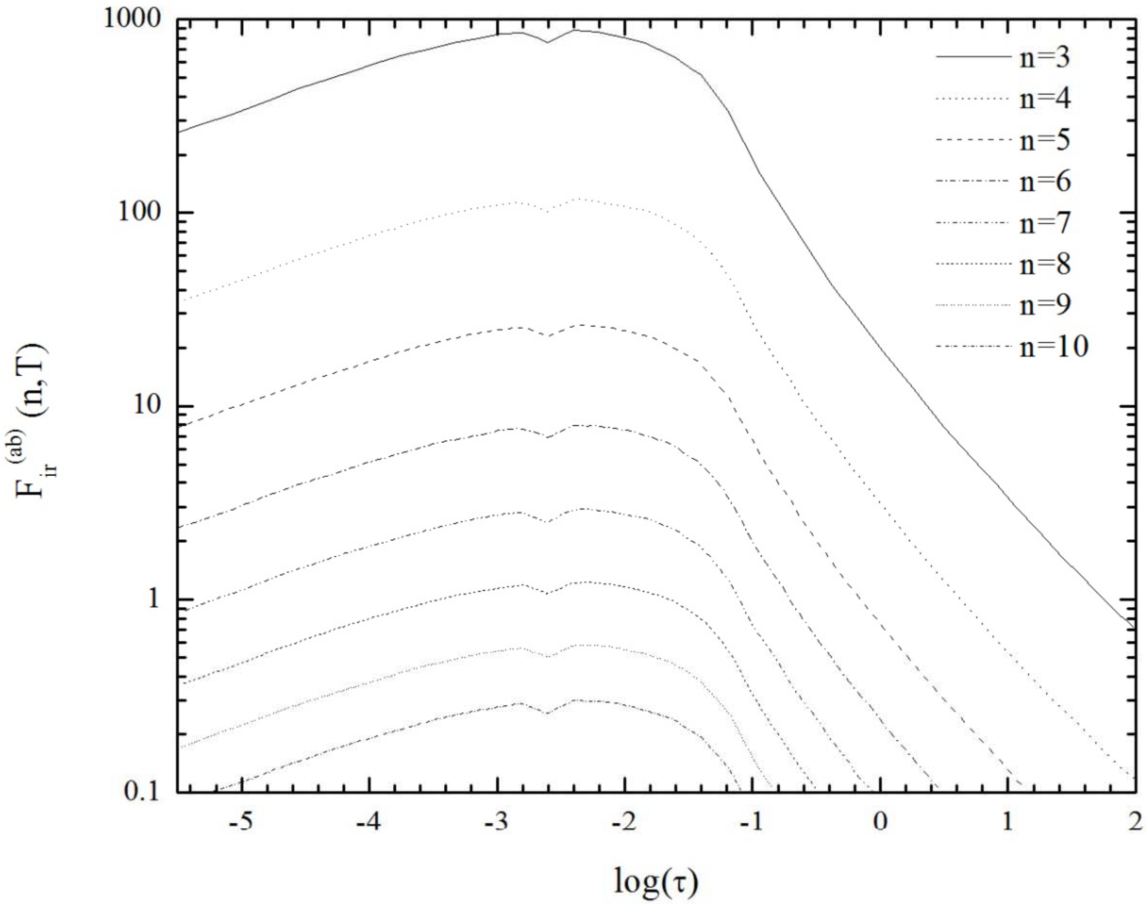

Figure 2. DB white dwarfs. Parameter F_{ir}^{ab} as a function of the logarithm of Rosseland optical depth log τ, for principal quantum numbers n = 3-10, with Teff=12000 K and log g =8.

Than, the influence of the chemi-ionization processes (4), (5) and the chemi-recombination processes (6), (7) with A=H on the excited hydrogen atom populations was examined in much more detail in Mihajlov, A.A., Jevremovic, D., Hauschildt, P.,Ignjatovic, & Alard 2003b, A&A, 403, 787 where these processes were included ab initio in a non-LTE modeling of an **M red dwarf atmosphere** with the effective temperature Teff = 3800 K, using PHOENIX code (see Baron, E. & Hauschildt, P.H. 1998, ApJ, 495, 370)

It 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 $2 \leq n \leq 20$. This is illustrated by **figure 3**.

