Rydberg atoms in astrophysics

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Abstract

Elementary processes in astrophysical phenomena traditionally attract researchers attention. At first this can be attributed to a group of hemi-ionization processes in Rydberg atom collisions with ground state parent atoms. This processes might be studied as a prototype of the elementary process of the radiation energy transformation into electrical one. The studies of nonlinear mechanics have shown that so called regime of dynamic chaos should be considered as typical, rather than exceptional situation in Rydberg atoms collision. From comparison of theory with experimental results it follows that a such kind of stochastic dynamic processes, occurred during the single collision, may be observed.

Key words: Rydberg atom, absorption, white dwarfs, stellar atmospheres

1. Introduction

If an atom is in a state of sufficiently high principal quantum number $n$ it means that the valence electron is far from the ionic core, and such atom appears hydrogenic. In such atoms the valence electron is influenced mainly by the positive charge of the ionic core, and not by its structure. The excited state of these hydrogen like atoms are commonly accepted to call Rydberg states, high Rydberg states, or simply highly excited states (Edelstein et al., 1985). For example the radius of Bohr orbit of Rydberg atom in the state $n = 110$ is equal to $6.4 \cdot 10^{-5}$ cm, i.e. very close to macroscopic size. Another
obvious property of such atom is the large transition dipole moment, which
simply reflects the separation between the valence electron and the positive
ionic core. Such atoms, as a result, provide the extremely high cross sections
of the relevant physical processes.

Although the study of Rydberg atoms has a long history, the develop-
ment of laser technique has led to a great experimental advances and in
recent years renewed interest for such researches. Another very important
field of researches for Rydberg atoms is astrophysics. The basic goal of our
paper is description of a various astrophysical situations that are responsible
for production of Rydberg states and their observational effects. Our paper
consists of three parts: (a) short review of astrophysical target of Rydberg
atoms (b) atom- Rydberg atom chemi-ionization collisional processes in stel-
lar atmospheres, and (c) description of dynamic chaos regime in Rydberg
atoms collisions.

1.1. The base astrophysical targets of searches for Rydberg atoms

Some models of big bang nucleosynthesis suggest that very high baryon
density regions were formed in the early universe. Then the most important
aspect is hydrogen recombination and Rydberg states can play important
role in this process. It is well known (Puy et al., 2007) that the chemical
composition of the primordial gas consists of electrons and:

- hydrogen: $H$, $H^-$, $H^+$, $H_2^+$ and $H_2$
- deuterium: $D$, $D^+$, $HD$, $HD^+$ and $HD^-$
- helium: $He$, $He^+$, $He^{2+}$ and $HeH^+$
- lithium: $Li$, $Li^+$, $Li^-$, $LiH^-$ and $LiH^+$

Their respective abundances are calculated from a set of chemical reac-
tions for the early universe (Puy et al., 2007). Evaluation of chemical abun-
dances in the standard BB model is presented at Fig. 1 from (Puy et al.,
2007).

Another probable regions of Rydberg atoms existence are the cool stars
and, firstly, the cool white dwarfs. Recently, a new effect has been noticed
from Spitzer observations of cool white dwarfs (Kilić et al., 2006). Namely,
these observations have demonstrated that some white dwarfs with $T <$
6100 K are found to display significant flux deficits in Spitzer observations,
Figure 1: Evaluation of chemical abundances in the standard Big Bang model. Vertical axes are the relative abundances and the horizontal axes are relative to the redshift.
Figure 2: Spectral energy distributions of cool white dwarfs observed with Spitzer space telescope (1Jy = $10^{-26} \cdot \text{W} \cdot \text{m}^{-2} \cdot \text{Hz}^{-1}$).

(see Figure 2 from Kilić et al. (2006)). These mid-IR flux deficits are not predicted by the current white dwarf models including collision induced absorption due to molecular hydrogen. This fact implies that the source of this flux deficit is not standard molecular absorption but some other physical process. We claim that such process may be absorption by atoms and molecules in highly excited Rydberg states.

