

# New approximate formulae for radiative accelerations in stars

G. Alecian<sup>1★</sup> and F. LeBlanc<sup>2★</sup>

<sup>1</sup>DAEC/LUTH, Observatoire de Paris, CNRS, Université Paris 7, Observatoire de Meudon, F-92195 Meudon Cedex, France

<sup>2</sup>Département de physique et d'astronomie, Université de Moncton, Moncton, New Brunswick, E1A 3E9, Canada

Accepted 2002 January 21. Received 2002 January 19; in original form 2001 November 23

## ABSTRACT

Radiative accelerations are quantities that are crucial in the study of diffusion processes in stars. Their calculation requires the use of large atomic and opacity data bases, and generally necessitates very heavy numerical computations. New approximate formulae for radiative accelerations in stars, arising from both bound–bound and bound–free transitions, are presented. These are written in a parametric form, which separate the terms depending on the local abundance of the element under consideration from those depending mainly on the atomic data. These formulae are shown to be significantly superior to those previously published. The main reason for this improvement comes from the use of monochromatic opacities instead of approximating these by the Rosseland mean. The principal advantage for the use of these parametric equations over other methods for calculating radiative accelerations is its numerical expediency. Results are shown for several elements (C, Ar, Ca and Fe) in a type A star.

**Key words:** diffusion – stars: abundances – stars: chemically peculiar.

## 1 INTRODUCTION

The transfer of momentum to atoms from the radiative field in stars during photoexcitation or photoionization can induce radiatively driven diffusion (Michaud 1970). In hydrodynamically stable stellar regions, radiative diffusion occurs and can cause elemental stratification and thus abundance anomalies. The diffusion velocity of each element depends on its radiative acceleration, which in turn depends on the capacity of its ions to absorb radiation.

Diffusion of the elements can modify the structure and evolution of stars. Evolutionary models including diffusion have been built for the Sun (Turcotte, Richer & Michaud 1998a) and AmFm stars (Turcotte et al. 1998b; Richer, Michaud & Turcotte 2000). In these stars, the outer regions are convective and diffusion is only dominant deeper in the interior. When the atmosphere of stars is stable, which seems to be the case for hotter stars, diffusion can be the dominant physical process in the line-forming region. Model atmospheres taking into account the effect of the stratification of the elements owing to diffusion on the atmospheric structure of blue horizontal-branch stars (Hui-Bon-Hoa, LeBlanc & Hauschildt 2000) and white dwarfs (Dreizler & Wolff 1999) have also been developed recently. Other studies have mainly focused on the creation of abundance anomalies in the atmospheres of Ap stars (Michaud 1970) and HgMn stars (Alecian & Michaud 1981; Seaton 1999).

In order to study properly the diffusion of the elements in stars it

is imperative to be able to evaluate precisely the radiative acceleration of each elemental species present. In stellar atmospheres (optically thin medium), the radiation transfer has to be solved explicitly [for the most recent studies see Hui-Bon-Hoa et al. 2002 in local thermodynamic equilibrium (LTE)/non-local thermodynamic equilibrium (NLTE), and Alecian & Stift (2002) for polarized radiation transfer in LTE]. In stellar interiors (optically thick), the diffusion approximation allows to simplify greatly the computation of the radiation flux. The results presented here are valid only in this last case.

Several methods have been employed to calculate radiative accelerations. The most direct, but also the most time-consuming, is the sampling method (e.g. Seaton 1997; Richer et al. 1998; LeBlanc, Michaud & Richer 2000, hereafter LMR2000). It consists of calculating the monochromatic opacity of each species at a sufficiently high number of frequency points in order to properly integrate the monochromatic opacity of the species under consideration, multiplied by the radiative flux, which intervenes in the radiative acceleration equation (see equation 11 of Gonzalez et al. 1995, hereafter GLAM). Seaton (1997) proposed the use of interpolation tables for radiative acceleration calculations. These tables were built with the OPACITY Project data (Seaton et al. 1992) available through TOPbase (Cunto et al. 1993). Although this scheme is numerically efficient, the tables are only valid for a narrow abundance domain and the inclusion of new atomic data, other species for instance, would require the elaborate task of recalculating all of these tables.

Another method, commonly called the GLAM method, uses an

★E-mail: georges.alecian@obspm.fr (GA); leblanfn@umoncton.ca (FL)

average value for the background opacity, i.e. the total opacity minus the opacity of the transition under consideration. In this method the frequency spectrum is divided into 4000 intervals in which this average background opacity is calculated. The total opacity is divided into two parts: the monochromatic opacity of the transition under consideration and the average background opacity. The radiative acceleration of each bound–bound and bound–free transition is then calculated by integrating the radiative acceleration equation. Unfortunately, this method suffers from the same lack of flexibility related to the atomic data as mentioned for the Seaton (1997) method.

Alecian (1985) and Alecian & Artru (1990) developed a semi-empirical parametric expression for radiative accelerations arising from bound–bound transitions in stellar interiors. Two parameters are found in this expression. They depend on the atomic data of the ion under consideration and on the plasma conditions, but are independent of the abundance of this ion. The first parameter depends on the oscillator strength of the transitions. The other parameter aims to characterize the saturation of the atomic lines. The principal advantage of this method is its numerical expediency. It should be noted that this method is very flexible and as more complete and precise data tables become available, the parameters can easily be recalculated. An approximate parametric formula has also been developed for bound–free transitions (Alecian 1994) by approximating the photoionization cross-sections of the ions considered by an analytical expression close to the hydrogenic case.

The aim of this paper is to improve the semi-empirical methods described above. It was shown in Alecian & LeBlanc (2000) that several assumptions on which Alecian & Artru’s (1990) method is based are not always respected, especially for the more abundant elements. Moreover, we will include the contribution of the bound–free transitions using an improved version of Alecian’s (1994) parametric method. The theoretical framework leading to these improved methods will be elaborated in Section 2. In Section 3, the radiative accelerations obtained with the new parametric equations will be compared to those obtained by the Seaton (1997) and Alecian & Artru’s (1990) methods. Finally, a brief conclusion will be presented.

## 2 THEORY

The semi-analytic approximations defined by Alecian & Artru (1990) for radiative accelerations of ions owing to bound–bound transitions are mainly based on the following assumptions: (i) effects of blends are negligible, (ii) the Rosseland opacity  $\bar{\kappa}_R$  is supposed to be independent of the ion concentration  $C_i$ , (iii) the total monochromatic opacities  $\kappa$  are close to  $\bar{\kappa}_R$  in the frequency domain where lines contribute to the radiative acceleration, (iv) all the lines of the ion saturate at the same concentration, (v) all the lines have a Lorentz profile, (vi) the radiative acceleration arising from photoionization is negligible. It should be remembered that the equations of Alecian & Artru (1990) are only valid for optically thick regions since the radiation flux used is the one given by the diffusion approximation. These semi-analytic approximations give good results for some elements (Ca for instance). However, comparisons with detailed computations show that these assumptions are not valid for several elements (especially for abundant elements in normal stars, like CNO and Fe) and when elements are strongly overabundant with respect to solar values. As stressed by Alecian & LeBlanc (2000), this is probably caused by assumptions (ii) and (iii), which are clearly not satisfied for abundant elements,

and also by assumption (vi) which is not satisfied for some ions and never satisfied when strong overabundances are considered. Approximations (i) and (iv) do not appear very constricting.