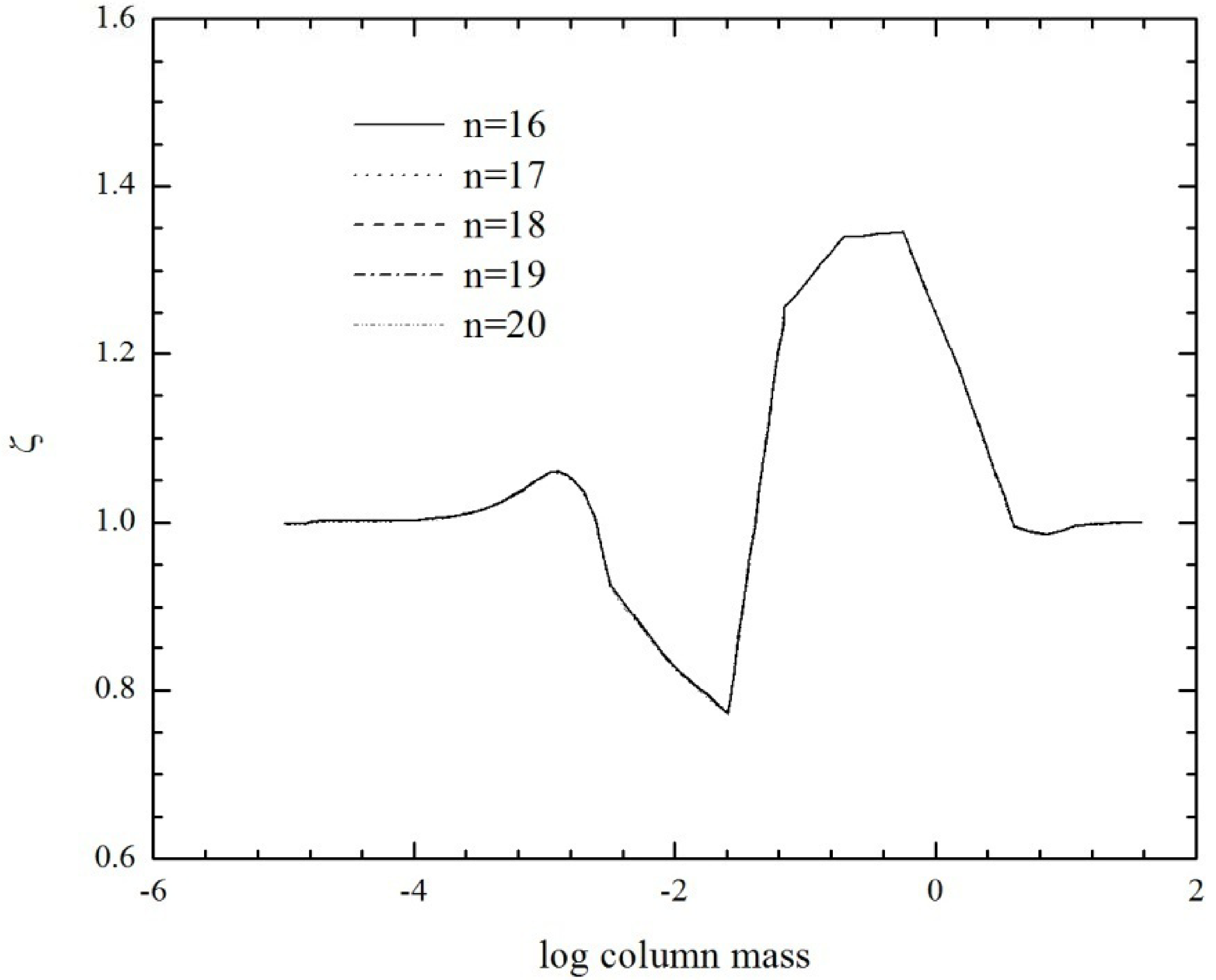

Figure 3: The behavior of the population ratio ζ for 16 ≤ n ≤ 20 as a function of the column mass.

