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IMPACT OF NEW ATOMIC DATA FOR THE FORMATION OF THE MG I 4571 Å LINE IN BENCHMARK STARS

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Abstract.
The Non-Local Thermodynamic Equilibrium (NLTE) formation of magnesium lines in cool stars can be improved by the inclusion of very recent quantum mechanical treatment of inelastic collisions with electrons and hydrogen atoms. We present the study of the intercombination line at 4571 Å in the atmosphere of four benchmark late-type stars: the Sun, Arcturus, HD 84937 (metal-poor dwarf) and HD 122563 (metal-poor giant). This preliminary study relies on a simplified model atom of Mg I with a consistent set atomic data rather than a complete model atom. In this context, results show that even if the 4571 Å line is formed close to LTE in the Sun, its line source function can be larger than the Planck function, especially in metal-poor giant for which we expect to have positive abundance corrections.

Keywords: Non-LTE, line formation, benchmark stars, magnesium, intercombination line

1 Introduction

The magnesium is one of the best α-element to understand the history of the chemical enrichment of our Galaxy and dwarf galaxies in the Local Group (Gehren et al. 2006; Andrievsky et al. 2010). But the departures from LTE suffer the lack of reliable data for the inelastic collisions with neutral hydrogen which could be non-negligible in atmosphere of cool stars (Mashonkina 1996; Barklem et al. 2011). Until recently, the inelastic collisions with H atoms in late-type stars have been neglected or treated with the Drawin's formula (Drawin 1969). This recipe, based on the corresponding oscillator strength of the radiative transition, is scaled by a fudge factor S_{H} to vary the intensity of the H collision rates (see e.g., for magnesium, Shimanskaya et al. 2000; Gehren et al. 2004; Mashonkina 2013).

With the computations of the accurate potentials for the MgH system (Guitou et al. 2010, 2011), the quantum cross-sections in Mg + H collisions (Belyaev et al. 2012) and their collisions rates (Barklem et al. 2012), it is now possible to explore the role of such inelastic collisions with hydrogen for Mg I in late-type stars. In this proceeding, we focus on the formation of the spin-forbidden intercombination line at 4571 Å which rises from the ground stage of Mg I. We performed calculations for benchmark stars for which high resolution and high signal-to-noise ratio are available for comparison. However, no NLTE abundance corrections are attempted here, since a more complete model atom is required to reach good accuracy on population densities.

2 A simplified model atom of Mg I

To assess the impact of the new atomic data on the NLTE abundance corrections, we decided to build a simplified model atom including only energy levels for which we have quantum mechanical data for collision with hydrogen. The model includes the first seven low-lying plus the continuum levels. The oscillator strengths are from the VALD database excepted for the Mg I triplet for which we used data from Aldenius et al. (2007),

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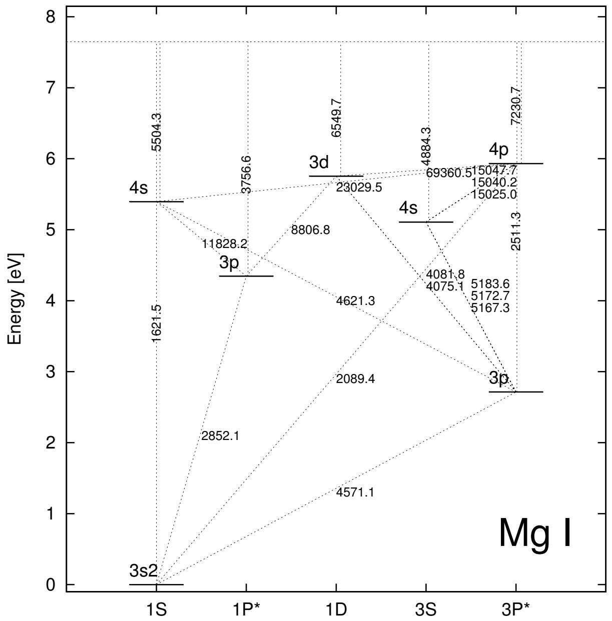

Fig. 1. Grotrian diagram of the Mg I model atom used in this work. Radiative bound-bound and bound-free at the threshold transitions are labeled in Å.

the 8806 and 11828 Å lines for which we use NIST data with an excellent accuracy. The oscillator strength of the 4571 Å is $\log gf = -5.69$. Photoionizations are from the TOPBASE with a treatment following Merle et al. (2011). The Grotrian diagram of the simplified model atom of Mg I is shown in Fig. 1.

