Improvements to the Single-Valued Parameter (SVP) Method for Radiative Acceleration Calculations: Preliminary Results

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Detailed calculations of radiative accelerations can be numerically onerous especially in stellar evolution modelling. Parametric equations for radiative accelerations that separate the terms depending explicitly on the atomic data from those depending on the physical properties of the stellar plasma have been developed in the past decades (and particularly since 2004). The parameters are calculated in advance and radiative acceleration calculations may then be carried out relatively quickly during stellar evolution simulations without the need for detailed atomic data. Several improvements regarding, for instance, the values of the parameters or the fitting procedure to more precisely calculate radiative accelerations are being developed. These parameters are generally tabulated using The Opacity Project atomic data and radiative accelerations. Results for certain elements of interest are shown in a typical A-type star.

1 Introduction

Atomic diffusion (Michaud, 1970) can be an important transport process in several types of stars for layers where mixing processes such as convection are weak enough. The modelling of this time-dependent physical process is complex and can affect the elements distribution inside stars (including superficial abundances), and therefore may modify the evolution of stars. For instance, evolutionary calculations have been carried out while including atomic diffusion for several types of stars (Turcotte et al., 1998; Richard et al., 2001; Vick et al., 2010) using the Montreal evolution code. In this paper, we only consider radiative acceleration $g_{\rm rad}$) calculations in stellar interiors. Some of the approximations used here at large optical depths are not valid in stellar atmospheres. Calculations of $g_{\rm rad}$ are numerically heavier than in interiors because the atomic lines are narrower there and it is essential to solve the equation of radiative transfer in detail. Model atmospheres while including abundance stratification due to atomic diffusion have been constructed for blue horizontal-branch stars (LeBlanc et al., 2010) and ApBp and HgMn stars (Alecian & Stift, 2019).

The principal ingredient for atomic diffusion and often the main competitor to gravity is $g_{\rm rad}$ due to momentum transfer to atoms following photon absorptions. Radiative acceleration of a given species therefore depends on its absorption spectrum due to both bound-bound and bound-free transitions. The calculation of $g_{\rm rad}$ is difficult since it necessitates the atomic data of all species present, or their detailed monochromatic opacity. To evaluate $g_{\rm rad}$, an integration over the spectrum (for instance see Section 2 of Gonzalez et al. 1995) of the product of the monochromatic opacity and the flux must be undertaken. The opacity spectrum and the flux must then be sampled on a sufficiently fine frequency grid that leads to a precise integration. This is commonly called the opacity sampling method, and the fineness of the grid required depends on the typical line widths and therefore on the stellar depth (i.e. LeBlanc et al. 2000) since the lines are wider deeper in the stars.

For instance, for the Montreal evolution code the monochromatic opacities used are those of OPAL (Iglesias & Rogers, 1996). These opacities are pretabulated on a given frequency, temperature and density grid.

Other methods have also been developed to calculate $g_{\rm rad}$. Gonzalez et al. (1995) developed a method to calculate $g_{\rm rad}$ in stellar interiors that uses approximate total opacity on a grid of 4000 frequency intervals. Atomic data from The Opacity Project (Seaton et al., 1992) was used for these calculations.

Seaton (1997, 2005, 2007) also calculated $g_{\rm rad}$ for the elements found in The Opacity Project using their atomic data and opacities. Their results for $g_{\rm rad}$ are given on two dimensional grids of temperature and the density of free electrons, which are well adapted for astrophysical applications. These grids may then be used to obtain $g_{\rm rad}$ by interpolation in a given stellar model.

More recently, Alecian & LeBlanc (2002) and LeBlanc & Alecian (2004) developed a numerically efficient method for calculating $g_{\rm rad}$ based on parametric equations. These equations were developed following the studies of Alecian (1985), Alecian & Artru (1990) and Alecian (1994). This method, that will be discussed in the next section, has the advantage of enabling the calculation $g_{\rm rad}$ from pretabulated parameters without having to access complete atomic data or detailed monochromatic opacities.

In this paper, we first describe the SVP method and then we outline the improvements brought to it. Preliminary results for Ar and Fe are shown. A short conclusion follows.

2 The SVP method

The SVP (for Singled-Valued Parameters) method is based on a simplified developments of $g_{\rm rad}$ equations such that the terms depending on atomic data are separated from those depending on the stellar model (i.e. local physical conditions). More details about the algebraic development are given in Alecian & LeBlanc (2002). The SVP method can only be used in optically thick regions and for stars with mass larger (or equal) to approximately one solar mass.

Several assumptions are made to lead to simplified parametric equations. For instance, for the acceleration due to bound-bound transitions, it is assumed that all atomic lines saturate according to the Lorentz line profiles. Voigt profiles are taken into account through the fitting procedure (see below). It is also assumed that the background opacity (i.e. due to all of the other opacity sources aside from the transition under consideration) is independent of the abundance of the atomic species under consideration and that it does not vary within the line profiles.

