Title : will be set by the publisher
Editors : will be set by the publisher
EAS Publications Series, Vol. ?, 2013

IMPACT OF NEW ATOMIC DATA FOR THE FORMATION OF THE MG I B TRIPLET LINES IN BENCHMARK STARS

Merle, T.[1], Thévenin, F.[2], Belyaev, A. K.[3,4], Guitou, M.[5], Feautrier, N.[6], Spielfiedel, A.[6] and Zatsarinny, O.[7]

Abstract. We aim to improve the calculation of the Mg I line profiles in benchmark stars and to assess the impact of the new quantum mechanical calculations of inelastic collisions with hydrogen. The method is based on the non-Local Thermodynamic Equilibrium (NLTE) line formation using updated atomic data for a simple model atom of Mg I. Focus on the formation of the Mg I b triplet lines at 5167, 5172 and 5183 Å is presented for the Sun, Arcturus, HD 84937 (metal-poor dwarf) and HD 122563 (metal-poor giant). This study is preliminary and essentially tests the new atomic data. In this context, we show that NLTE effects are smaller for this triplet when quantum mechanical H collisions are included compared with the use of the semi-classical Drawin's formula.

1 Introduction

Magnesium is an α-element whose abundance values are important for understanding the chemical evolution of our Galaxy (Gehren et al. 2006, Andrievsky et al. 2010). The magnesium is essentially first ionized in the atmospheres of late-type stars where the local temperature is larger than 3500 K. Then, the Non-Local Thermodynamic Equilibrium (NLTE) effects from the minority species Mg I, can potentially affect the Saha-Boltzmann equilibria, leading to abundance corrections from LTE. It is then necessary to investigate the formation

[1] IAA, Université Libre de Bruxelles, CP 226, Bvd du Triomphe, 1050 Brussels, Belgium
[2] Lagrange, UMR7293, Université de Nice Sophia-Antipolis, CNRS, OCA, 06300 Nice, France
[3] Department of Theoretical Physics, Herzen University, St. Petersburg 191186, Russia
[4] Department of Physics & Astronomy, Uppsala University, Box 515, 75120 Uppsala, Sweden
[5] Université Paris-Est Marne-la-Vallée, MSME, UMR 8208 CNRS, 77454, France
[6] LERMA, Observatoire de Paris, 92195 Meudon Cedex, France
[7] Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA

DOI: (will be inserted later)

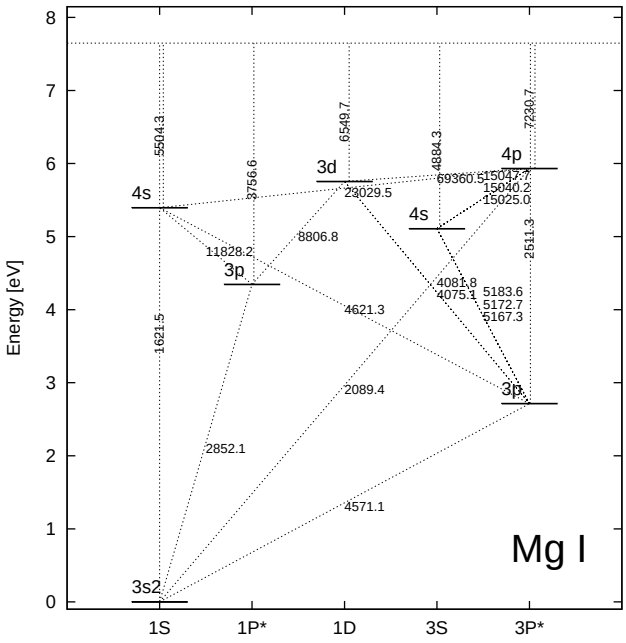

Fig. 1. Grotrian diagram of the Mg I model atom used in this work. Radiative bound-bound and bound-free at the threshold transitions are labeled in Å.

of the lines of this element to predict for which lines and in which atmospheres NLTE abundance corrections are negligible or not. Moreover, recent detail quantum calculations are available for this element concerning inelastic collisions with electrons (Zatsarinny 2009) and hydrogen (Barklem et al. 2012). In this proceeding, we focus on the formation of the optical green triplet at 5167, 5172 and 5183 Å which is visible in all range of metallicity. 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 Atomic data

The choice of consistency in atomic data are made here. We build a simplified model atom including only energy levels for which we have quantum mechanical data for collisions 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, the 8806 and 11828 Å lines for which we use NIST data with an excellent accuracy.