The similar effect have been recently discovered and for magnetic white dwarfs from spectropolarimetric observations made at Russian BTA-6m telescope and NIR photometric observations of magnetic white dwarfs at Russian-Italian AZT-94 telescope located at Campo Imperatore. The details can be found in Gnedin et al. (2006).
2. Atom Rydberg atom chemi-ionization collision processes in stellar atmospheres

Besides of the star atmospheres with strong magnetic fields, the processes with the participation of the Rydberg’s atoms could be of interest in the atmospheres of other types of stars where the presence of magnetic field can be neglected in the first approximation. As an example, within this study is considered the significance of the chemi-ionization processes

\[
H^*(n) + H \rightarrow e + H^+ + H \\
H^*(n) + H \rightarrow e + H_2^+ 
\]

\[
He^*(n) + He \rightarrow e + He^+ + He \\
He^*(n) + He \rightarrow e + He_2^+ 
\]

and inverse chemi-recombination processes

\[
e + H^+ + H \rightarrow H^*(n) + H \\
e + H_2^+ \rightarrow H^*(n) + H \\
e + He^+ + He \rightarrow He^*(n) + He \\
e + He_2^+ \rightarrow He^*(n) + He
\]

for some stellar atmospheres. Here \( H \) and \( He \) are the atoms in the ground states, \( H^*(n) \) and \( He^*(n) \) - the Rydberg atoms (in the states with the principal quantum number \( n \gg 1 \)), \( H_2^+ \) and \( He_2^+ \) - the molecular ions in the ground electronic states, and \( e \) - free electron.

In accordance with Mihajlov et al. (1996) and Mihajlov et al. (1997) it is assumed that:

- the processes (12) occur at the parts of the trajectories of the atom-projectile, \( H \) or \( He \), which lie deeply inside the orbit of the outer electron in the Rydberg atom, \( H^*(n) \) or \( He^*(n) \) and are caused by dipole part of the interaction of this electron with the ion-atom complex \( H + H^+ \) or \( He + He^+ \);

- the considered processes are treated as the result of the resonant conversion of the energy within the electron component of the collision atom-Rydberg atom system, what understands that the transition of the outer electron from the initial bound (Rydberg) state with given \( n \) to the final free state with some momentum \( k \) occurs simultaneously with the transition of ion-atom complex from the first excited electronic state to the ground electronic state;
- the processes can be described by means of the decay velocity of the initial electronic states which depends only from the internuclear distance.

From the results of Mihajlov et al. (1996) and Mihajlov et al. (1997) it follows that the processes (1-4) are significant for such hydrogen and helium plasmas with $\frac{Ne}{Nat} < 10^{-3}$, where $Ne$ and $Nat$ are the free electron and ground state atom density. This means that these processes could be significant for the stellar atmospheres which contain the corresponding weakly ionized layers. Here, this assumption is illustrated by the results related to one of M red star (in the hydrogen case) and to some of DB white dwarfs (in the helium case).

2.1. M red star

In Mihajlov et al. (2003) it is shown that the processes (1) and (3) in the region of $n$ from 4 to 8 influence to the populations of all hydrogen atom excited states with $n > 3$ what is illustrated by next figures 3 and 4 which show the behavior of the ratio of the excited states population calculated with and without these processes.

Then, in Mihajlov et al. (2003) is shown that the processes (1) and (3) in the whole region of $n > 1$ also influence to the free electron density what is illustrated by figure 5 which shows the behavior of free electron density calculated with these processes (solid curve) and without of them (dashed curve).

The presented results suggest that the processes (1) and (3), due to their influence on the excited state populations and the free electron density, also should influence on the atomic spectral line shapes. This assumption is confirmed by the figures 6 and 7 which show the profiles of some of hydrogen spectral lines calculated with and without these processes.

2.2. DB white dwarfs

The previous research show that in the helium case the situation should be similar to the hydrogen case. This assumption is based on the results obtained in Mihajlov et al. (2003), where the processes (2) and (4) were considered from the aspect of their efficiency in comparison with the other
As expected, the additional collisional term in statistical equilibrium brings the solution closer to local thermodynamical equilibrium (LTE). In terms of our population ratios, in the parts of atmosphere where populations, determined in our calculations using \( \mathbb{P}_{\text{cal}} \), are larger than LTE populations (departure coefficients 1), our parameter is larger than one. This means that in such a case, chemi-ionization processes depopulate excited states and dominate in comparison with chemi-recombination processes. The result is that populations determined with processes (1, 2) included are smaller in comparison with populations calculated without them and consequently is larger than one. In the reverse case (1), parameter is smaller than one, which means that in this case chemi-recombination processes dominate over chemi-ionization ones and increase the population of excited levels. As a result, in both cases, processes (1, 2) act as important factors closing the difference between the calculated and LTE populations.