Alecian (1994) developed a parametric formula that approximates the radiative acceleration arising from bound–free transitions. In this method, the photoionization cross-sections are approximated by an expression close to that of the hydrogenic ion and autoionization lines are neglected. This method also assumes that the opacity arising from the photoionization of the ion under consideration does not contribute significantly to the total opacity.

We present here new semi-analytic approximations obtained in the same spirit than those of Alecian & Artru (1990) and Alecian (1994), but which correct the main drawbacks mentioned above. These new approximations now involve a more precise treatment of the opacities.

### 2.1 Approximate formulae for the contribution arising from bound–bound transitions

We consider an element  $A$  with atomic mass  $A$  (in atomic units),  $A^{+i}$  stands for the ion with charge  $+i$  (0 for neutral).

Let us define the following quantities (symbol ‘–’ stands for frequency averaged values):  $\kappa_A$ : monochromatic opacity of element  $A$ ,  $\kappa_{il}$ : opacity arising from transition  $l$  of ion  $A^{+i}$  (at line centre frequency). The background opacity (other sources of opacity than  $A$ ) in the medium is

$$\kappa_{\text{med}} = \kappa - \kappa_A, \quad (1)$$

where  $\kappa$  is the total opacity of the medium.

Its average over frequency  $\nu$  is defined in the same way as the Rosseland average:

$$\bar{\kappa}_{\text{med}} = \frac{\int_0^\infty \frac{\partial B_\nu}{\partial T} \partial \nu}{\int_0^\infty \frac{1}{\kappa_{\text{med}}} \frac{\partial B_\nu}{\partial T} \partial \nu}, \quad (2)$$

where  $B_\nu$  is the Planck function at the local temperature  $T$ .

We define a contribution of element  $A$  to the Rosseland average:

$$\bar{\kappa}_A = \bar{\kappa}_R - \bar{\kappa}_{\text{med}}. \quad (3)$$

It is also convenient to define

$$\begin{aligned} \kappa_{A-il} &= \kappa_A - \kappa_{il}, & \varepsilon_{A-il} &= \frac{\kappa_{A-il}}{\kappa_{\text{med}}}, \\ \bar{\varepsilon}_A &= \frac{\bar{\kappa}_A}{\bar{\kappa}_{\text{med}}}. \end{aligned} \quad (4)$$

Note that  $\bar{\kappa}_R = \bar{\kappa}_{\text{med}}(1 + \bar{\varepsilon}_A)$ .

In this paper we consider concentrations with respect to hydrogen,  $C_A = N_A/N_H$  and  $C_i = N_i/N_H$ , where  $N_A$ ,  $N_i$  and  $N_H$  are respectively the number densities (per unit volume) of element  $A$ , ion  $A^{+i}$  and hydrogen.

Finally, we define two quantities that can be reasonably considered as independent of the concentration of element  $A$ ,

$$\delta_{il} = \frac{\varepsilon_{A-il}}{C_A} \quad \text{and} \quad \bar{\delta}_A = \frac{\bar{\varepsilon}_A}{C_A}. \quad (5)$$

Integrating the detailed radiative acceleration equation (for instance see equation 5 of Alecian, Michaud & Tully 1993) for a single bound–bound transition and assuming it has a Lorentz profile with a full line width at half maximum of  $\gamma_{il} N_e T^{-1/2}$ , where  $N_e$  is the electronic density and  $\gamma_{il}$  is a factor that depends on the

transition under consideration (see Alecian & Artru 1990), the acceleration arising from the line  $l$  of  $A^{+i}$  is given by (see Appendix A for more details)

$$g_{il} = d_{il} \frac{(1 + \bar{\epsilon}_A)}{(1 + \epsilon_{A-il})} \left[ 1 + \frac{h_{il} C_i}{(1 + \epsilon_{A-il})} \right]^{-1/2} \quad (6)$$

where

$$d_{il} = q \frac{\bar{\kappa}_{\text{med}}}{\kappa_{\text{med}}} \eta_{il} P_l,$$

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

$$\eta_{il} = \frac{N_{il}}{N_i} f_l,$$

$$P_l = u_l^4 \frac{e^{u_l}}{(e^{u_l} - 1)^2} \quad \text{with } u_l = \frac{h \nu_l}{kT}, \quad (7)$$

and

$$h_{il} = \frac{\eta_{il}}{b \kappa_{\text{med}} \gamma_{il}},$$

$$b = 9.83 \times 10^{-23} \frac{N_e T^{-1/2}}{X_H}, \quad (8)$$

where  $\nu_l$  is the line centre frequency,  $T_{\text{eff}}$  and  $R$  are respectively the effective temperature and radius of the star,  $r$  is the radius at the layer with temperature  $T$ ,  $N_{il}$  is the number density of the ion  $i$  in the initial level of the transition in that same layer,  $f_l$  is its oscillator strength, and  $h$  and  $k$  are respectively the Planck and the Boltzmann constants. Equation (8) includes the mass fraction of hydrogen ( $X_H$ ), which was neglected in Alecian & Artru (1990).

The main approximations made to obtain equation (6) are that line  $l$  has a Lorentz profile and that  $\kappa_{\text{med}} + \kappa_{A-il}$  varies weakly over the frequency interval where the line contributes significantly to  $g_{il}$ . To go further in our analytical development we need to make some more assumptions. The first one is to suppose that  $\kappa_{\text{med}}$  does not vary significantly when the element's concentration  $C_A$  varies. In main-sequence stars, this assumption is clearly justified (except for hydrogen and helium) when element  $A$  has an abundance  $\chi$  with respect to the Sun (according to the same definition as Seaton 1997) smaller than around 100 (see Alecian & LeBlanc 2000). This approximation ensures that  $d_{il}$  and  $h_{il}$  do not depend on  $C_A$ . At this stage, one other assumption is useful to proceed to the series expansion of equation (6):  $\epsilon_{A-il} \ll 1$ . This last assumption means that the contribution  $\kappa_{A-il}$  of element  $A$  to the background opacity is negligible at frequency  $\nu_l$ . It will be seen below (see Section 3.2) that this is generally the case except for some blended lines (mutual blends between lines of the same element) of abundant metals (mainly CNO and Fe) when  $\log \chi \geq 1$ . In the following, we define  $C_{A,\text{critical}}$  as the concentration above which this approximation is not valid. The above hypothesis regarding  $\kappa_{\text{med}}$  and  $\epsilon_{A-il}$ , and neglecting second order terms in equation (6), allows us to write the radiative accelerations  $g_{il}$  as

$$g_{il} \approx d_{il} [1 + C_A (\bar{\delta}_A - \delta_{il})] \times (1 + h_{il} C_i)^{-1/2}. \quad (9)$$

Compared with the original approximation of Alecian (1985), this expression differs from his equation (1) by the new term which is in brackets and by the fact that  $d_{il}$  and  $h_{il}$  depend explicitly on the opacities.

