Modelling the spectrum of Mg in cool stars

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Abstract. The astrophysical importance of Mg, together with its unique range of spectral features in late-type stars, plus its relative simplicity from an atomic physics point of view, makes it a prime target and test bed for detailed *ab initio* non-local thermodynamic equilibrium (NLTE) modelling in stellar atmospheres. In this paper, we present example first results for calculations of NLTE Mg line based on a new model atom with significant improvements in the collision data for neutral Mg. We perform calculations for excitation of the lower-lying levels due to electron impacts using the R-matrix method. Recent data for excitation and charge transfer due to hydrogen atom impacts involving low-lying levels are now employed. Further, we have made efforts to use physically-motivated methods for calculating radiative and collisional data involving Rydberg states. The results are compared with observed spectra and the impact of the new calculations briefly explored.

1. Introduction

Neutral magnesium creates a broad range of spectral features in late-type stars, including some of the strongest lines in their spectra. Consequently, Mg is detectable even in low-quality spectra and in old, metal-poor stars, making Mg an excellent tracer of alpha-element abundances. At T > 5000 K, Mg I is a minority species and as a result is expected to be sensitive to departures from local thermodynamic equilibrium (LTE) in stellar atmospheres due to photoionization by non-local radiation. While in the sun non-local thermodynamic equilibrium (NLTE) effects on lines in the optical are relatively small [1], significant departures from LTE are seen in calculations for metal-poor dwarfs and giants [2]. However, past studies such as these have often been forced to use atomic collision data for inelastic and line broadening processes of questionable quality, frequently approximate formulae, and this is a significant source of uncertainty in the NLTE modelling. Ref. [3] showed that such atomic data was the largest source of uncertainty in their calculations of the solar 12 micrometer lines (see also Ref. [4]). [1] demonstrated the particular sensitivity of the 8806 Å line to the rates for inelastic collisions with neutral hydrogen.

The astrophysical importance of Mg, together with the unique range of spectral features in late-type stars, plus its relative simplicity from an atomic physics point of view, makes it a prime target and test bed for detailed *ab initio* NLTE modelling in stellar atmospheres. Here we present some initial results, noting that a far more detailed study is underway [5].

2. NLTE modelling using new collision data

We have performed NLTE Mg line formation calculations using the MULTI code [3] based on a new model atom with significant improvements in the collision data for neutral Mg.

Calculations for excitation of the lower-lying levels due to electron impacts are performed using the R-matrix method [5-12] based on configuration interaction calculations of the electronic structure employing polarization pseudostates [13-15]. In Figure 1 the resulting rate coefficients at a representative temperature are compared with the data from [16], which is the data employed in most recent studies. It is seen that the general agreement is reasonable, though there is a large scatter with some transitions differing by around 3 orders of magnitude. In particular, data for optically forbidden transitions are always larger in our calculations, often significantly so. Such processes correspond to spin-changing transitions, which are often important in NLTE modelling (see below). For transitions involving high-lying states, more approximate methods must be employed. The two most commonly used are the semi-empirical Bethe-Born formula of van Regemorter [17], and the impact parameter method of Seaton [18]. Figure 2 compares the rate coefficients from the two methods, which are seen to have significant differences for many transitions, often van Regemorter giving larger rates. As we will see in the next section, the choice has significant impact on the solar 12 micrometer lines.

Recent data for excitation and charge transfer involving low-lying levels due to hydrogen atom impacts from full quantum scattering calculations by some of us [19-21] are now employed. Prior to these calculations, the classical "Drawin formula" was often used, which has been shown to be completely unsatisfactory [22]. In particular, it cannot be used for charge transfer processes, or spin-changing processes, which are exactly those processes that have been found to be most important in NLTE modelling, e.g. [23, 24].