Later, again using the **PHOENIX code** for the case of the atmosphere of the same **red dwarf**, the influence was examined of the processes (4-7) 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 Ne, is also generated and, as one of further consequences, significant changes in hydrogen line profiles. This fact is illustrated by **figure 4**.

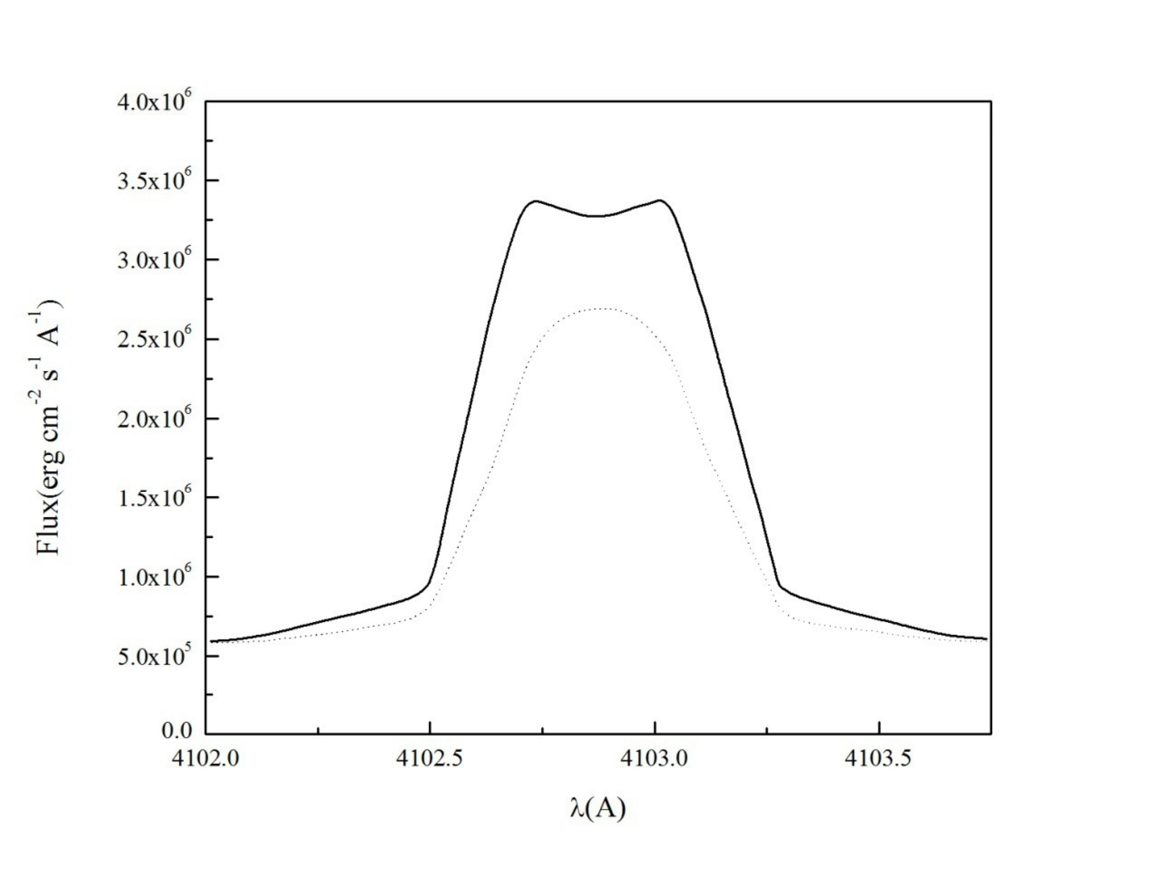

Figure 4: Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for Hβ line.