The total contribution of lines of ion  $A^{+i}$  to the radiative acceleration  $g_{i,\text{line}}$  is obtained after summation of  $g_{il}$  over all the

bound-bound transitions of the ion. However, to sum equation (9) directly over  $l$  cannot lead to any useful formula. Therefore, we proceed here as in Alecian (1985): (i) to propose a parametric expression for  $g_{i,\text{line}}$  and (ii) to express analytically the various coefficients in this parametric expression, of the radiative acceleration arising from bound-bound transitions, according to the known asymptotic behaviour with respect to the concentration.

As a parametric expression for  $g_{i,\text{line}}$  we propose the following one:

$$g_{i,\text{line}} = g_{i,0} (1 + \xi_i C_i) \times \left( 1 + \frac{C_i}{C_{i,S}} \right)^\alpha. \quad (10)$$

Compared with the original approximation of Alecian (1985), this expression differs from his equation (5) by the new  $\xi_i$  term and by the exponent  $\alpha$ , which is no longer fixed to  $-1/2$ , as could be expected if the lines had a pure Lorentz profile.  $C_{i,S}$  can be considered as the ion concentration above which saturation of lines is strong.

The best known asymptotic behaviour of the radiative acceleration is that it tends to be constant with respect to the concentration of  $A^{+i}$  when  $C_i$  is vanishing (or  $C_i \ll C_{i,S}$ ). Identifying (10) and  $\sum_l g_{il}$  for  $C_i = 0$  allows us to set

$$g_{i,0} = \sum_l d_{il} = q \bar{\kappa}_{\text{med}} \sum_l \frac{\eta_{il} P_l}{\kappa_{\text{med}}}. \quad (11)$$

Note that in this expression,  $\bar{\kappa}_{\text{med}}$  and  $\kappa_{\text{med}}$  are kept equal to their values at current concentration  $C_i \neq 0$ .

The two other coefficients,  $C_{i,S}$  and  $\xi_i$ , will be determined considering, this time, large concentrations. We suppose first that  $C_{i,S} \ll C_{A,\text{critical}}$ . This hypothesis will be justified below.

Assuming  $C_{i,S} \ll C_i \ll C_{A,\text{critical}}$  (condition denoted by  $\infty$ ), equation (10) can be approximated as

$$g_{i,\text{line}}|_\infty \approx g_{i,0} C_{i,S}^{-\alpha} C_i^\alpha + g_{i,0} \xi_i C_{i,S}^{-\alpha} C_i^{\alpha+1}. \quad (12)$$

If one uses the exact expression of  $g_{i,\text{line}}$  obtained by a summation of  $g_{il}$  from equation (9), one obtains

$$g_{i,\text{line}}|_\infty = \sum_l g_{il} = \left( \sum_l h_{il} d_{il}^{-1/2} \right) C_i^{-1/2} + \left[ \frac{N_A}{N_i} \sum_l h_{il} d_{il}^{-1/2} (\bar{\delta}_A - \delta_{il}) \right] C_i^{+1/2}. \quad (13)$$

Note that the ratio  $N_A/N_i$  does not depend on the concentration.

To find an analytic expression for  $C_{i,S}$  and  $\xi_i$ , we identify both terms ahead of  $C_i$  in equations (12) and (13) for  $\alpha = -1/2$ . This leads to

$$C_{i,S} = b \left[ \frac{\sum_l \left( \frac{\eta_{il} \gamma_{il}}{\kappa_{\text{med}}} \right)^{1/2} P_l}{\sum_l \frac{\eta_{il}}{\kappa_{\text{med}}} P_l} \right]^2 \quad (14)$$

and

$$\xi_i = \frac{N_A}{N_i} \frac{\sum_l (\bar{\delta}_A - \delta_{il}) \left( \frac{\eta_{il} \gamma_{il}}{\kappa_{\text{med}}} \right)^{1/2} P_l}{\sum_l \left( \frac{\eta_{il} \gamma_{il}}{\kappa_{\text{med}}} \right)^{1/2} P_l}. \quad (15)$$

We will use the above expressions for  $C_{i,S}$  and  $\xi_i$ , for  $\alpha \neq -1/2$  assuming that these parameters are not too sensitive on deviation of  $\alpha$  from  $-1/2$ .

To conclude this subsection, it should be noted that if one assumes that element  $A$  does not contribute to the background opacity, and if one neglects the departure of monochromatic opacities from the Rosseland average (i.e. approximations of Alecian 1985), then equation (10) reduces to the approximate formulae and parameters of Alecian (1985) and Alecian & Artru (1990).

## 2.2 Approximate formulae for the contribution due to bound–free transitions

Momentum transferred to ions through bound–free transitions can contribute significantly to the total radiative acceleration. Generally, for many metals with solar abundances, this contribution is smaller than the one due to bound–bound transitions ( $g_{i,\text{line}}$ ). The acceleration owing to photoionization  $g_{i,\text{cont}}$  presents some different behaviours than  $g_{i,\text{line}}$ : (i) it is less subject to saturation effects because bound–free cross-sections spread over much larger frequency intervals (and more smoothly) compared with bound–bound cross-sections, (ii) the momentum received by  $A^{+i}$  is redistributed to  $A^{+(i+1)}$ , (iii) photoionization is a three-body interaction and thus a fraction of the momentum is taken away by the ejected electron (e.g. Massacrier 1996). Several papers have discussed the bound–free acceleration (e.g. Alecian 1994 and GLAM) and it is outside the scope of the present paper to discuss in more details the properties of  $g_{i,\text{cont}}$ .

According to Alecian (1994), assuming that photoionization cross-sections follow a power law close to the hydrogenic one, and neglecting the momentum taken away by electrons,  $g_{i,\text{cont}}$  (for  $i > 0$ ) can be approximated by the following formulae:

$$g_{i,\text{cont}} \approx 7.16 \times 10^{-26} \frac{N_e T_{\text{eff}}^4}{T^{\frac{3}{2}}} \left(\frac{R}{r}\right)^2 \frac{1}{A i^2} \Theta_i, \quad (16)$$

where

$$\Theta_i = a_i \frac{\bar{\kappa}_{\text{med}} N_{i-1,0} p_{i-1}}{N_{i-1} p_i g_0} \sum_k \frac{n_k g_k Q_k}{\kappa_{\text{med},k}} \quad (17)$$

and

$$Q_k \approx u_k^3 \left[ \frac{u_k}{1 - e^{-u_k}} - e^{u_k} \ln(1 - e^{-u_k}) \right], \quad (18)$$

where  $N_{i-1,0}$  is the number density of the ground level of  $A^{+(i-1)}$  and  $N_{i-1}$  is the number density of this ion,  $p_i$  the partition function of  $A^{+i}$ ,  $n_k$ ,  $g_k$ , are respectively the main quantum number and the statistical weight of energy level  $k$  of  $A^{+(i-1)}$ ,  $u_k$  and  $\kappa_{\text{med},k}$  are respectively  $u$  and  $\kappa_{\text{med}}$  at the frequency threshold for photons to ionize from level  $k$ . The factor  $a_i$  has a value of unity by default, but we have introduced it to correct possible discrepancies with respect to hydrogenic cross-sections. In equation (17), to be consistent with  $g_{i,\text{line}}$ , we have chosen to approximate  $\Theta_i$  in terms of  $\bar{\kappa}_{\text{med}}$  and  $\kappa_{\text{med}}$  rather than  $\bar{\kappa}_R$  and  $\kappa$  as in Alecian (1994). As stressed by Alecian (1994), the main contribution to  $\Theta_i$  comes from the ground level of  $A^{+(i-1)}$  and, owing to the rapid decrease of  $Q_k$  when higher energy levels are considered, we never encounter situations where the sum over  $k$  has any tendency to diverge. Note that contrarily to  $g_{i,\text{line}}$  (if redistribution is negligible),  $g_{i,\text{cont}}$  is not zero for the state in which the ion is completely ionized (C VII for instance).