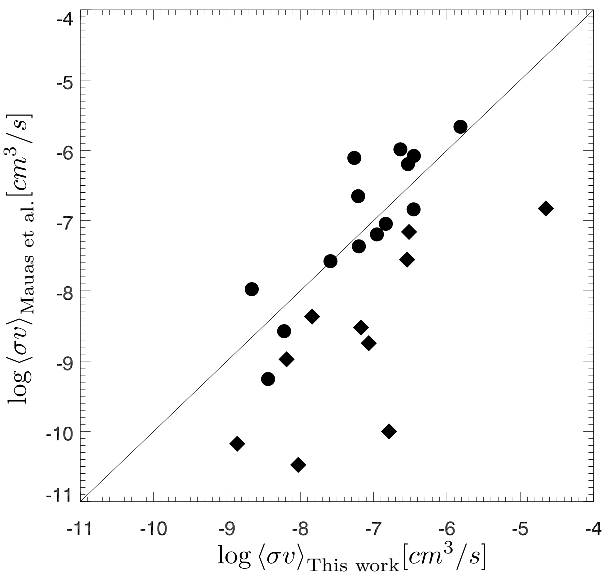

Figure 1. Comparison between the electron collisional rates at T=5000 K calculated by us and those used by [16]. Circles correspond to the optically allowed transitions, and diamonds are the optically forbidden transitions.

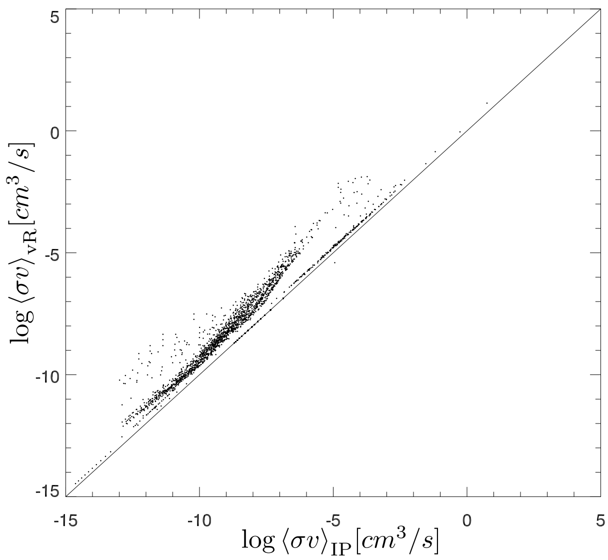

Figure 2. Comparison of electron collision rate coefficients at T=5000 K using the impact parameter (IP) approximation and the van Regemorter formula (vR).

3. Comparison with observed spectra

A few example comparisons of predicted and observed spectra are now shown to demonstrate the effects.

Figures 3 and 4 compare spectra for the 12 micrometer lines in the solar spectrum. Here we see that the predicted spectrum is rather sensitive to the choice of method for estimating the electron collision rates among high-lying states, as these transitions take place among Rydberg states. It is well known that the Born approximation overestimates cross sections at low energies and that the impact parameter method gives better results; see [18, 26]. Here we see the astrophysical comparison is also significantly improved by favouring the impact parameter method.

Figure 5 compares spectra of the quite strong 8806 Å absorption line with observations for 6 standard benchmark stars with relatively well-known stellar parameters. One sees directly that the NLTE models provide much better overall fits to the lines, especially in the cores of the lines which form high in the stellar atmospheres where collisions are relatively inefficient, and thus NLTE effects start to become very important.

