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Non-LTE line formation in the atmospheres of Ap stars: importance for pulsational analysis of roAp stars

T. Ryabchikova,[1,2] L. Mashonkina,[1] A. Ryabtsev,[3] R. Kildiyarova,[3] M. Khristoforova[4]

[1] Institute of Astronomy, Pyatnitskaya 48, 119017, Moscow, Russia
[2] Institute of Astronomy, University of Vienna, 1180 Vienna, Austria
[3] Institute of Spectroscopy, Troitsk, Moscow region, Russia
[4] Institut für Astronomie und Astrophysik der Universität München, München, Germany

Abundance analyses of cool Ap stars have revealed a huge ionization imbalance in Pr II – Pr III and Nd II – Nd III which may reach 2 dex in the atmospheres of rapidly oscillating (roAp) stars (Ryabchikova et al. 2001). In an LTE analysis of one of these stars, γ Equ, Ryabchikova et al. (2002) interpreted the observed imbalance as a stratified Pr and Nd distribution with an accumulation of the elements above $\log\tau_{5000} = -8$. In upper atmospheric layers departures from LTE are expected. Therefore non-local thermodynamical equilibrium (NLTE) line formation should be considered to obtain theoretical line profiles and equivalent widths for a range of effective temperatures and Pr-Nd overabundances typical for cool Ap stars. Also, for a correct analysis of bisector pulsational measurements across the core of the H_α line, NLTE formation of hydrogen lines has to be taken into account. NLTE formation of Nd II/Nd III lines was studied by Mashonkina et al. (2005). Here we present calculations of the statistical equilibrium of Pr II – Pr III in the atmospheres of A-type stars, and NLTE formation of the hydrogen lines.

The code DETAIL (K. Butler, private communication) based on the Accelerated Lambda Iteration method was used in Pr and Nd calculations and the NONLTE3 code (Sakhibullin 1983) was used for the hydrogen lines. The final model atoms include:

- 19 levels of H I,
- 203 Pr II combined levels + 54 Pr III combined levels + the Pr IV ground state,
- 247 Nd II combined levels + 68 Nd III combined levels + the Nd IV ground state.

In this study, we calculated energy levels and transition probabilities for Pr II – III and Nd II – III. For other atoms/ions, the data were extracted from the NIST (Martin et al. 1978) and VALD (Kupka et al. 1999) databases. We used photoionization cross-sections for hydrogen. For the REE elements, electron collision cross-sections were calculated for allowed transitions following van Regemorter (1962). For hydrogen, the recent electron-impact excitation data of Przybilla & Butler (2004) were used for transitions between energy levels with $n \leq 7$ and the approximation formula of Johnson (1972) for the remainder. Electron-impact ionization rates were calculated applying the Seaton formula as described by Mihalas (1978). In the atmospheres with Teff between 7250 K and 7700 K H I is still the dominant ionization stage and at each depth point the ground state keeps its thermodynamical level population. However, excited levels are subject to non-thermal excitation effects such that the second level is underpopulated and the third one is overpopulated relative to the corresponding LTE number densities in the layer between $\log\tau_{5000} = -1$ and -3. In the upper layers, up to $\log\tau_{5000} = -4.5$, the second level shows an opposite effect and its departure coefficient, $b_2 > 1$, decreases outwards, while b_3 reaches its maximum value around $\log\tau_{5000} = -3$. This behaviour explains the weakening of the core-to-wing transition in the NLTE Hα profile compared to the LTE one.

Our calculations for chemically homogeneous Ap atmospheres with +3 dex Pr overabundance show that the NLTE corrections for Pr II lines grow rapidly with the effective temperature, but they stay nearly constant for Pr III lines. NLTE effects in chemically homogeneous atmospheres may explain no more than 0.6 dex in the 1 – 2 dex ionization imbalance (REE anomaly), observed in cool roAp stars.

Because a statistical equilibrium of Pr II and Nd II depends strongly on radiative b-f transitions, the test NLTE calculations have been made for the stratified abundance distribution with multiplying the photoionization cross-sections for hydrogen by scaling factors of 100 and 0.01. An increase of the photoionization cross-sections for hydrogen does not, in fact, affect NLTE line formation, while a decrease of the cross-sections leads to a reduction of the NLTE effects. A step distribution of Pr and Nd with a steep 4 dex increase of the abundance of both elements towards the upper layers starting at $\log \tau_{5000} \approx -3.5$ in the atmosphere of roAp star HD 24712 allows to explain the observed REE abundance anomalies.

In the first approximation an influence of the star's ~ 3 kG magnetic field was accounted for by using a pseudo-microturbulence of $1\,\mathrm{km\,s^{-1}}$. We checked a change in line depth formation caused by Zeeman splitting. The line profile of Pr III 5300 calculated with the magnetic spectral synthesis code SYNTHMAG (Piskunov 1999) was approximated by a sum of triplet Zeeman components. Magnetic desaturation results in a shift of the line depth formation by 0.6 dex (in $\log \tau_{5000}$ scale) towards the deeper atmospheric layers. Taking into account both the photoionization cross-section uncertainty and magnetic effects we conclude that the error in the position of the Pr and Nd abundance jumps may be as large as $\pm 0.5 - 0.6$ dex.

NLTE depth formation of the H_α core, Pr and Nd lines was used to explain the observed pulsational radial velocity (RV) amplitudes and phases in the atmosphere of HD 24712 (see Fig. 1 by Kochukhov 2007). Tracing the region between H_α core formation and the upper atmosphere, pulsational phase values of different elements gradually increase. A step in pulsational phase between the H_α core and Pr lines may be caused by limitations of our modelling, e.g. the model fit to the H_α core is still unsatisfactory and vertical Pr and Nd distributions can only be schematically determined. However, we can reconstruct and explain pulsational phenomena in atmospheres of roAp stars only by detailed studies of spectral line formation.

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