- here, one of our main aims is to draw attention to the importance of all processes (1) - (5) 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 (8) - (10) 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 (4) and (5) was qualitatively shown that for $4 \leq n \leq 8$ their efficiency is comparable to the efficiency of the concurrent processes (9) and (10) in a part of the solar photosphere (see Mihajlov et al. (1997a)).

The fact that the processes (1) - (5) can be important for the solar photosphere is supported by the results obtained in Mihajlov et al. (2003a, 2007b) for an M red dwarf atmosphere (Teff = 3800 K). Namely, the compositions of the solar and the considered M red dwarf's photospheres are practically the same and the values of hydrogen-atom density, Ne and T in these photospheres change within similar regions (Vernazza, J., Avrett, E., & Loser, R. 1981, ApJS, 45, 635; Mihajlov et al. 2007b), so that one can expect that the influence of processes (1) - (5) on the hydrogen-atom excited states and free-electron populations in the solar atmosphere will be at least close to their influence in that of the M red dwarf, and that these processes will be very important for weakly ionized layers of the solar atmosphere.

THE RATE COEFFICIENTS OF THE CHEMI-IONIZATION/RECOMBINATION PROCESSES

- partial rate coeffcients of the chemi-ionization processes (4) and (5)
$K^{(a;b)}_{ci}(n; T)$

- partial rate coeffcients of the inverse chemi-recombination processes (6) and (7) $K^{(a;b)}_{cr}(n; T)$

-total rate coeffcients for chemi-ionization and chemi-recom. processes

$$K_{ci;cr}(n; T) = K^{(a)}_{ci;cr}(n; T) + K^{(b)}_{ci;cr}(n; T) \qquad (12)$$

- $I_{ci}(n; T)$, $I_{cr}(n; T)$ be the total chemi-ionization and chemi-recombination fluxes caused by the processes (1,2) and (4,5)

$$I_{ci}(n; T) = K_{ci}(n; T)\, Nn\, N1 \quad \text{and} \quad I_{cr}(n; T) = K_{cr}(n; T)\, N1\, Ni\, Ne; \qquad (13)$$

- $I_{i;ea}(n; T)$, $I_{r;eei}(n; T)$ and $I_{r;ph}(n; T)$ be the (8), (9) and (10). fuxes caused by ionization and recombination processes

$$I_{i;ea}(n; T) = K_{ea}(n; T)\, Nn\, Ne; \quad I_{r;eei}(n; T) = K_{eei}(n; T)\, Ni\, Ne\, Ne;$$
$$I_{r;ph}(n; T) = Kph(n; T)\, Ni\, Ne \qquad (14)$$

- **quantities Fi(n; T)** which characterize the relative effciency of partial chemi-ionization processes (4) and (5) together and the impact electron-atom ionization (8)

$$Fi(n, T) = \frac{Ici(n, T)}{Ii,ea(n, T)} = \frac{Kci(n, T)}{Kea(n, T)} \cdot N1Ne \qquad (15)$$

- **quantities $F_{i;ea;2\text{-}8}(T)$** characterize relative influence of the chemi-ionization processes (4) and (5) together to that of the impact electron-atom ionization process (8) on the whole block of the excited hydrogen atom states with 2 ≤ *n* ≤ *8,*

$$F_{i,ea;2\text{-}8}(T) = \frac{\sum_{n=2}^{8} Ici(n, T)}{\sum_{n=2}^{8} Ii,ea(n, T)} = \frac{\sum_{n=2}^{8} Kci(n, T)\, N_n}{\sum_{n=2}^{8} Kea(n, T)\, N_n} \cdot N1Ne \qquad (16)$$

- In **Figure 5** 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

- In **Figure 6** the behavior of the quantity $F_{i;ea}(2\text{-}8)(T)$ 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).