Photoionizations are from the TOPBASE. The Grotrian diagram of the simplified model atom of Mg I is shown in Fig. 1.

Bound-bound collisions with electrons are treated using the quantum mechanical (QM) approach based on the R-matrix close coupling method (Zatsarinny 2009). From the collision cross-sections $\sigma_{ij}^{\rm e}$ (expressed in units of πa_0^2, with a_0 the Bohr radius) we calculated the (dimensionless) effective collision strength as a function of the temperature T:

$$\Upsilon_{ij}^{\rm e}(T) = g_i \frac{kT}{E_{\rm H}^{\infty}} \int_0^{\infty} \sigma_{ij}^{\rm e}(x)(x + x_{ij}){\rm e}^{-x}{\rm d}x \tag{2.1}$$

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

Collisions with neutral hydrogen are treated in two ways. First, using the Drawin's formula (Drawin 1969) which is a SC approach based on the corresponding oscillator strength value of the radiative transition. Second, using the new QM calculations from Barklem et al. 2012. They published collision rates per unit of hydrogen density number $\langle \sigma_{ji} v \rangle$ for 28 transitions between the seven low-lying + ionic levels. These included the charge exchange process (ion-pair production and mutual neutralization). From these values, we computed the corresponding effective collision strengths for bound-bound collisions:

$$\Upsilon_{ij}^{\rm H}(T) = 4.965 \times 10^6 g_j \sqrt{T}\ \langle \sigma_{ji} v \rangle \tag{2.2}$$

and for charge exchange process (ce):

$$\Upsilon_{\rm ce}^{\rm H}(T) = 2.483 \times 10^6 g_c \sqrt{T} \langle \sigma_{ci} v \rangle \tag{2.3}$$

where g_j and g_c are the statistical weights for the upper and for the ionic levels respectively, $\langle \sigma_{ji} v \rangle$ and $\langle \sigma_{ci} v \rangle$ are tabulated in Barklem et al. 2012.

As an illustrative example, we show in Fig. 2 comparison of atomic data for the b multiplet. The oscillator strength (red line) does not depend on the temperature and it is close to unity. Effective collision strength with electrons (in blue) using SC approach (from Impact Parameter Method, Seaton 1962a) is around three order of magnitudes larger than the QM approach. The difference in effective collision strength with hydrogen (in green) between SC and QM approaches reach one order of magnitude at low temperature. It has to be mentioned that a little difference in $\Upsilon_{ij}^{\rm H}$ could have a larger impact on the statistical equilibrium than a large difference in $\Upsilon_{ij}^{\rm e}$ since the rates are proportional to Υ times the number density which is higher for hydrogen, especially in metal-poor stars.

3 Theoretical results

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

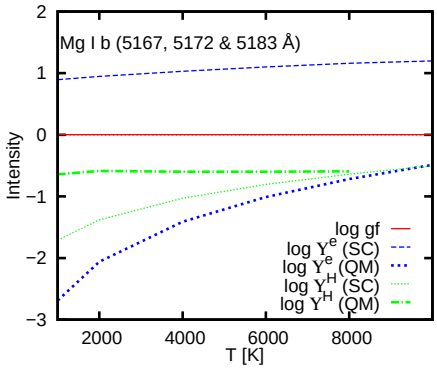

Fig. 2. Comparison of oscillator/collision strengths for the b triplet. Semi classical (SC) formulae are used for effective collision strengths with electrons $\Upsilon^{\rm e}_{ij}$ from Seaton 1962a and with neutral hydrogen $\Upsilon^{\rm H}_{ij}$ from Drawin 1969. Quantum mechanical (QM) cross-sections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

strengths with electrons and hydrogen atoms. 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: $4500/1.5/-2.50/+0.40$).