LeBlanc & Alecian (2004) and Alecian & LeBlanc (2002) found that the $g_{\rm rad}$ due to lines in optically thick regions can be expressed as:

$$g_{i,\mathrm{line}} = q\varphi_i^* \left(1 + \xi_i^* C_i\right) \left(1 + \frac{C_i}{b\psi_i^{*2}}\right)^{\alpha_i}, \tag{1}$$

where

$$q = 5.575 \times 10^{-5} \frac{T_{\mathrm{eff}}^4}{T} \left(\frac{R}{r}\right)^2 \frac{1}{A}, \tag{2}$$

and

$$b = 9.83 \times 10^{-23} \frac{N_{\mathrm{e}} T^{-1/2}}{X_{\mathrm{H}}}. \tag{3}$$

The parameters ${\varphi_i}^*$, ${\psi_i}^*$ and ${\xi_i}^*$ are the values of φ_i , ψ_i and ξ_i (see Eqs. 10 to 15 and Section 3.3 of Alecian & LeBlanc (2002) for more details) calculated where the population of ion i is close to its maximum. These parameters are therefore calculated at a single value of temperature and density for a given stellar mass (which is the source of the acronym SVP for the method in question). The parameter ${\varphi_i}^*$ depends on the oscillator strengths of the bound-bound transitions of the ion. The ${\psi_i}^*$ parameter is related to the line widths and therefore affects saturation. The third parameter ${\xi_i}^*$ depends on the contribution of the ion to the total opacity and also affects the dependence of the acceleration on abundance. These three parameters are calculated with the atomic data from The Opacity Project. The quantities T_{eff} and R are the effective temperature and radius of the star, while T and r are the local temperature and radius. The variable N_{e} represents the density of free electrons, X_{H} the hydrogen mass fraction, A the atomic mass in atomic units of the species under consideration and C_i the concentration (in number) of the ion relative to hydrogen.

For pure Lorentzian profiles, the parameter α_i is -0.5. It is written as a free parameter in Eq. 1 to take into account the fact that the lines are not all Lorentzian in nature. This should therefore better represent the saturation effect.

A more approximate parametric equation for the bound-free transition was also developed by Alecian (1994) and Alecian & LeBlanc (2002). This equation has two free parameters that must be fitted. These two parameters along with α_i are obtained by fitting the parametric g_{rad} to those obtained using the method proposed by Seaton (1997, 2005, 2007).

Once the six parameters are obtained for each ion (${\varphi_i}^*$, ${\psi_i}^*$, ${\xi_i}^*$ and the three fitted parameters discussed above), g_{rad} calculations are numerically economical, since complete atomic or opacity data are not required. This method has been used in the Toulouse-Genève Evolution Code (Hui-Bon-Hoa, 2008; Théado et al., 2009) and the CESTAM code (Deal et al., 2018).

3 Preliminary results

A revised and improved version of the parameters of the SVP method originally published by LeBlanc & Alecian (2004) is in preparation and some preliminary results are presented here. The parameters will be calculated for the elements C, N, O, Ne, Na, Mg, Al, Si, S, Ar, Ca and Fe. In this section, preliminary results for Ar and Fe for three abundances will be shown in a $2\,\mathrm{M}_{\odot}$ stellar model. These calculations are performed in LTE and no magnetic effects are included. Also, no redistribution effects among the ions are considered in the SVP method, in other words, it is assumed that the momentum gained through a bound-bound transition of a given ion for instance is spent in this same ion state (more details concerning redistribution is given in Section 5 of Gonzalez et al. 1995). However, a weighting of each ion's contribution with its diffusion coefficient is possible, since the SVP method calculates radiative accelerations of ions to evaluate the total $g_{\rm rad}$ of the element.

Even though the results of LeBlanc & Alecian (2004) are relatively precise in most cases, some important differences relative to the results of Seaton (1997) remain. For instance, the results of LeBlanc & Alecian (2004) are relatively poor for larger abundances for certain elements such as C, N, O and Fe. The improvements brought to the SVP method here aims to improve the results in these cases.

The first improvement consists of using up-to-date data from The Opacity Project (i.e. version OPCD3.3, Seaton 2005) to calculate ${\varphi_i}^*$, ${\psi_i}^*$ and ${\xi_i}^*$ for each ion for the elements considered. In this version of OPCD, the inner-shell contributions (Badnell et al., 2005) are now included in both monochromatic opacities and $g_{\rm rad}$ calculations (Seaton 2005, 2007). Another improvement was brought in the estimation of ${\psi_i}^*$ for the Stark broadening. The criteria in calculating ${\xi_i}^*$ was also revised: this parameter obtained through a Taylor expansion of first order is now kept equal to zero for most species because ${\xi_i}^*$ does not always improve results.

