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IMPROVEMENT OF ATOMIC MODELS FOR NLTE RADIATIVE TRANSFER IN ATMOSPHERES OF LATE TYPE STARS

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Abstract. We present our first results on NLTE line transfer for Mg I, Ca I and Ca II in atmospheres of late type stars. This work prepares for the analysis of future spectroscopic data of the Gaia mission. To do this, we have updated atomic models of magnesium and calcium. This work on NLTE effects will also be applied to correct the determination of LTE chemical abundances for late type stars.

Keywords: radiative transfer, stars: abundances, stars: atmospheres, stars: late type

1 Introduction

The determination of stellar chemical abundances is an important clue to understand chemical evolution of galaxies. The classical line formation synthesis is based on a strong assumption: the Local Thermodynamic Equilibrium (LTE) which means that Boltzmann and Saha laws are verified everywhere in the line forming region. This assumption leads to consider independently all the lines of the same element as two level atom models. But several radiative mechanisms can affect a level population using all the other excited levels or other ionization stages making the two level atom model poorly realistic. To improve accuracy in the abundance analyses, we relax the assumption of LTE and build atoms taking into account as many energy levels as possible with all available radiative and collisional transitions between them: this is the Non LTE (NLTE) approach.

In this work, we focus on α elements, starting with magnesium and calcium, because they are good tracers of stellar populations in galaxies, with several optical and Infra-Red (IR) lines. Moreover, these elements are crucial for the Gaia spatial mission (Katz et al. 2004). A medium resolution spectrograph RVS (Radial Velocity Spectrometer) will observe in the region of the Ca II IR triplet lines with few iron, silicon and magnesium lines, doing hundreds of million of spectra to analyze. Therefore, it will be necessary to have a grid of synthetic spectra and NLTE corrections for realistic abundance determination.

In the first part, we present the atom modelling, then we test the validity of these model atoms on solar line profiles and finally we present the NLTE computations for a grid of stellar parameters using the NLTE 1D radiative transfer code MULTI (Carlsson 1986) and the MARCS model atmospheres (Gustafsson et al. 2008).

2 Atom modelling

In order to model an atom, one has to collect:
– the excited levels with their energies, statistical weights and electronic configurations;
– the ionization cross sections of these levels caused by the radiative field and by the collisions;
– the oscillator strengths and spectral broadening parameters of the radiative transitions;
– the cross-sections (when available, otherwise semi-empirical formulae) for the collisional transitions.

We have developed a code that compiles data from atomic databases like NIST[*], TopBase[†], VALD[‡], Kurucz[§], from literature for electronic collisional cross-sections (Burgess et al. 1995; Samson & Berrington 2001), Van

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[*]available at: `http://physics.nist.gov/asd3`
[†]available at: `http://cdsweb.u-strasbg.fr/topbase/topbase.html`
[‡]available at: `http://vald.astro.univie.ac.at/$\sim$vald/php/vald.php`
[§]available at: `http://www.cfa.harvard.edu/amp/ampdata/kurucz23/sekur.html`