Figure 3: The behavior of the population ratio \( \zeta \) for \( 3 \leq n \leq 9 \) as a function of the column mass.
As can be seen from Fig. 2, the behaviour of $\zeta$ for 6 ≤ $n$ ≤ 9 shows a tendency to converge to a pattern, which may differ up to 40% from unity. For higher levels (Figs. 3 and 4) the convergence to a pattern is complete and it can be understood by assuming that highly excited hydrogen level populations have quasi-Boltzman distributions different from distributions for partial LTE. It is not surprising that the population ratios for the levels up to 30 and the proton density show the same behaviour as levels with 15. One also has to remember that in the layers with temperatures lower than 4500 K the main electron contributors are metals so, as expected, there is very little change in electron density.

5. Conclusion

We have demonstrated the importance of the inclusion of chemi-ionization (1a,b) and chemi-recombination (2a,b) processes in modeling of atmospheres of late type stars.

Figure 4: The behavior of the population ratio $\zeta$ for 3 ≤ $n$ ≤ 9 as a function of the column mass.
Figure 5: Structure of model atmosphere - temperature $T_e$ and electron density $N_e$ vs. column mass.
Figure 6: Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for $H_\alpha$ line
Figure 7: Line profiles with (full) and without (dashed) inclusion of chemi-ionization and chemi-recombination processes for $H_\beta$ line
relevant ionization/recombination processes, for the $n$ from 3 to 10, in the atmospheres of some of DB white dwarfs. This results are illustrated by the figures 8 and 9 which shows the behavior of the ratios of the ionization/recombination fluxes caused by the processes (2) and (4) and the relevant electron-atom and electron-electron-ion processes.

1. The results presented in the helium case show that the processes (2) and (4) in the atmospheres of the considered DB white dwarfs should make the similar effects as the processes (1) and (3) in the considered M red dwarf atmosphere.

2. The processes (2) - (4) should be included in the models of stellar atmospheres from the beginning in a consistent way.
Figure 9: Parameter $F^{(ab)}_{ir}(n, T)$ as a function of the logarithm of Rosseland optical depth $\log(\tau)$, for principal quantum numbers $n = 3-10$, with $T_{\text{eff}} = 14000K$ and $\log(g) = 8$
3. Concerning one potential cause of anomalies in Rydberg atoms spectra

Recent spectroscopic measurements of white dwarfs IR spectra reveal a gap in the radiation emitted by Rydberg atoms (RA) having values of the principal quantum number $n \approx 10$ (Afanasiev et al., 2006). Among possible reasons of these anomalies a number of publications consider the following processes: (i) collision induced absorption (CIA), (ii) relativistic quantum effects of ”vacuum polarization” under the super strong magnetic fields $B \geq 10^{13}$G, (iii) Stark-effect under the electric fields with intensities $E \geq 10^6$V/cm.

The threshold of the electric field intensity for an auto ionization process is equal to $E \approx 3 \cdot 10^4$V/cm for RA with $n > 10$. This means that the lines in RA spectra emitted with $n \geq 10$-states should be blocked with a strong electric field. The RA lifetime $\tau_{CH}$ is formed mainly due to intensive chemi ionization collisions and appears to be $\leq 10^{-8}$s ($n \approx 10$) if the following realistic conditions are realized in white dwarfs atmospheric plasma: the concentration of ground state particles $N_0 \geq 3 \cdot 10^{17}$cm$^{-3}$, the electron concentration $N_e \geq 10^8$ cm$^{-3}$, RA concentration $N_R^* \geq 10^{13}$cm$^{-3}$, and the constant $k$ of the chemi ionization reaction (CHR) $k \approx 10^{-9}$cm$^3$s$^{-1}$.

$$RA + A \rightarrow A^+_2 + e$$  \hspace{1cm} (5)

The mentioned value of the collision lifetime $\tau_{CH}$ is seen to be by two orders of magnitude less than the RA’s reference radiation values $\tau_R$ occurring due to photon spontaneous emission. Note, moreover, that maximum $k(n)$ corresponds to $n \approx 10$ (see Klyucharev et al. (2007)), that should bring to ”selectivity” of the process (5) by $n$ when an external electric field is absent.