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 at unity) 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 departure from LTE are more reduced if the QM H collisions are used. This is contrary to what is expected since it was claimed that Drawin formula give an upper limit toward the thermalization of the departure coefficients. Indeed, only 11 bound-bound transitions with oscillator strengths contribute to the H collision rates in the SC approach whereas all the bound-bound transitions (21) in the QM approach contribute to the rates. Moreover, the QM $\Upsilon^{\rm H}_{ij}$ for the Mg I b triplet is larger than the SC one.

Results for the 3p ^{3}P and 4s ^{3}S energy levels are given in left panels of Fig. 3. Departure coefficients with no H collisions are computed for comparison (black lines). In all cases, line opacities of the Mg I b triplet is reduced due to the depopulation of the lower level. Excepted in Arcturus, the upper level (thin line) is more depopulated than the lower one (thick line). This will influence the line

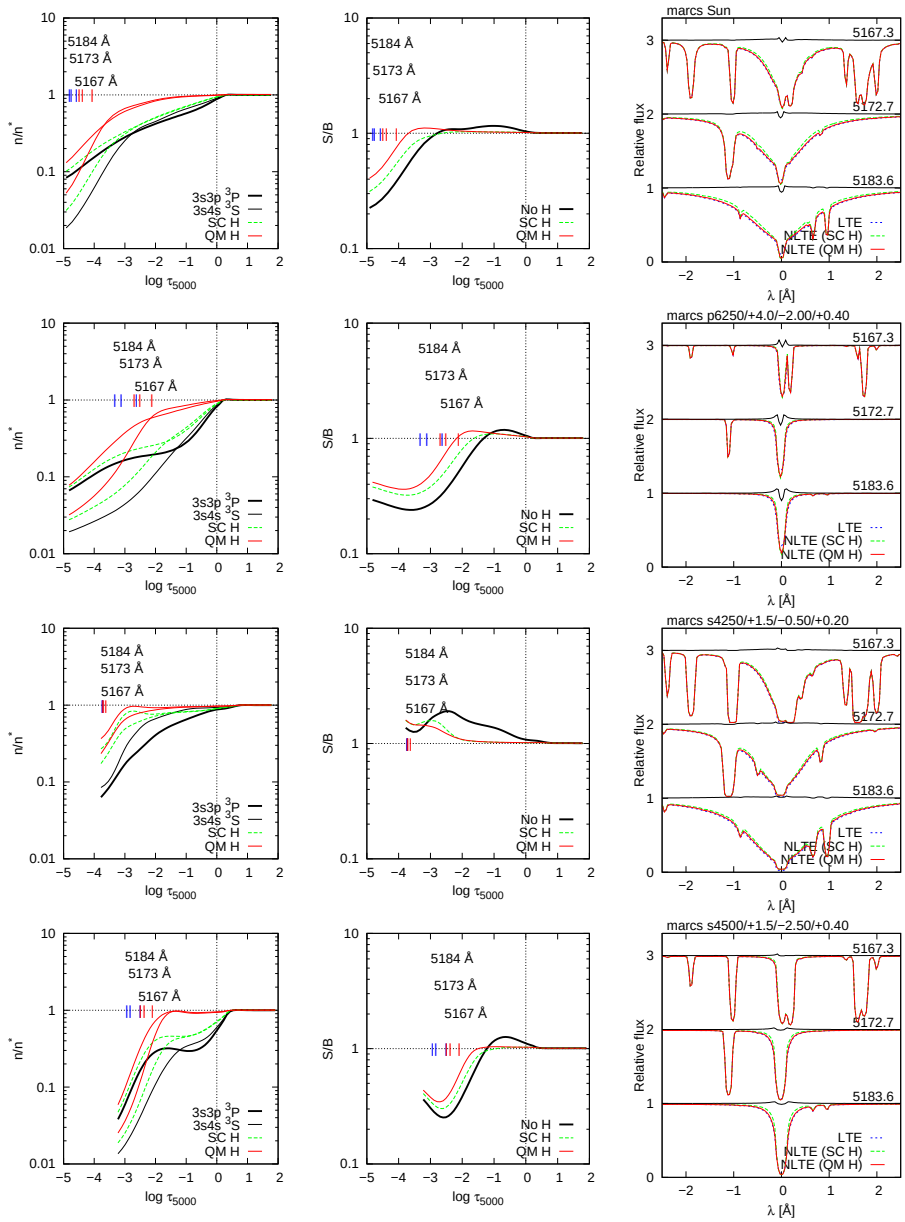

Fig. 3. Formation of the Mg I b triplet in model atmospheres of benchmark stars (atmospheric parameters given at the top of right panels with $T_{\rm eff}/\log g/[{\rm Fe/H}]/[\alpha/{\rm Fe}]$). Black profiles are NLTE results with no H collisions; green profiles with Semi-Classic (SC) H collisions 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 levels implied in the b triplet. **Middle:** line source function of the b triplet. **Right:** theoretical line profiles of the b triplet.

source functions as shown in middle panels of Fig. 3, normalized to the Planck function. In the Wien regime, $S_{ij}/B_{ij} = b_j/b_i$. When the source function is lower than the Planck function where the core line formed, the flux in the line is lower than in LTE. A weaker opacity line compared with LTE combined with a weaker source function make the strength of the NLTE line profile unpredictable. Only in Arcturus for which the source function is larger than in LTE lead to stronger flux in the line core (see right panels of Fig. 3). Overplotted to the theoretical