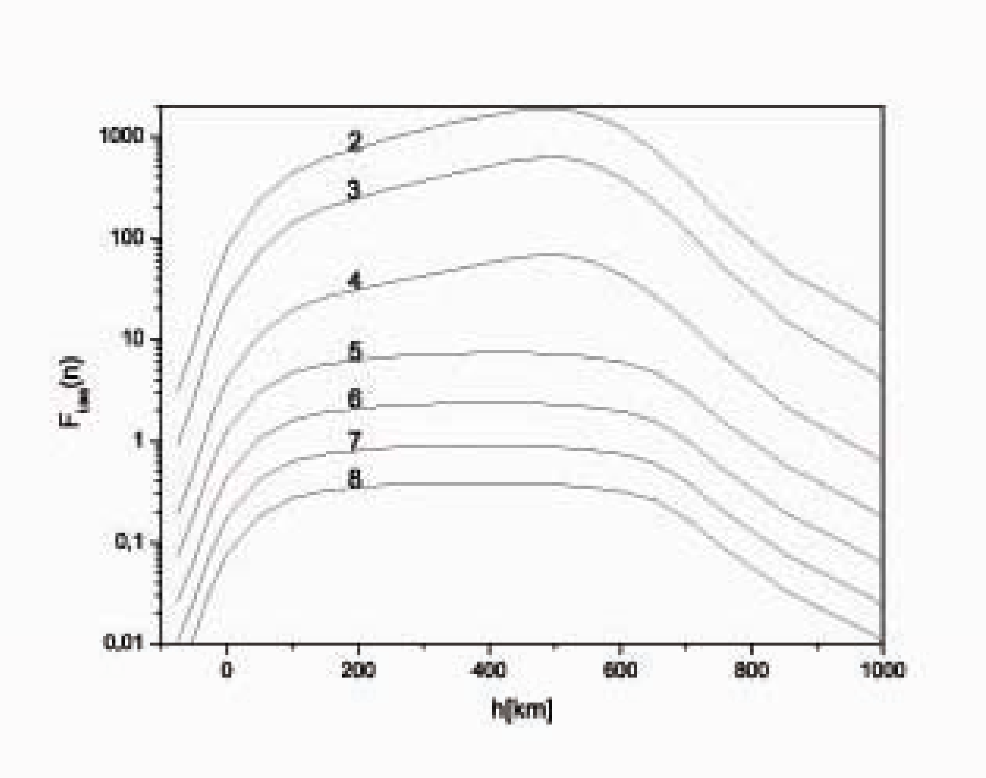

Fig 5: Behavior of the quantity $F^{(ab)}_{i;ea}$ (n) *given by Equation (8), as a func*tion of height h.