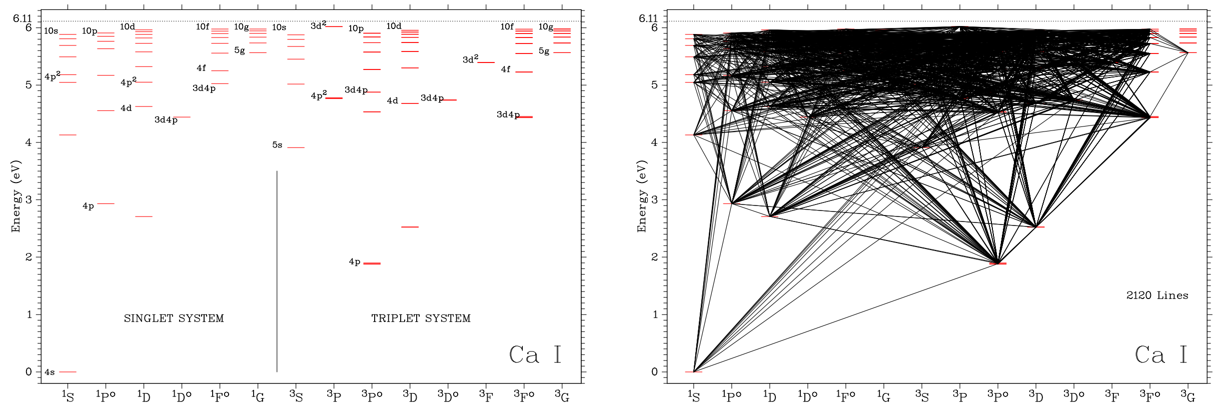

Fig. 1. Grotrian diagram of Ca I. Neutral calcium is a two-electron atom which implies two multiplicity systems: a singlet system and a triplet system where each level contains three fine levels except for ^{3}S terms. Left panel: energy levels; fine structure is presented but not visible at this scale. Right panel: radiative transitions; all transitions between fine levels considered are identified from VALD.

der Waals broadening parameter (Anstee & O'Mara 1995; Barklem & O'Mara 1997, 1998) and semi-empirical formulae for electronic collisional transitions (Van Regemorter 1962; Seaton 1962). In this work, we have neglected the contribution of inelastic collisions with neutral hydrogen (because there is a lack of accurate quantum mechanical calculations to determine their importance) and the Stark effect in the line broadening parameters. Some of the best complete atoms for Mg I and Ca I/II were constructed respectively by Przybilla et al. (2001) and by Mashonkina et al. (2007) but without taking the fine structure into account. We have included it for all levels until $n = 10$ and $l = 4$ for Mg I, Ca I and Ca II. An example of a Grotrian diagram for Ca I is presented in Fig. 1.

We have tested model atoms on solar lines, using theoretical LTE 1D MARCS solar atmosphere, chemical mixture from Grevesse et al. (2007) and opacities from the Uppsala package (Gustafsson 1973). The code MULTI2.2 (Carlsson 1986), slightly modified for the collisional transition part, solves the radiative transfer and statistical equilibrium equations consistently and computes line intensities, equivalent widths and contribution functions for all the radiative transitions. We are able to reproduce the main solar lines for Mg I, Ca I and Ca II in a good agreement with the LTE computations and solar atlas¶ from Brault & Neckel (1987), except for the Mg I optical triplet (5167, 5172, 5183 Å) and the line cores of Ca II IR triplet because they are formed in atmospheric layers not included in the theoretical MARCS models (see Merle et al., in prep., for more details).

3 NLTE equivalent width corrections for a grid of stellar parameters

We have selected stellar parameters for late type stars with an effective temperature range of $[5000, 7000]$ K with a 500 K step, a logarithm of surface gravity of 3, 4 and 4.5 and a range of metallicity of $[-3, 0]$ with 1 dex step. Plane parallel model atmospheres with standard composition from the MARCS site‖ (Gustafsson et al. 2008) have been adopted. We have computed LTE equivalent widths W^* and NLTE equivalent widths W for all lines of Mg I, Ca I and Ca II model atoms. Fig. 2 and Fig. 3 show variations of the W/W^* ratio for the Mg I 8736 Å and the Ca II 8542 Å lines with stellar parameters. We have chosen these lines because they are in RVS wavelength range.

For stars with solar abundance [Fe/H] $= 0$, we can see a negligible deviation from LTE whatever the effective temperature and surface gravity for Ca II 8542 Å line. Concerning the Mg I 8736 Å line, we find a deviation from LTE of about +20%. As shown in the other panels of Fig. 2 and Fig. 3 and for late type stars with [Fe/H]< -1, the general trend is that the LTE deviation increases with the decreasing metallicities for both lines but not in the same way; this implies a negative correction for the magnesium LTE abundance deduced from the 8736 Å line and a positive correction for the calcium LTE abundance deduced from the 8542 Å line. At metallicity of