We’d like to pay attention to one more possibility of RA reallocation within excited states resulted from the Rydberg electron (RE) motion chaos-tization in a single $RA + A$ collision event. The nature of the so called stochastic dynamics arises due to nonlinear energy behavior of RE as a function of its principal quantum number $n$. In an external microwave field the most important contribution to the coupling between the atom and the field occurs in the vicinity of the atomic core where the optical electron has the maximum velocity. Even small energy changes result in strong motion period variations for RE. The latter leads to a comparatively rapid (in the scale of the period) dephasing within the electron and the microwave field oscillations
Figure 10: RE trajectories (upper Figs) and RE energy dynamics (lower Figs) in the hydrogen atom for free atom (a) and in the presence of a microwave field (b).
and to the RE dynamic randomization (Fig. 10). As it was shown in an accurate CHR treatment (Klyucharev et al. 2007) the processes (5) goes through the formation of the intermediate quasi molecular complex $(AA^+) + e$, (see Fig. 11), in which RE $e_{nl}$ becomes common for the nuclei. The two atomic ions $A^+$ exchange the inner valence electron $e_1$ and produce a variable dipole moment that oscillates at the exchange interaction frequency. The latter perturbs RE with an effective microwave electrical field and eventually manifests itself in the diffusion ionization (Fig. 12a).

The key point of our treatment related to astrophysical applications is the observation that an external statistic magnetic or electric field may strongly modify the futures of the dynamic chaos (see Fig. 12) if the atomic state \{n, l\} of RE satisfies the so called Föster or double Stark resonance. The latter is realized when the RE energy $E_{nl}$ appears to locate exactly between any two adjoining states belonging to $l' = l \pm 1$ series: $2E_{nl} \equiv E_{n'l'} + E_{n'+1'l'}$.

$$U_Z(r) = -\frac{z}{r} + \frac{a}{2r^2}$$  \hspace{1cm} (6)

Figs. 12 and 13 demonstrate the RE stochastic dynamics in the model

Figure 11: Formation of a microwave electric field in the quasi molecular complex due to the exchange of the inner valence electron.
Figure 12: (a) Random dynamics of RE energy E in the hydrogen atom due to coupling with an external microwave field resulting in the diffusion (chaotic) ionization ($E > 0$). (b) The same for the model Zommerfield atom under the realization of Föster (the double Stark) resonance. The details of the interatomic potential \[\text{(6)}\] are seen to dramatically modify the chaotic dynamics (absence of ionization).
Figure 13: Dependence of the diffusion lifetime ($\tau_{CH}$) $\sim N$ (the number of the RE orbital rounds) on the parameter $a$ of the model Zommerfeld atomic potential (6). The peaks correspond to occurring different Föster resonances. The value $a = 0$ corresponds to the hydrogen atom case.
Zommerfield potential \( U_Z \) (atomic units) which covers the hydrogen case \( (z = 1, \ a = 0) \). Zommerfield atom is known to well describe real alkali atoms and it provides a simple analysis (both analytical and numerical) of the Föster resonance situation. Importantly, in the vicinity of the Föster resonance the diffusion coefficients of the Fokker-Plank equation describing RE random walk within the energy levels (Fig[11]) appears to be very sensitive to details of the internuclear potential. One should expect, correspondingly, an irregular (anomaly) behavior of the diffusion auto ionization time \( \tau_{CH} \) for reaction \( (5) \) on the intensities of the external statistic fields. Since the auto ionization time \( \tau_{CH} \) determines the concentration of RAs in white dwarfs atmospheric plasmas, its anomalies should directly manifest themselves in the anomalies of RA spectra.

4. Conclusions

In this paper it was shown that the atoms and molecules in Rydberg’s states play an are important role in the astrophysics from at least two reasons:

• They are large and weakly bound, because the probable astrophysical targets for searching Rydberg atoms are the cold stars and cosmic objects including standard Big Bang chemistry, late M-dwarfs, brown dwarfs and white dwarfs. The basic effect producing by Rydberg atoms in atmospheres of these stars is significant flux deficits in Spitzer observations of these stars. In cool stars atom-Rydberg atom chemionization collision processes become very important. It was shown also that so-called regime of dynamic chaos should be considered as typical rather than exceptional situation in Rydberg atoms collisions.

• Much of their atomic structure and behavior in external fields can be understood on the basis of straightforward extension of hydrogenic theory. For example, it is interesting to consider the behavior of Rydberg atoms and molecules in the atmospheres of the white dwarfs with extremely strong magnetic fields. In such strong magnetic fields Rydberg atoms become anisotropic producing special features in the spectra of polarized radiation.

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