line profiles are the difference (black line) between NLTE QM H profile (red) and LTE one (blue). From these differences, we can infer that NLTE abundance corrections are weak, the largest correction being for the metal-poor dwarf HD 84937. In that case, NLTE line core is deeper than LTE whereas the wings are slightly less pronounced than in LTE. This is due to a source function larger than the Planck function for $-2 < \log \tau_{5000} < 0$ as seen from the middle panel in Fig. 3 for this star.

4 Conclusion

This theoretical study is dedicated to the formation of the Mg I b triplet in four benchmark stars using a simplified model atom of Mg I including only levels for which new quantum mechanics data are available for inelastic collisions with hydrogen. This preliminary study shows that NLTE line formation diverge from LTE one but with very little impact on the NLTE abundance correction (certainly less than 0.1 dex). In particular, the line cores are formed deeper in the atmosphere due to the reduction of the line opacity compared with LTE. The use of QM H collisions give smaller corrections than with SC H collisions (Drawin's formula) even with a scaling factor of unity. This last result is in disagreement with what is claimed in the literature that Drawin's formula gives too small NLTE abundance corrections. Nevertheless, a more detailed study with a more complete model atom will firmly confirms/invalidates this assertion.

References

Aldenius, M., Tanner, J. D., Johansson, et al. 2007, A&A, 461, 767
Andrievsky, S. M., Spite, M., Korotin, S. A., et al. 2010, A&A, 509, A88
Barklem, P. S., Belyaev, A. K., Spielfiedel, et al. 2012, A&A, 541, A80
Carlsson, M. 1986, Uppsala Astronomical Observatory Reports, 33
Drawin, H. W. 1969, Zeitschrift fur Physik, 225, 483
Gehren, T., Shi, J. R., Zhang, H. W., Zhao, G., et al. 2006, A&A, 451, 1065
Gustafsson, B., Edvardsson, B., Eriksson, K., et al. 2008, A&A, 486, 951
Seaton, M. J. 1962a, Proceedings of the Physical Society, 79, 1105
Seaton, M. J. 1962b, in Atomic and Molecular Processes, ed. D. R. Bates, 375+
Zatsarinny, O., Bartschat, K., Gedeon, S., et al. 2009, Phys. Rev. A, 79, 052709