¶available at: ftp://ftp.hs.uni-hamburg.de/pub/outgoing/FTS-Atlas

‖available at: `http://marcs.astro.uu.se`

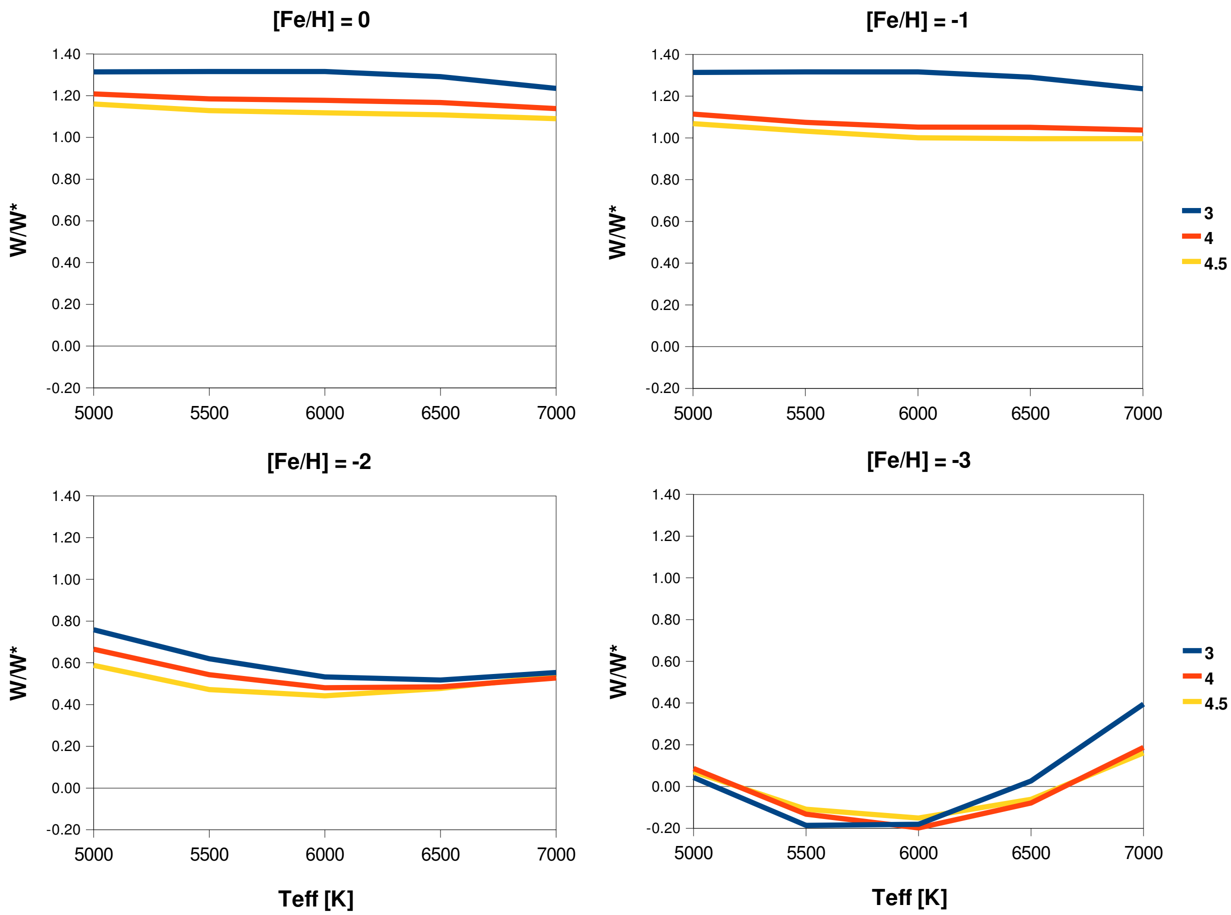

Fig. 2. W/W^* ratio vs effective temperature $T_{\rm eff}$ for Mg I 8736 Å. W stands for the NLTE theoretical equivalent width whereas W^* is the LTE theoretical one. Each of the four panels corresponds to a global metallicity [Fe/H] as indicated. The W/W^* are plotted for surface gravities: $\log g = 3$ (blue), $\log g = 4$ (red) and $\log g = 4.5$ (yellow).

[Fe/H] $= -3$, the W/W^* ratio of Mg I 8736 Å line has negative values corresponding to an emission line but it may not be observable since the line is very weak. The W/W^* corrections for more lines in optical and RVS domains will be available in Merle et al. (in prep).

4 Conclusions

We have performed a realistic atom modelling for Mg I, Ca I and Ca II with more energy levels, more transitions than we can be found in the literature, taking into account fine structure of energy levels, and the best physics available concerning photo-ionization, electronic collisions and hydrogen elastic collisions. Then, we computed a grid of NLTE equivalent width corrections for late type stars that will be useful to study galactic abundances and its evolution. We confirm that NLTE effects are important for metal poor stars, but need to be studied line by line for a quantitative prediction of the error on the LTE abundance determinations.