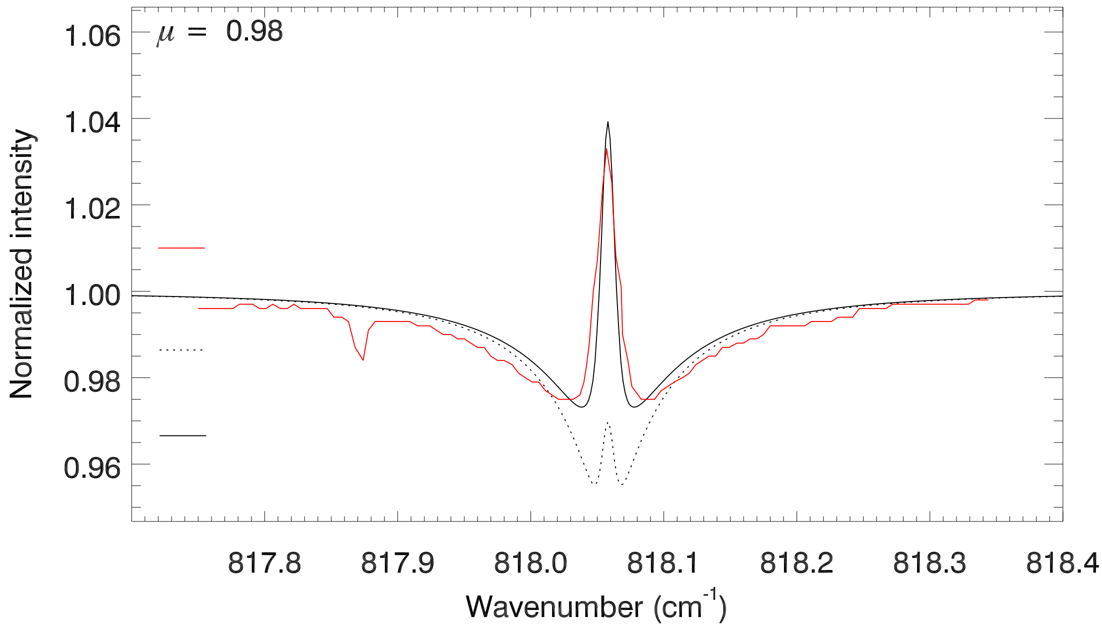

Figure 3. Infrared 12.2 micrometer line profile at solar disc centre calculated using all the available atomic data and using impact parameter method (solid black line) or the van Regemorter formula (dashed lines) formula where no R-matrix calculations were available. Observed spectrum (solid red line) is from [25].

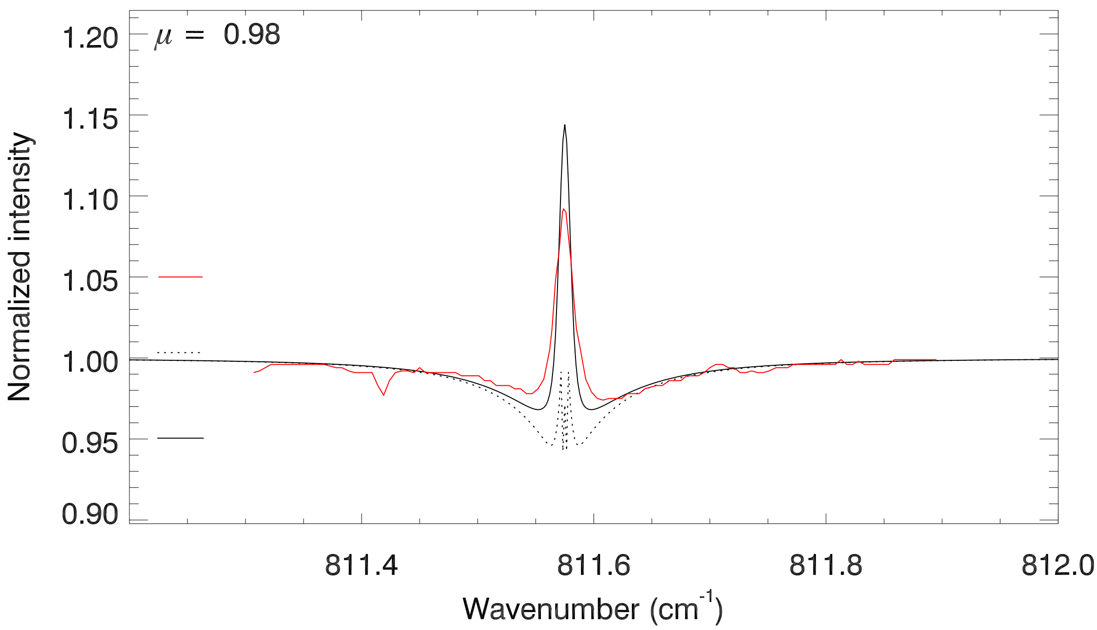

Figure 4. As for figure 3, but for the 12.3 micrometer line.