For the treatment of inelastic collisions we compute from published rates or cross-sections the effective collision strength Υ as a function of the local temperature T for bound-bound transitions (i lower level $\rightarrow j$ upper level) with electrons (e) and with hydrogen atoms (H). The collisions rates can be then computed as follows:

$$C^{\mathrm{e}}_{ij}(T) = 8.629 \times 10^{-6}\ n_{\mathrm{e}}\ \frac{\Upsilon^{\mathrm{e}}_{ij}(T)}{g_i\sqrt{T}}\mathrm{e}^{-E_{ij}/kT} \quad [\mathrm{s}^{-1}] \tag{2.1}$$

$$C^{\mathrm{H}}_{ij}(T) = 2.014 \times 10^{-7}\ n_{\mathrm{H}}\ \frac{\Upsilon^{\mathrm{H}}_{ij}(T)}{g_i\sqrt{T}}\ \mathrm{e}^{-E_{ij}/kT} \quad [\mathrm{s}^{-1}] \tag{2.2}$$

where n_{e} and n_{H} are the number density of electrons and hydrogen atoms respectively, g_i the statistical weight of the lower level, k the Boltzmann constant and E_{ij} the energy of the transition. $\Upsilon^{\mathrm{e}}_{ij}$ and $\Upsilon^{\mathrm{H}}_{ij}$ are dimensionless quantities symmetric with respect to the transition $i \iff j$ ($\Upsilon_{ij} = \Upsilon_{ji}$).

The effective collision strengths with electrons $\Upsilon^{\mathrm{e}}_{ij}$ we used are based on quantum mechanical (QM) cross-sections of Zatsarinny et al. (2009) for resonance transitions and on unpublished data of the same author for the remaining transitions. The QM approach is based on the R-matrix close coupling method. From the collision cross-sections σ^{e}_{ij} (expressed in units of πa_0^2, with a_0 the Bohr radius) we calculate:

$$\Upsilon^{\mathrm{e}}_{ij}(T) = g_i \frac{kT}{E^{\infty}_{\mathrm{H}}} \int_0^{\infty} \sigma^{\mathrm{e}}_{ij}(x)(x + x_{ij})\mathrm{e}^{-x}\mathrm{d}x \tag{2.3}$$

where g_i is the statistical weight of the lower level implied in the collision, E^{∞}_{H} the Rydberg energy and $x_{ij} = E_{ij}/kT$. Bound-free collisions with electrons are treated using the traditional semi-classical (SC) approach of Seaton (1962b).

The effective collision strengths with hydrogen atoms we used are based on either the SC approach of Drawin (1969), using the formulation of Lambert (1993) to deduce:

$$\Upsilon^{\mathrm{H}}_{ij}(T) = 4\sqrt{2}\ \frac{m_{\mathrm{e}}(m_{\mathrm{H}} + m_{\mathrm{Mg}})}{m^2_{\mathrm{H}}}\ g_i f_{ij}\ \frac{E^{\infty}_{\mathrm{H}}}{E_{ij}}\ \frac{1 + 2/x_{ij}}{x_{ij}} \tag{2.4}$$

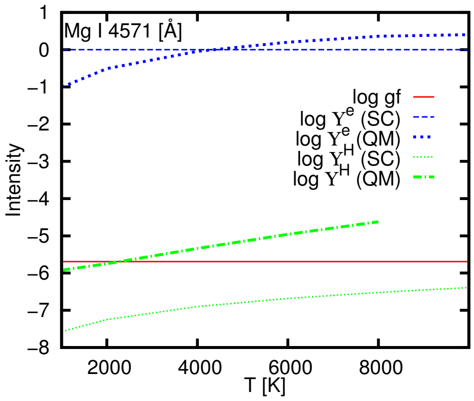

Fig. 2. Comparison of oscillator/collision strengths for the 4571 Å line. Semi-classical (SC) formulae are used for effective collision strengths with electrons $\Upsilon^{\rm e}_{ij}$ from Seaton (1962a) and with neutral hydrogen $\Upsilon^{\rm H}_{ij}$ from Drawin (1969). Quantum mechanical (QM) cross-sections are used for effective collision strengths with electrons $\Upsilon^{\rm e}_{ij}$ from Zatsarinny et al. (2009) (and private communication) and with neutral hydrogen $\Upsilon^{\rm H}_{ij}$ from Barklem et al. (2012).

or on the QM approach of Guitou et al. (2011); Belyaev et al. (2012); Barklem et al. (2012) to deduce:

$$\Upsilon^{\rm H}_{ij}(T) = 4.965 \times 10^6 g_j \sqrt{T}\ \langle \sigma_{ji} v \rangle \tag{2.5}$$

where $\langle \sigma_{ji} v \rangle$ is the downward rate coefficient, in units of cm^3 s^{-1}, computed for the transitions between the seven lowest states of Mg I by Barklem et al. (2012).