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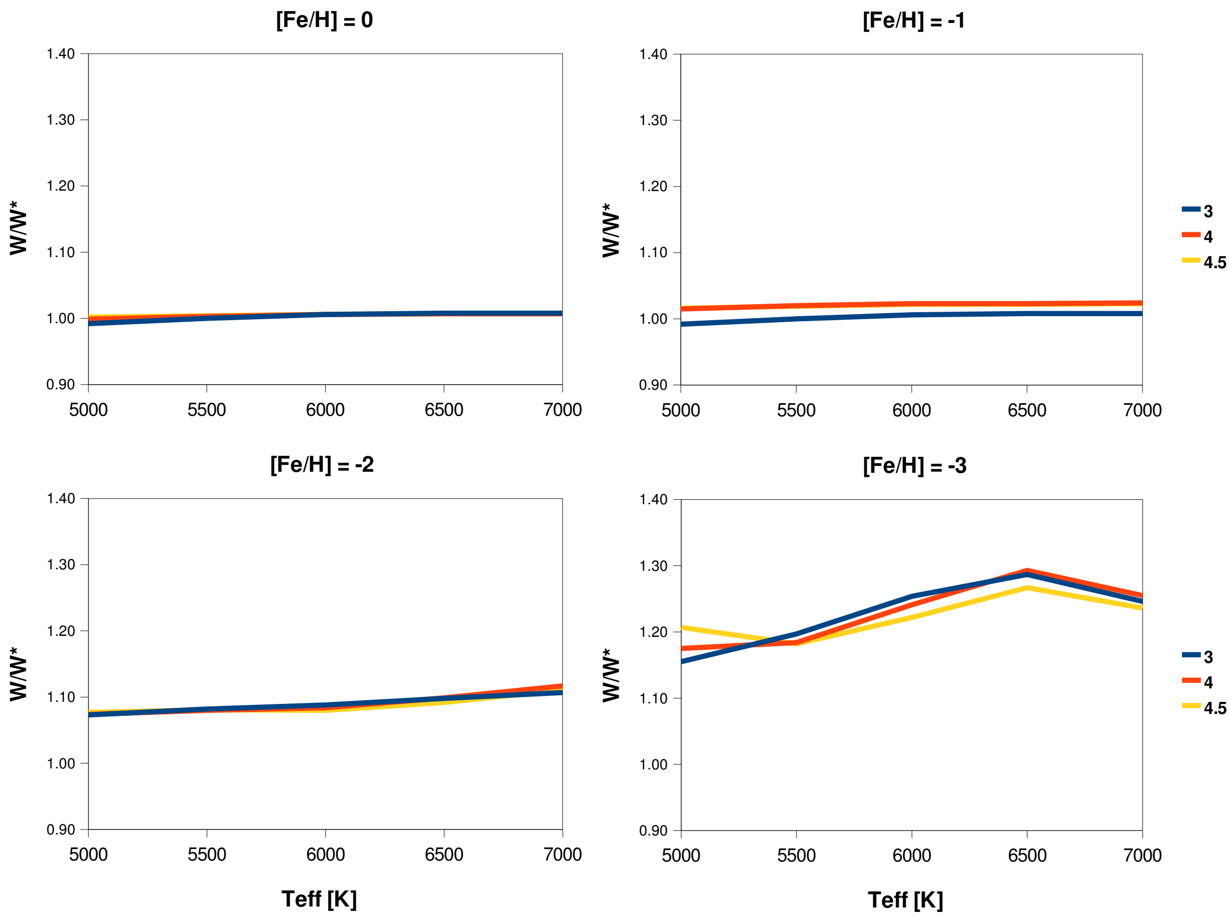

Fig. 3. W/W^* ratio vs effective temperature $T_{\rm eff}$ for Ca II 8542 Å. W stands for the NLTE theoretical equivalent width whereas W^* is the LTE theoretical one. Each of the four panels corresponds to a global metallicity [Fe/H] as indicated. The W/W^* are plotted for surface gravities: $\log g = 3$ (blue), $\log g = 4$ (red) and $\log g = 4.5$ (yellow).

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