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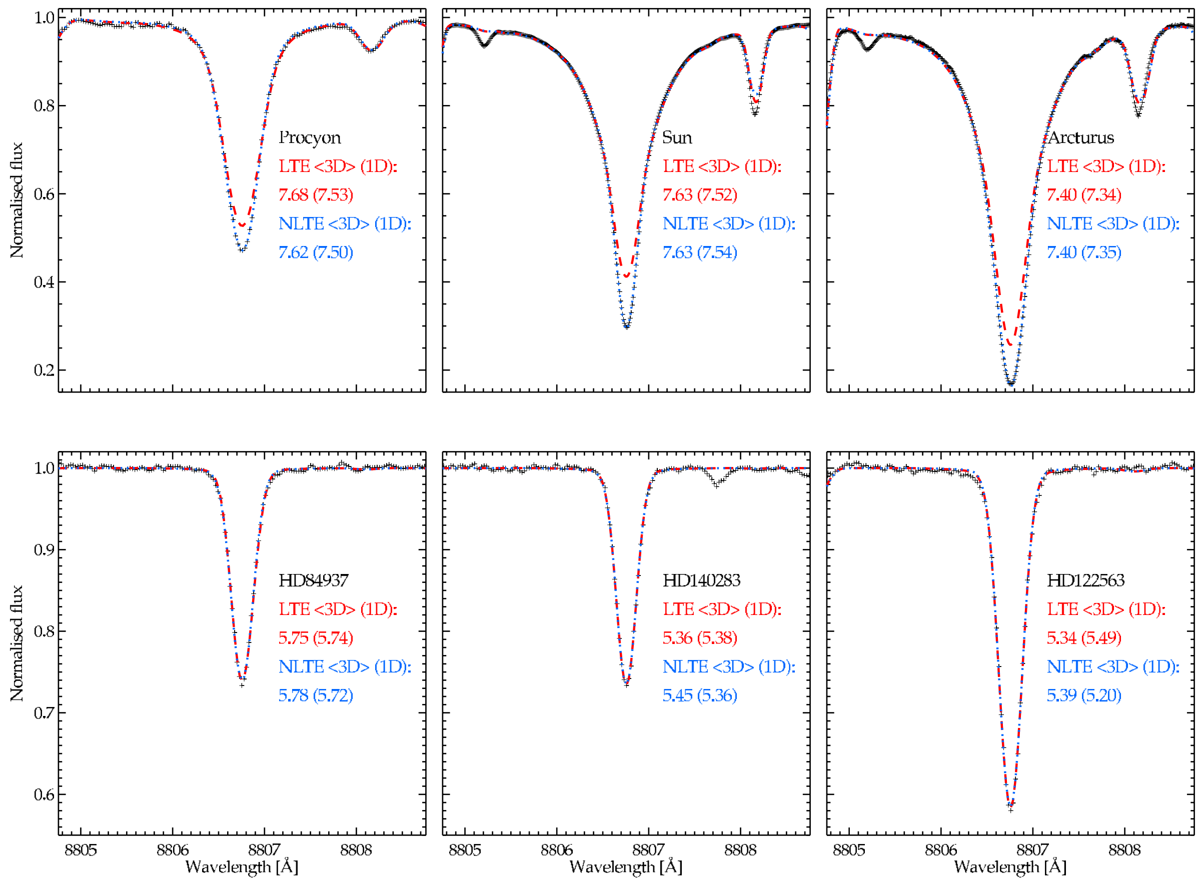

Figure 5. Observed spectra of the NLTE sensitive Mg I 8806Å line (pluses). The best fitting <3D> (3D averaged model atmosphere) LTE (red dashed line) and NLTE profile (blue dotted line) are overplotted and the corresponding Mg abundances stated in each panel. The abundances from classical 1D models are given in parentheses (spectra not plotted). Plot by Karin Lind, from [5].

4. Discussion

We have shown some preliminary example results of NLTE modelling of Mg I in stellar atmospheres. In particular, we have seen the diagnostic value of the 12 micrometer lines in differentiating between two possible descriptions for electron collision rates among high-lying states. We have also seen the general improvement of fits to the near infrared 8806 Å line from our NLTE modelling compared to LTE modelling. This work is ongoing, but we expect final and more extensive results, along with significantly more details of the model atom, to be published in the near future [5].

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