An important mechanism to account for is the charge exchange process Mg I+ H $\Longleftrightarrow$ Mg II+ H$^-$ for which we can also define an effective collision strength $\Upsilon^{\rm H}_{\rm ce}$:

$$\Upsilon^{\rm H}_{\rm ce}(T) = 2.483 \times 10^6 g_c \sqrt{T} \langle \sigma_{ci} v \rangle \tag{2.6}$$

where g_c is the statistical weight of the ionic state and $\langle \sigma_{ci} v \rangle$ is tabulated in Barklem et al. (2012).

We compare the SC and QM effective collision strengths with electrons and hydrogen atoms for the 4571 Å line in Fig. 2. The oscillator strength (red line) does not depend on the temperature and its value is very small compared with values for allowed transitions. Effective collision strength with electrons (in blue) using SC approach (here default value set to one for an intercombination line) is of the same order of magnitude as in the QM approach excepted at very low temperature for which the difference can reach one order of magnitude. The difference in effective collision strength with hydrogen (in green) between SC and QM approaches reaches two orders of magnitude at high temperature.

3 Theoretical results for the 4571 Å line

We used the 1D NLTE radiative transfer code MULTI (Carlsson 1986) version 2.2, modified to read and compute properly collision rates from effective collision strengths with electrons and hydrogen atoms. Line blanketing effect is taken into account through the inclusion of background atomic lines of other main species. Statistical equilibrium are computed using model atmospheres from MARCS database (Gustafsson et al. 2008) for the Sun, a metal-poor dwarf HD 84937 (model: $6250/4.0/-2.00/+0.40$), Arcturus (model: $4250/1.5/-0.50/+0.20$) and a metal-poor giant HD 122563 (model: $4500/1.5/-2.50/+0.40$). Excepted for the Sun, the atmospheric parameters are rough estimates that have to be refined for detailed comparisons with observations which is under the scope of this study.

Computations of statistical equilibrium are done with QM approach for collisions with electrons and with (i) no H collisions, (ii) SC H collisions (Drawin's formula with a scaling factor $S_{\rm H} = 1$) or (iii) QM H collisions (including charge exchange process). The departure coefficients are defined by: $b_i = n_i/n_i^*$ where n_i^* is the number density of level i at LTE. The computed statistical equilibrium for the 4 benchmark stars show a general depopulation of the levels due to the overionization of Mg I by UV radiation of non-local origin (trend well known for neutral minority species in atmosphere of late-type stars). Computations including H collisions reduce departures from LTE. The departures from LTE are more reduced if the QM H collisions are used.