In the present work, in order to be able to compare our results with the accelerations obtained using the tables and codes of Seaton (1997) and LMR2000, the total radiative acceleration for element  $A$  is expressed as

$$g_{\text{tot}} = \frac{\sum_i N_i (g_{i,\text{line}} + g_{i,\text{cont}})}{\sum_i N_i}. \quad (19)$$

This expression does not take into account the redistribution effects between ions nor their mobility, which should be considered when accurate diffusion velocities are needed.

## 3 RESULTS

Numerical calculations of radiative accelerations are presented using the formulae developed in the previous section. Their accuracy and their range of validity are verified by comparing them to accelerations obtained by detailed methods (Seaton 1997 and LMR2000). These computations were performed for a main sequence star with  $T_{\text{eff}} = 10000$  K and  $\log g = 4.314$  (model communicated by J. Richer, see Richer & Michaud 1993).

### 3.1 Atomic data and opacities

The above formulae involve atomic data for bound–bound transitions, and monochromatic opacities arising from each element separately. We have used the data produced by the OPACITY Project (hereafter OP, Seaton et al. 1992) because these atomic and opacity data are consistent and the radiative accelerations obtained with the improved approximate formulae presented here can be compared with those computed using the tables and codes of Seaton (1997). The atomic data have been loaded from TOPbase in CDS (Strasbourg). The opacities have been computed with the OP-tables and codes (2000 version) kindly communicated by M. J. Seaton and C. Zeippen. The OP-tables consist of original OP cross-sections files (the total cross-sections of each element are tabulated with respect to  $u$ ). The OP-codes compute  $\bar{\kappa}_R$  and  $\bar{\kappa}_{\text{med}}$  from these files for a given mixture, temperature and density. We have included these codes in ours, and we have developed our own utilities to compute (using the same tables) the monochromatic opacities needed in the formulae presented in the previous section.

### 3.2 Numerical computations of radiative accelerations

For the sake of clarity, we have chosen to present our computations for only four metals, C, Ar, Ca and Fe, which are representative of the different behaviours we have encountered among the ten elements we have considered (C, N, O, Ne, Mg, Si, S, Ar, Ca and Fe).

To validate the approximations made in Section 2 for bound–bound transitions, we want to verify if the new parametric equations can reproduce two basic aspects: (i) the ability of equation (11) to provide accelerations for vanishing concentrations, and (ii) the ability of equation (10) to reproduce the saturation effect over a large range of concentrations.

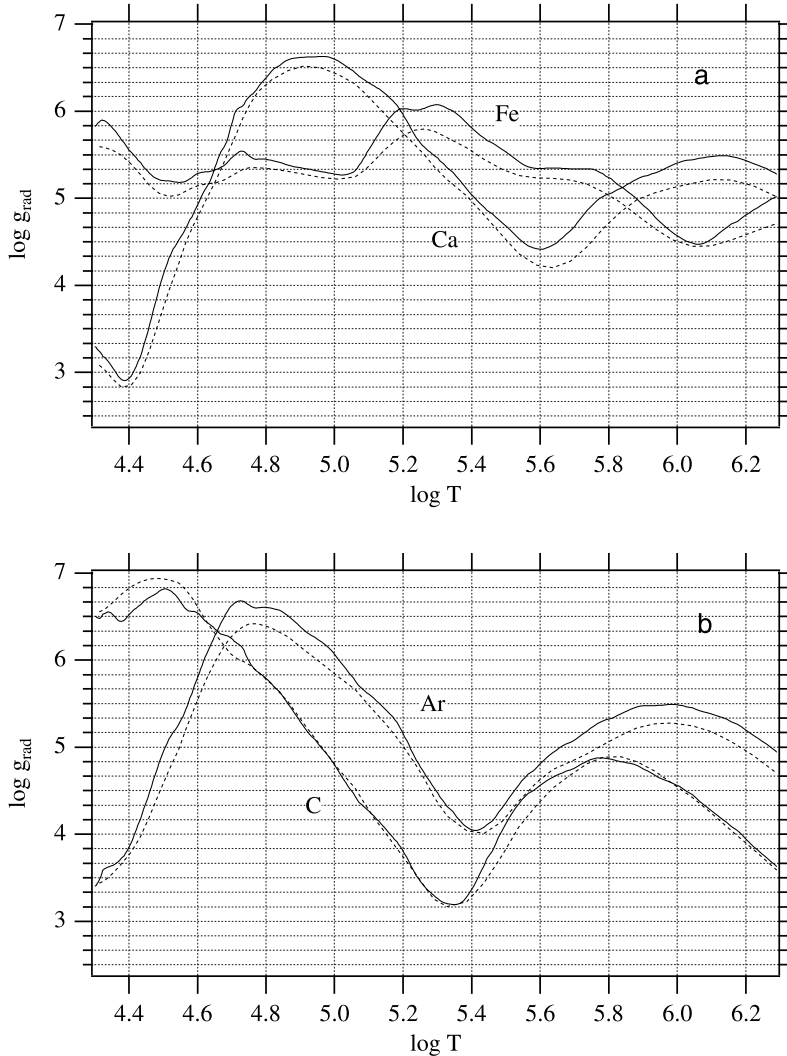
In the computations presented below, we have found that when  $\log \chi \geq 1$  for abundant elements (CNO and Fe), the assumption  $\varepsilon_{A-ii} \leq 1$  used in Section 2 is not always satisfied and even  $\varepsilon_{A-ii} > 1$  can be encountered. This means that  $C_A$  is larger than or close to  $C_{A,\text{critical}}$ . In that case we force  $\varepsilon_{A-ii} = 0.99$ . This certainly

introduces an error in the evaluation of the first term  $(1 + \xi_i C_i)$  of equation (10). When  $\log \chi = 1$ , we have found that for carbon  $0.8 < (1 + \xi_i C_i) < 1$ , therefore, we assume that this error does not have strong consequences in what follows.