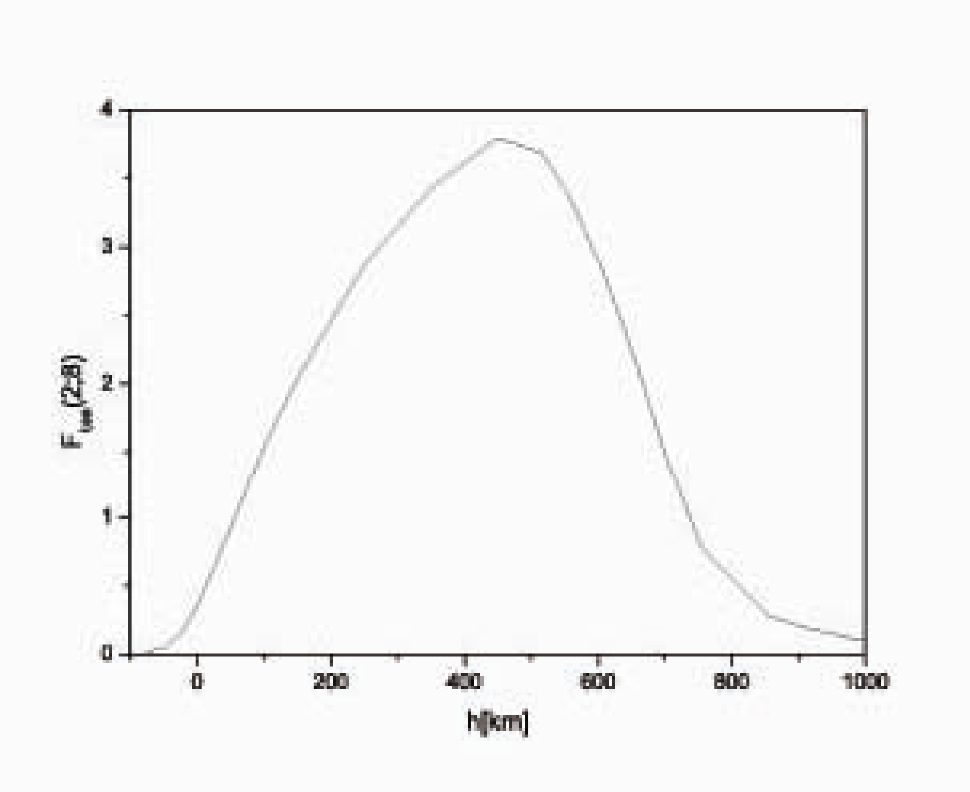

Fig 6:Behavior of the quantity $F_{i;ea}(2; 8)$ *given by Eq. (17), as a func*tion of height h.

we **compared** the relative influence of the **chemi-recombination processes** (6) and (7) together and total influence of the electron - electron - H^+ recombination process (9) and photo-recombination electron - H^+ process (10) 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 $< h < 600$ km).

Conclusions

Chemi-ionization and chemi-recombination in the atmospheres of the **Sun,** some **M red dwarfs** and **DB white dwarfs** have been investigated.

- 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.
- it is shown that these processes and their importance for non-local thermodynamic equilibrium modeling of the solar atmospheres should be investigated further.

Conclusions

- the **chemi-ionization** processes in atom - Rydberg atom collisions, as well as the corresponding **chemi-recombination** processes are factors of influence on the atom excited-state populations in weakly ionized layers of stellar atmospheres.
- 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**.

Conclusions

- the **chemi-ionization** processes in atom - Rydberg atom collisions, as well as the corresponding **chemi-recombination** processes are factors of influence on the atom excited-state populations in weakly ionized layers of stellar atmospheres.
- 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**.

Conclusions

We should note that a group of collision ion-atom radiative processes was investigated by us in several papers:

Ermolaev, A.M., Mihajlov, A.A., Ignjatovi c, L.M., & Dimitrijevic, M.S. 1995, J. Phys. D., 28, 1047

Ignjatovic, L.M., Mihajlov, A.A., Sakan, N.M., Dimitrijevic, M.S., & Metropoulos, A. 2009, MNRAS, 396, 2201

Mihajlov, A. A. & Dimitrijevic, M.S. 1986, A&A, 155,319

Mihajlov, A.A. & Dimitrijevic, M.S. 1992, A&A, 256, 305

Mihajlov, A.A., Dimitrijevic, M.S., & Ignjatovic, L.M. 1993, A&A, 276, 187

Mihajlov, A.A., Dimitrijevic, M.S., & Ignjatovic, L.M. 1994a, A&A, 287, 1026

Mihajlov, A.A., Dimitrijevic, M.S., Ignjatovic, L.M., & Djuric} Z. 1994b, A&AS, 103, 57

Mihajlov, A.A., Ignjatovic, L.M., Sakan, N.M., &Dimitrijevic, M.S. 2007a, A&A, 469, 749

Conclusions

It was suggested that these processes should be included in the stellar atmosphere models, and recently it was actually realized in Fontenla, J.M., Curdt, W., Haberreiter, M., Harder, J., & Tian, H. 2009, ApJ, 707, 482, and Koester, D. 2010, private communications. Due to a principal similarity between the mechanisms of processes (1) - (5) and these radiative processes, one can hope that the chemi-ionization/recombination processes will be also included in the stellar atmosphere models.

Thank you for attention