Improvements were also brought to the fitting procedure used to obtain the values of the three free parameters found in the $g_{\rm rad}$ equations for bound-bound and bound-free transitions (LeBlanc & Alecian, 2004). These parameters are now simultaneously fitted for five abundances (for -2 to $+2$ solar in dex) to the $g_{\rm rad}$ of Seaton (2007). The error due to each abundance are now also weighted by giving more weight to values surrounding the solar abundance. For the results shown here, the following weights were used: 5 was used for the solar abundance, 3 for abundances of ±1 dex relative to solar and 1 for abundance of ±2 dex relative to solar. The errors may be therefore increasingly larger for abundances above 10 times solar and below 0.1 times solar. When this study is completed, values for the six parameters for each ion considered will be generated for 17 stellar models (calculated with the CESTAM code) from 0.9 to $10\,{\rm M}_\odot$.

Figs. 1 and 2 show $g_{\rm rad}$ for Ar and Fe respectively in a $2\,{\rm M}_\odot$ stellar model. The fundamental parameters for this model are $T_{\rm eff} = 8200\,{\rm K}$ and $\log g = 4.0$.

The $g_{\rm rad}$ naturally varies with depth since the dominating ion changes. For instance, minima in the curves of Fig. 1 and 2 are associated to regions where a noble gas configuration ion dominates. The discontinuity observed at roughly $\log T = 4.8$ is caused by the underlying stellar model and is related to the transition between convective and radiative zones.

The results for Ar using the SVP method is very good when comparing to the detailed results of Seaton (2007). The precision of these results are similar to those found in LeBlanc & Alecian (2004). The anomaly seen at $\log T = 5.4$ for an abundance of 0.1 times the solar value for Ar is related to insufficient opacity sampling for low abundances. This was already reported in Seaton (2005). However, such inaccuracies are not important since they often occur when the value of $g_{\rm rad}$ is much less than gravity.

For Fe, the improved fitting procedure used here leads to results that are much better than those found in LeBlanc & Alecian (2004) as compared to the accelerations calculated by The Opacity Project. Our new results much better simulate saturation effects for larger abundances. Previous results for an abundance of +1 dex relative