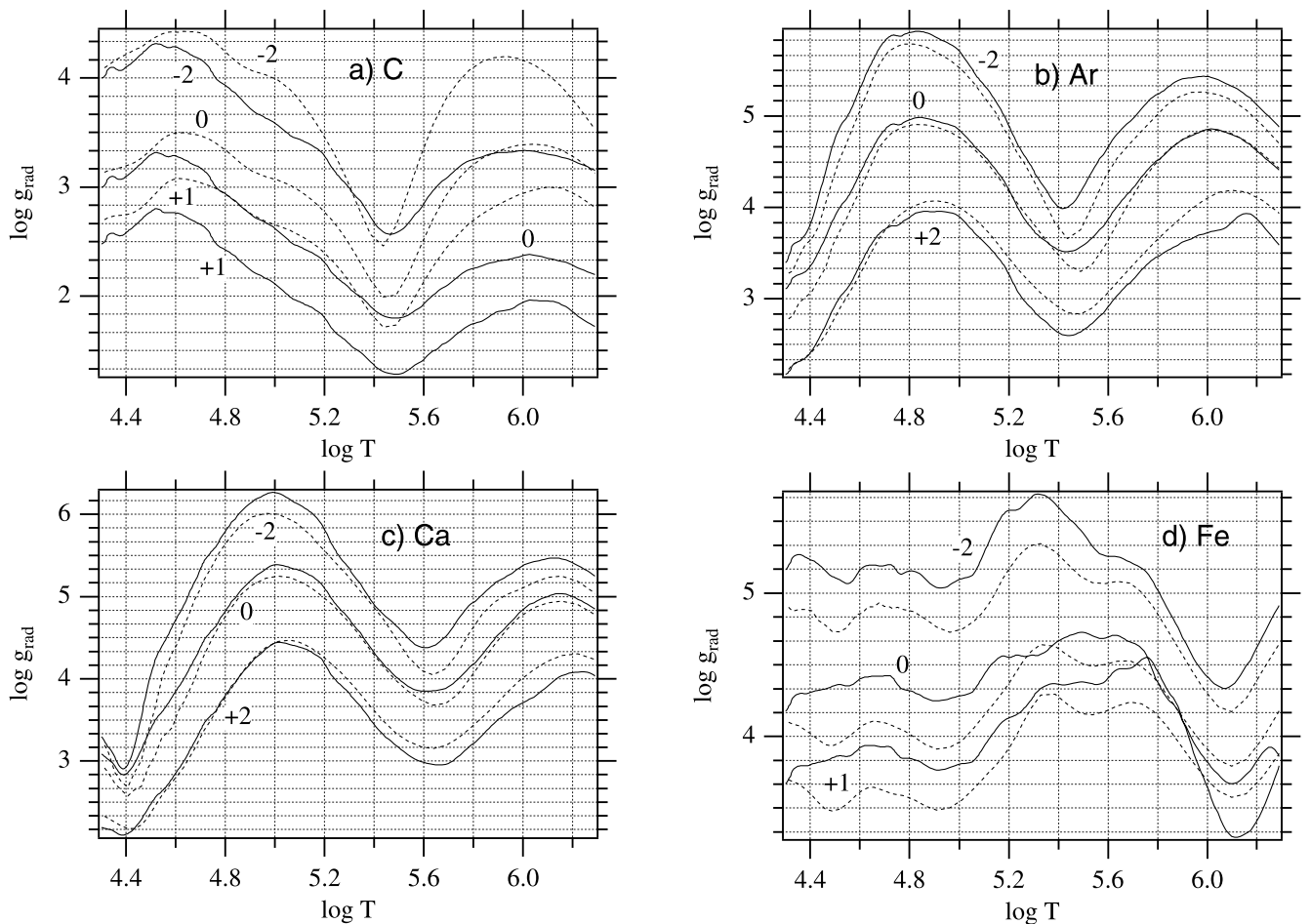
Solid lines in Figs 1(a) and (b) show  $\log(g_0)$  versus  $\log T$ , for C and Ar, and Ca and Fe, respectively. We have defined  $g_0$  as  $(\sum_i N_i g_{i,0})/N_A$ , which can be interpreted as the total acceleration arising from bound-bound transitions when the abundance of the element is vanishing. Dashed lines are the accelerations arising from lines using the detailed sampling method of LMR2000 computed for a very small abundance ( $\log \chi = -8$ ) in order to compare with  $\log(g_0)$ . However, in order to be consistent with the results of Seaton (1997) which will be used in comparisons below, the frequency grids used to calculate the radiative accelerations are not those presented in LMR2000 but are those employed in Seaton (1997). We have used the method of LMR2000 because the tables and codes of Seaton (1997) do not allow calculations at such low abundance and do not allow the separation of the contribution from bound-bound transitions from the total radiative acceleration. We

find that for a vanishing abundance ( $\log \chi = -8$ ),  $g_{i,\text{line}} \approx g_{i,0}$ , and that  $g_{i,0}$  is not sensitive to  $\log \chi$ .

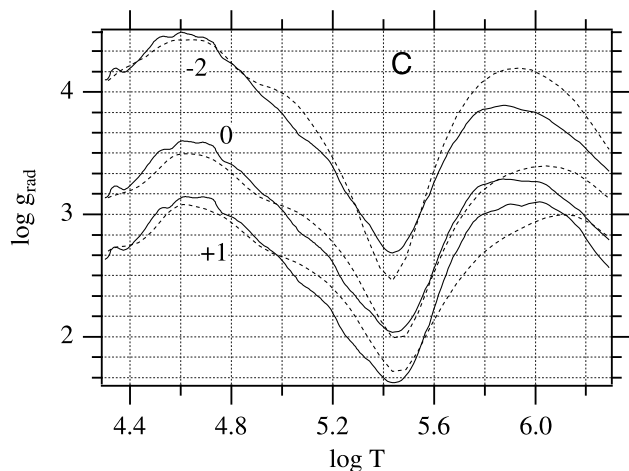
Figs 2(a)–(d) show the logarithm of the accelerations arising from bound-bound transitions of a given element  $g_{\text{line}}$ , defined as  $(\sum_i N_i g_{i,\text{line}})/N_A$ , for  $\log \chi = -2, 0, +1$  (for C and Fe) or  $+2$  (for Ar and Ca). In these figures,  $g_{i,\text{line}}$  have been computed using equation (10) while assuming  $\alpha = -1/2$ . As in Fig. 1, solid lines are the accelerations obtained using approximations of Section 2, and dashed lines those obtained by the sampling method. It appears that comparison of  $g_{\text{line}}$  against sampling is rather good for Ar and Ca over a wide range of concentrations. For both elements, the difference between the accelerations calculated using the two methods is around 0.2 dex, it tends to be around 0.4 dex for temperatures larger than  $\log T = 5.4$ . For Fe, the departure is more systematically around 0.4 dex. For C, the effect of saturations is not well reproduced. This is most likely caused by our assumption that  $\alpha = -1/2$ . In order to evaluate the importance of the role of  $\alpha$ , we have calculated radiative accelerations trying several values of  $\alpha$  around  $-1/2$ , for each ionization state of carbon. The same curves



**Figure 1.** Accelerations arising from bound-bound transitions for vanishing abundances for each element considered. The logarithm of the acceleration is shown versus the depth (logarithm of temperature). Solid lines correspond to  $g_0$  and dashed lines to accelerations obtained through the sampling method for  $\log \chi = -8$ . The acceleration  $g_0$  for a given element is a weighted sum of  $g_{0,i}$  over the ionization stages of that element (see text). (a) Calcium and iron; (b) carbon and argon.