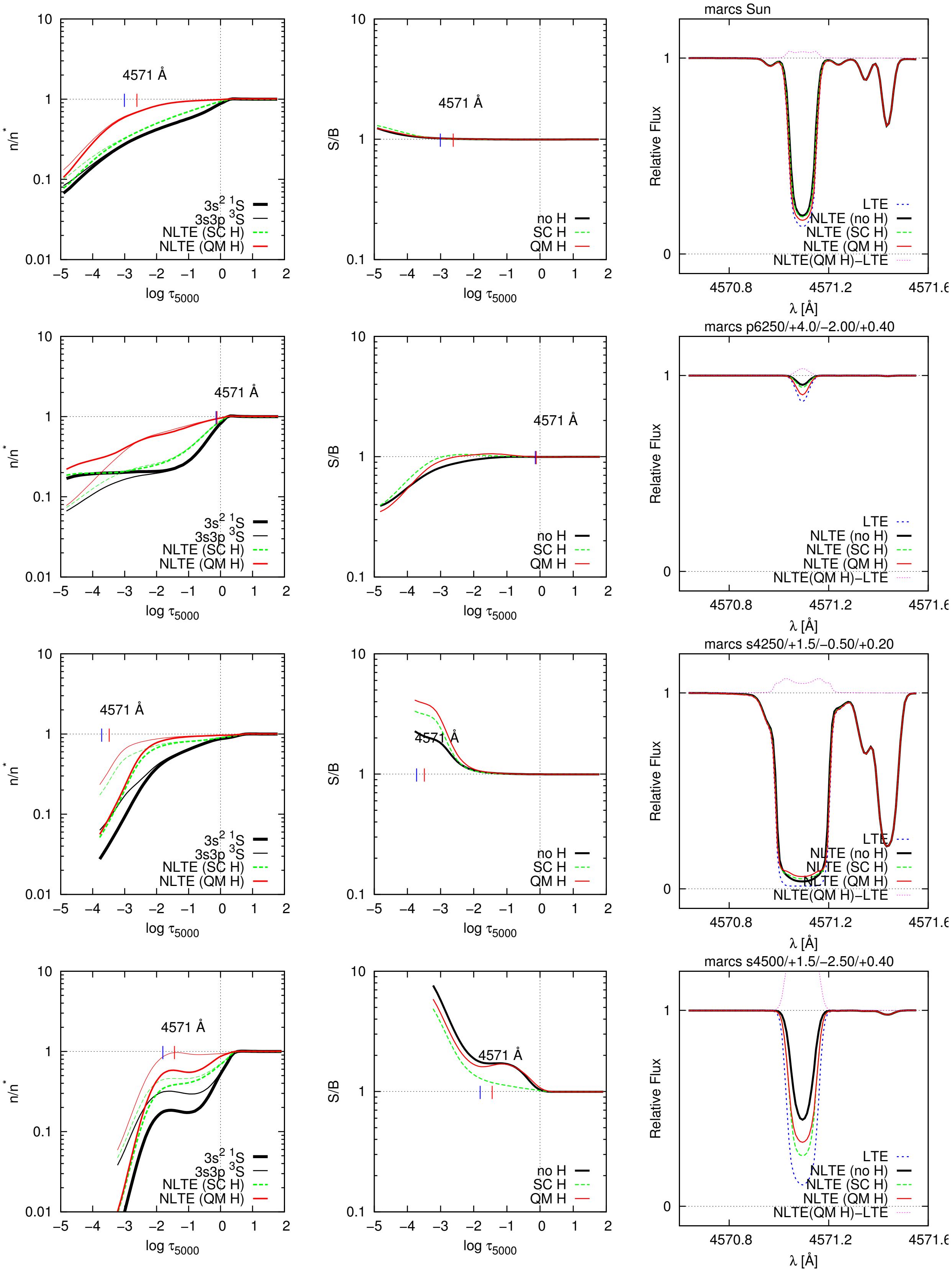

Fig. 3. Formation of the Mg I 4571 Å line in model atmospheres of benchmark stars (atmospheric parameters given at the top of right panels with $T_{\rm eff}/\log g$/[Fe/H]/[α/Fe]). Black profiles are NLTE results with no H collisions; green profiles with Semi-Classic (SC) H collisions and red profiles with quantum mechanical (QM) H collisions. Blue profiles are LTE results. Vertical dashes show the optical depths where the line cores are formed in LTE (blue) and in NLTE (red). **Left:** departure coefficients of the implied levels. **Middle:** line source functions. **Right:** line profiles.

This is contrary to what is expected since it was claimed that Drawin formula gives an upper limit toward the thermalization of the departure coefficients. At solar and subsolar metallicities (in the Sun and Arcturus) the line forms in the upper part of the atmosphere whereas in metal-poor stars the line forms deeper due to a lower abundance value.

In the dwarf stars (two upper series of panels in Fig. 3), upper and lower departure coefficients follow the same trend leading to a source function equals to the Planck function at the line core formation depth. Thus the divergence of the NLTE and LTE profiles is entirely due to the NLTE effect on the line opacity. The reduction of the line opacity induced a weaker line in NLTE. As the depopulation is the lower when using QM H collisions, then the corresponding profile is the closest to the LTE profile.

In the giants (two lower series of panels in Fig. 3), the line formation follow a different process since the upper and lower departure coefficients diverge at the line core formation depth. This will influence the line source functions as shown in middle panels of Fig. 3, normalized to the Planck function. In the Wien regime, $S_{ij}/B_{ij} = b_j/b_i$. The line source function is larger than the Planck function at the line core formation depth leading to weaken the line. NLTE effects on line opacity and source function act in the same way to reduce the line profile. For this line in giants, SC H collisions will give lower abundance correction than QM H ones. And specifically for Arcturus, taking no H collisions into account will provide the lower abundance correction since the divergence between upper and lower departure coefficient is the smallest in this case. In the metal-poor giant, the source function is lower when using SC H collisions leading to a profile closer to the LTE one. Whatever SC or QM H collision, we expect to have strong positive NLTE abundance correction (> 0.1 dex) in metal-poor giants for this line.

4 Conclusion

We have studied the NLTE line formation of the intercombination line at 4571 Å of neutral magnesium in four benchmark stars with the use of semi-classic or quantum mechanical treatment of inelastic collisions with hydrogen atoms. The formation of this spin-forbidden line is known to be controlled by collisions (at least in the Sun) giving a line source function very close to LTE. This is no longer the case in giants stars where departures from LTE also affect the line source function especially in metal-poor giants for which we expect to have strong positive abundance correction (probably larger than $+0.1$ dex).

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