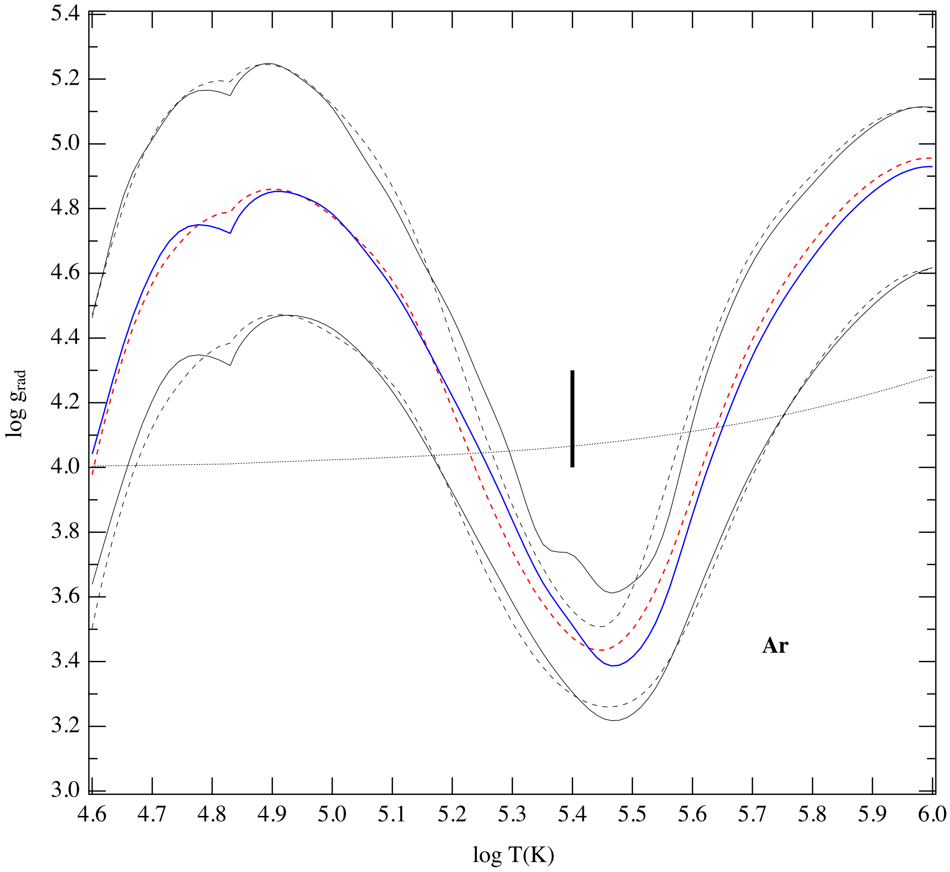

Fig. 1: Argon radiative acceleration with respect to the depth (expressed as temperature) in a $2\,\mathrm{M}_\odot$ model obtained through the SVP method (dashed lines) and with the procedure proposed by Seaton (2007) (solid lines) for three concentrations of Ar from 10^{-1} (the upper curves) to 10 times the solar value, using the same set of optimized parameters. The blue and red lines are for solar abundances.The vertical bar represents 0.3 dex, and the pointed curve is the local gravity.

to solar did not properly fit those of Seaton (1997). However, the curve for an abundance of -1 dex relative to solar shows that the $g_{\rm rad}$ due to the FeXII ion near $\log T = 5.55$ is not well reproduced in our results. A similar effect was also seen to a lesser degree in the results of LeBlanc & Alecian (2004).

4 Conclusion

Preliminary results shown here for two elements in an A-type star, illustrate the present status of our SVP method, including some improvements made to obtain more precise $g_{\rm rad}$. In addition to the use of more recent monochromatic opacities and $g_{\rm rad}$ from The Opacity Project, improvements were also brought to the fitting procedure used for adjusting certain parameters to better reproduce the detailed

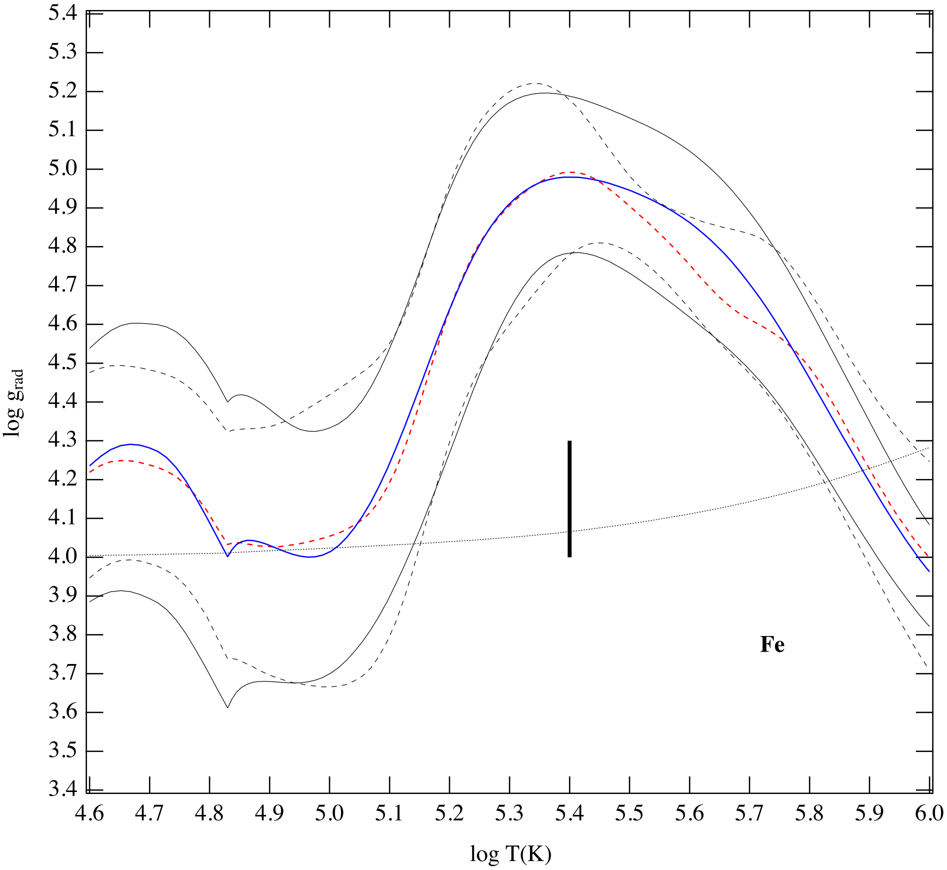

Fig. 2: Same as Fig. 1 but for iron.

$g_{\rm rad}$ calculations of Seaton (2007). These improvements are especially important for the most abundant elements at large overabundances (i.e. at +1 dex relative to solar values).

Calculations for all 12 trace elements for which detailed atomic data are available in The Opacity Project are underway. The parameters for each ion for 17 stellar models from 0.9 to 10 $M_\odot$ will be made accessible to the scientific community via the web site `gradsvp.obspm.fr`. These results may then be used to more easily calculate $g_{\rm rad}$ and study atomic diffusion in stellar interiors.

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