**Figure 2.** Accelerations arising from bound–bound transitions for each element considered, obtained using equation (10), and assuming  $\alpha = -1/2$ , for three different abundances. Dashed lines are accelerations obtained through the sampling method, the  $\log \chi$  is indicated on each curve. (a) Carbon for  $\log \chi = -2, 0, +1$ ; (b) argon for  $\log \chi = -2, 0, +2$ ; (c) calcium for  $\log \chi = -2, 0, +2$ ; (d) iron for  $\log \chi = -2, 0, +1$ .



**Figure 3.** Acceleration arising from bound–bound transitions for carbon using the values of  $\alpha$  shown in Table 1. This plot can be compared with Fig. 2(a).

as in Fig. 2(a) are shown in Fig. 3 but using the values of  $\alpha$  given in Table 1. This result is quite satisfactory since the discrepancies between detailed and approximate calculations fall around 0.2 dex, except for the highest temperatures. However, these discrepancies at high temperatures could be explained by some missing atomic

**Table 1.** Adjustable parameters.

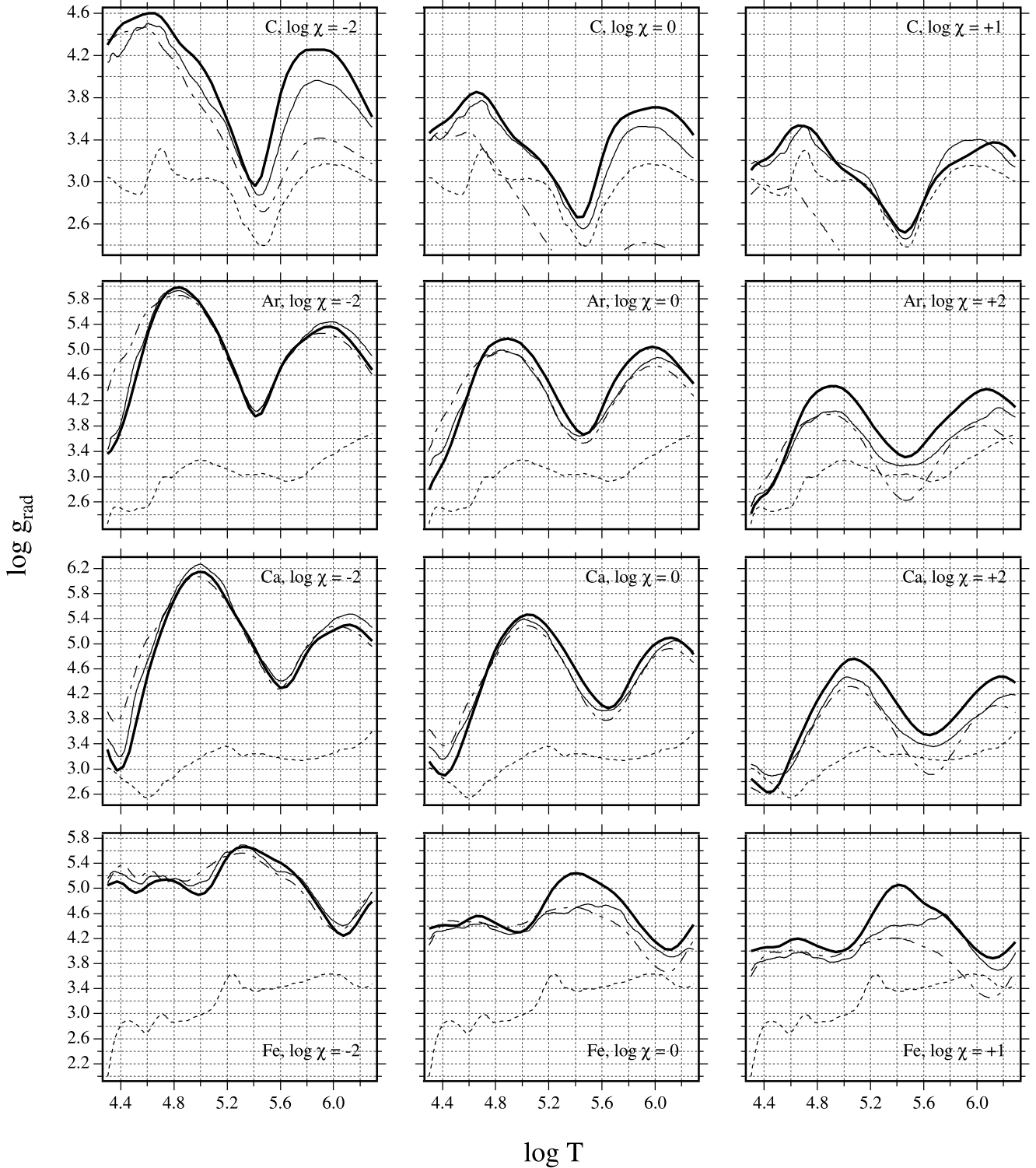
Ion	$\alpha$	$a_i$	$a_i^*$
C I	-0.5	1.	1.
C II	-0.48	1.	1.
C III	-0.48	1.	0.4
C IV	-0.4	1.	0.6
C V	-0.41	1.4	0.8
C VI	-0.29	0.3	0.1
C VII	No lines	0.15	0.25
All ions of Ar, Ca and Fe	-0.5	1.	1.

species, as compared with those included in Seaton (1997), for the evaluation of the background opacities in the detailed sampling method of LMR2000. We have not attempted to obtain more suitable values of  $\alpha$  for the ions of the other elements (Ar, Ca, Fe) since the purpose of the present paper is to validate the approximate formulae of Section 2 and not to furnish exhaustive data to use these formulae. This will be the scope of a forthcoming paper.

The final step in this study is to compare the full  $g_{\text{tot}}$  given by equation (19) to the accelerations obtained using the codes and tables of Seaton (1997). These comparisons are shown in Fig. 4. The thick solid lines are the accelerations of Seaton (1997), the thin solid lines are those obtained through equation (19), the dashed line

is the contribution of photoionization (weighted sum of  $g_{i,\text{cont}}$ ), and the short–long dashed lines are the accelerations obtained by the approximate formulae of Alecian & Artru (1990). The grid step is 0.2 dex in all of the panels. All  $g_{i,\text{cont}}$  have been computed with  $a_i = 1$  except for carbon for which they have been adjusted

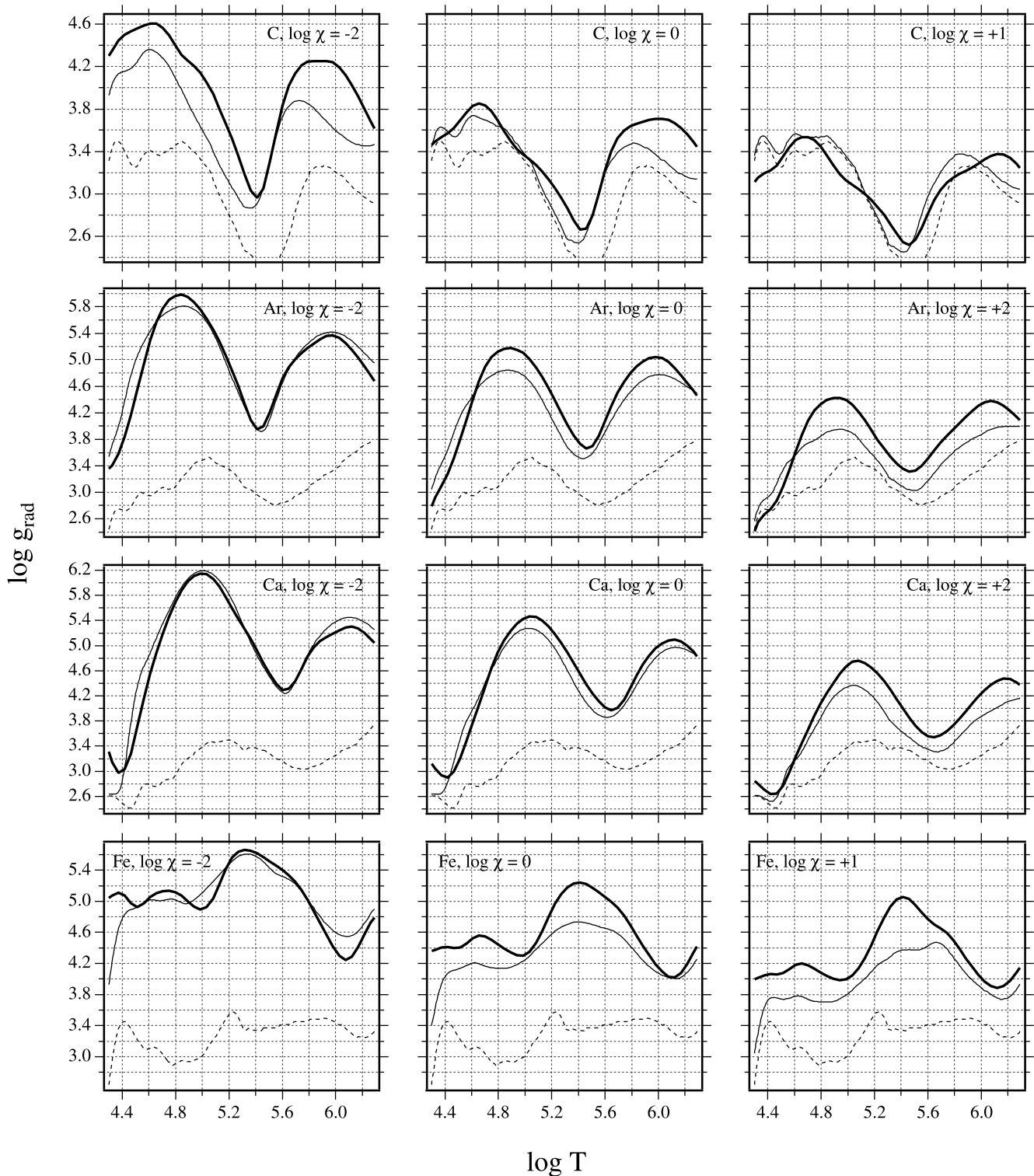
manually (see Table 1) to minimize the discrepancy with the accelerations obtained with the codes and tables of Seaton (1997). The values of  $\alpha$  are those found in the previous paragraph (see Table 1). The agreement, better than 0.2 dex for a large part of the stellar model and for a large range of concentrations, is quite



**Figure 4.** Total accelerations for each element considered and for three different abundances. The thin solid lines are total accelerations obtained using equation (19) (with the values of  $\alpha$  and  $a_i$  shown in Table 1), the dashed lines are the contributions of photoionization given by equation (16), the thick solid lines are total accelerations obtained using the codes and tables of Seaton (1997), and finally, the dashed dotted lines are the accelerations given by the formulae of Alecian & Artru (1990).

satisfactory. The discrepancy which appears for Fe around  $\log T = 5.3$  for  $\log \chi = 0, +1$ , can be explained by the fact that Seaton's tables are based on more complete atomic data than available in TOPbase, since he has included atomic fine structures for iron (OP 'PLUS' data, not used in our work). Therefore, we overestimate the

saturation effect of lines. Note also that our data for Fe do not include data for Fe I and Fe II because they are not available in TOPbase. In all cases, our equation (19) gives significantly better agreement with Seaton's accelerations than the formulae of Alecian & Artru (1990), especially, and as expected, for large



**Figure 5.** The SVP approximation for each element considered and for three different abundances. The thin solid lines are total accelerations obtained using equation (19) (with the values of  $\alpha$  and  $a_s^*$  shown in Table 1) where  $g_{i,\text{line}}$  are the SVP accelerations defined by equation (20), the dashed lines are the contributions of photoionization given by equation (16) but assuming  $\kappa_{\text{med}}/\kappa_{\text{med},k} = 1$ , the thick solid lines are total accelerations obtained using the codes and tables of Seaton (1997).



abundances and for C and Fe. For C, the better agreement at  $\log \chi = +1$  is caused by  $g_{i,\text{cont}}$  (with adjusted  $a_i$  of Table 1) which dominates  $g_{\text{tot}}$ .

### 3.3 The SVP approximation

Approximations proposed in Section 2, and leading to equation (10), separate the concentration term from those depending explicitly on the atomic data. As a consequence, detailed computation is no longer needed each time the local concentration of the element under consideration changes. This is especially useful to shorten the calculations necessary to describe the building-up of the time-dependent stratification of elements inside stars. However, the computation of expressions (11), (14) and (15), i.e.  $g_{i,0}$ ,  $C_{i,S}$  and  $\xi_i$ , has to be done at least once for each layer of a given model, and requires a large amount of atomic data. In this section, we examine the efficiency of an additional approximation we have chosen to name ‘SVP approximation’ (for Single Valued Parameters approximation). This approximation, inspired from the one proposed by Alecian & Artru (1990), reduces drastically the amount of atomic data to be processed.

Let us define two dimensionless functions  $\varphi_i$  and  $\psi_i$  such as, according equations (11) and (14):  $g_{i,0} = q\varphi_i$  and  $C_{i,S} = b\psi_i^2$ . SVP approximation is based on the fact that  $\varphi_i$ ,  $\psi_i$  and  $\xi_i$  (the dimensionless function given by equation 15) vary weakly around the layers where ion  $A^{+i}$  gives its maximum contribution to the total radiative acceleration of element A. Moreover, these quantities are weakly dependent on the stellar model.

SVP approximation consists in writing  $g_{i,\text{line}}$  as:

$$g_{i,\text{line}} = q\varphi_i^* (1 + \xi_i^* C_i) \times \left( 1 + \frac{C_i}{b\psi_i^{*2}} \right)^\alpha, \quad (20)$$

where the parameters  $\varphi_i^*$ ,  $\psi_i^*$  and  $\xi_i^*$  are the numerical values of the functions  $\varphi_i$ ,  $\psi_i$  and  $\xi_i$  in a layer where  $T = T_{\text{ion},i}$  which corresponds to the temperature of the layer where  $A^{+i}$  has its maximum relative population. Note that there is only one set of three parameters for each ion. One important point to emphasize is that equation (20) is valid only for temperatures around  $T_{\text{ion},i}$ , but allows the computation of  $g_{\text{tot}}$  for any layer in the model since the weighting by  $N_i$  in equation (19) ensures that contributions of  $g_{i,\text{line}}$  far from  $T_{\text{ion},i}$  are negligible.

The SVP approximation cannot be safely extended to the acceleration due to bound–free accelerations because  $\Theta_i$  is too sensitive to the local temperature. The only simplification we propose is to impose  $\bar{\kappa}_{\text{med}}/\kappa_{\text{med},k} = 1$  in equation (17).

Fig. 5 shows the results obtained for  $g_{\text{tot}}$  using SVP approximation for  $g_{i,\text{line}}$  and the simplification mentioned in the previous paragraph for  $g_{i,\text{cont}}$ . The parameters  $\varphi_i^*$ ,  $\psi_i^*$  and  $\xi_i^*$  are obtained using the computations presented in Fig. 4 for the largest abundances. We emphasize that the same set of these parameters (three per ion) has been used to compute  $g_{\text{tot}}$  whatever the abundance. The agreement is not as good as the one found in Fig. 4, especially for carbon for which we had to change the value of  $a_i$  for C III to C VII to reduce the discrepancy we encounter for this element (column  $a_i^*$  in Table 1). This discrepancy is mainly due to the approximation  $\bar{\kappa}_{\text{med}}/\kappa_{\text{med},k} = 1$  in the computation of  $g_{i,\text{cont}}$ . But, this simplification has been proposed only to avoid explicit use of any opacity tables in the computations of  $g_{\text{tot}}$  shown in Fig. 5, it is not necessary when  $\kappa_{\text{med}}$  and  $\kappa_{\text{med},k}$  are available. We have also verified that keeping  $\kappa_{\text{med}}$  and  $\kappa_{\text{med},k}$  in equation (17) improves the results significantly. Another source of error for carbon comes from

the fact that CV has an ideal gas configuration and is the dominating ion for a large temperature domain, and thus it is difficult to properly define  $T_{\text{ion},i}$ . It should also be noted that the values of  $\alpha$  and  $a_i$  used here were manually adjusted to obtain better results for a solar abundance of the element. A more systematic algorithm will have to be devised to adjust these parameters, but this is outside the scope of this paper. Finally, the SVP approximation appears to be rather good for the other elements (Ar, Ca and Fe), noting that no adjustments were made to the values of  $\alpha$  or  $a_i$  for these elements in the results presented here.

## 4 CONCLUSION

The new approximations proposed in this paper are undoubtedly a major improvement over the semi-analytic approximations defined by Alecian (1985), Alecian & Artru (1990) and Alecian (1994). Of course, this improvement has a cost: detailed monochromatic opacities are now involved in the functions  $\varphi_i$  and  $\psi_i$ , and a new function  $\xi_i$  (depending also on opacities) has been introduced. However, the new approximations have kept several advantages.

(i) The terms depending strongly on the local abundance are separated from those depending mainly on the atomic data. This allows much faster computation of time dependent stratifications in stars, with reasonable accuracy even for abundant elements. The requirement is to tabulate  $\varphi_i$ ,  $\psi_i$  and  $\xi_i$  for each layer of the stellar model, before the first time step of the computation.

(ii) The new approximations include an analytic approximation of the radiative acceleration arising from photoionization.

(iii) Equation (10) models the radiative acceleration on a physical basis. This is more satisfactory for understanding of the behaviour of radiative accelerations than a method using large interpolation tables. It could be easily implemented in any application where detailed opacities and atomic data are available and it can also bring us to define additional approximations (see below).

We have also proposed the SVP approximation, which is less accurate, but is extremely fast in numerical applications. In SVP approximation, the computation of the acceleration needs neither large atomic data bases nor detailed opacity tables (except if higher accuracy is needed for the contribution of photoionization). The requirement is to have tables of  $\varphi_i^*$ ,  $\psi_i^*$  and  $\xi_i^*$ . They will be produced exhaustively, with the  $\alpha$  and  $a_i$ , in a forthcoming paper. The other requirement is to have a table of atomic energy levels which are needed to compute  $\Theta_i$ , but, in any case, these atomic data are the same as those needed to compute the relative population of ions.

## ACKNOWLEDGMENTS

This research was partially funded by NSERC, and La Faculté des Études Supérieures et de la Recherche de l’Université de Moncton. One of us (FL) is grateful for a one month Visiting Professorship at the Observatoire de Paris and Université Paris 7 – Denis Diderot. We are indebted to RQCHP and CERCA for computing time with which some of our calculations were made. We also thank M. J. Seaton and C. Zeppen to have kindly communicated some parts of the OP codes and tables necessary to compute the opacities and J. Richer for providing the stellar model used for our calculations.

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## APPENDIX A

The radiative acceleration arising from a bound–bound transition  $l$  (from level  $k$  to  $m$ ) of ion  $A + i$  is given by

$$g_{il} = \frac{N_{ik}}{Am_p c N_i} \int_0^\infty \sigma_{km} F_\nu d\nu, \quad (\text{A1})$$

where  $F_\nu d\nu$  is the net energy flux transported by photons with frequency between  $\nu$  and  $\nu + d\nu$ ,  $\sigma_{km}$  is the absorption cross-section for a transition from energy level  $k$  to  $m$  at frequency  $\nu$ ,  $m_p$  is the mass of the proton,  $N_{ik}$  the number density of ion  $A^{+i}$  in level  $k$  and  $c$  is the velocity of light. Other symbols are defined in the main text.

Since we consider an optically thick medium, the diffusion approximation can be used to express the net energy flux. Then, according to the definition of the effective temperature of stars, the radiative acceleration, using same notations as equation (7), can be written as (see for instance Vauclair, Michaud & Charland 1974 and GLAM)

$$g_{il} = \frac{\pi k^4}{2h^3 c^3} \left(\frac{R}{r}\right)^2 \bar{\kappa}_R T_{\text{eff}}^4 \frac{N_{ik}}{Am_p N_i} \int_0^\infty \sigma_{km} \kappa^{-1} P(u) du. \quad (\text{A2})$$

One can note that, according to the definitions in Section 2,

$$\kappa = \kappa_{\text{med}} + \kappa_{A-il} + \frac{N_{ik} \sigma_{km}}{\rho}, \quad (\text{A3})$$

where  $\rho$  is the mass density.

The cross-section for a bound–bound transition  $l$  (from level  $k$  to  $m$ ), with normalized profile  $\phi_\nu$ , can be approximated by the classical formula (see for instance Mihalas 1978, p. 278):

$$\sigma_{km} = \frac{\pi e^2 f_l}{m_e c} \phi_\nu, \quad (\text{A4})$$

where  $e$  and  $m_e$  are respectively the values of the charge and the mass of the electron.

If we assume that the profile  $\phi_\nu$  is a Lorentz profile, and that  $\kappa_{\text{med}}$  and  $\kappa_{A-il}$  do not vary significantly in the frequency interval where the line  $l$  contributes to the acceleration, the integral in (A2) can be calculated analytically and leads to equation (6) for the radiative acceleration.