Radiation forces on highly ionized elements in stellar envelopes

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Abstract. Approximations for radiation forces are developed to study the diffusion processes of elements in stellar envelopes. This paper gives a method for computing easily radiation forces in the case of extensive atomic data base or, on the contrary, when atomic data are unknown. These approximations provide an expression for the radiation force, which is well suited for an analytical approach of the diffusion mechanisms.

The general trends of radiation forces are analyzed from the point of view of their dependence on the spectroscopic properties of different atomic ions. The whole atomic effects in the expression for radiation forces have been separated from the effects of element concentration and local plasma conditions, and then have been gathered into two parameters. The behavior of these parameters is analyzed for two isoelectronic sequences with respect to the ionic charge (up to +30). An estimation of the data at high ionization is derived on the basis of the known properties of isoelectronic sequences.

The accuracy of the proposed approximations is also discussed.

Key words: acceleration mechanisms – stars: abundances – stars: chemically peculiar

1. Introduction

Some of the abundance anomalies observed in peculiar Am and Ap stars are explained by diffusion processes occurring in internal layers (below the superficial convection zone for the Am stars) rather than in external layers as for the other anomalies. In order to study these processes, one needs to compute the forces due to absorption of photons by highly ionized elements far below the photosphere, in optically thick regions. This requires atomic data concerning mainly the bound-bound transitions (energy levels, oscillator strengths and line widths) for ions that are found in each layer. The deeper one computes the forces, the higher are the ionization stages to be considered.

There are three main reasons which lead to the development of approximations for the radiative accelerations:

(i) To achieve a rigorous computation one has to consider the momentum transferred through each atomic transition of each ion and in each layer of the stellar envelope. But the large amount of atomic data to be treated could be prohibitive. Such complete atomic data are expected to be available soon, as the result of scientific projects such as "OPACITY" (Seaton, 1987a).

(ii) It also happens that some of the atomic data are not available. At the present time, there is no data bank available for highly charged ions. A lack of precision in the computation of radiative accelerations in deeper layers makes impossible the prediction of the superficial abundance anomalies of peculiar stars older than some 10^6 yr, which is roughly the time required by elements to diffuse from deeper layers to the stellar surface (or to the bottom of the superficial convection zone).

(iii) The detailed expression of the radiative acceleration (see for instance Alecian and Vauclair, 1983; for a general review on diffusion processes) may be used in numerical computations but not easily in analytical approaches of diffusion processes in stars. An approximate expression would help to point out the dependences of the building up of abundance peculiarities on the different physical parameters.

The purpose of the present work is to find approximations for the radiative accelerations that are well fitted to the above motivations.

Michaud et al. (1976) have proposed an approximate method which is very useful for a rough estimation of the radiative accelerations. However, this method does not consider the specific atomic characteristics of the different ions (except for those with a noble-gas configuration). On the other hand, these authors use an approximate broadening formula based on the atomic data for the first ionization stages of manganese for which thermal broadening plays a dominant role. This is equivalent to consider that the line broadening is mainly thermal. Such an approximation may be justified in the stellar atmospheres, but not in deeper layers (when the optical depth at 5000 Å is stronger than about 10) where collisional broadening increases slightly faster than the thermal one. Indeed, taking into account the collisional broadening of lines may change strongly the radiation forces in the case of very saturated lines (even if the collisional line width is smaller than the thermal one by a factor of 10, see Alecian, 1979). The approximations of Michaud et al. (1976) have the advantage of being simple and they provide radiation forces for any kind of ion within a factor of about 3 in atmospheric regions (note that these approximations have still not been checked for highly ionized elements). This allows one to identify which element may be strongly over-abundant. It does not, however, lead to any quantitative prediction of observable peculiarities, especially when internal layers are involved.

On the other hand, Alecian (1985) proposed an approximate formula for radiative accelerations which is more accurate than the previous one but which requires some knowledge of the atomic data. This author gives an analytical expression for the radiative acceleration as a function of the local temperature T and two parameters depending on atomic properties (η and ζ) which are to be tabulated for each ion. In order to use this formula in deep layers of stars, one must either find the energy levels and the transition probabilities for many lines of the considered ions, or find a way to extrapolate the parameters known for low degrees of ionization towards higher ones.

In Sect. 2, some improvements of the approximations of Alecian (1985) are presented. Section 3 gives a detailed study of the previous approximations for two isoelectronic sequences and analyses the general behavior expected at high ionization degrees, using the characteristic trends of the spectroscopic properties. Section 4 presents an extensive computation using a tape recorded database. The complete results obtained for 21 isoelectronic sequences, with tables and graphs, are published in Alecian and Artru (1990, hereafter referred to as Paper II). Section 5 shows how to compute radiative accelerations using the present approximations. A discussion is presented in Sect. 6.

2. Approximate formulae for the radiative acceleration

The approximation of the radiative acceleration used in this work is basically the same as that proposed by Alecian (1985) where the radiative acceleration g_i^{rad} is expressed in the form:

$$g_i^{\text{rad}} = g_{i,0}^{\text{rad}} \left(\frac{1}{1 + \dfrac{C_i}{C_{i,0}}} \right)^{1/2}. \tag{1}$$

Here $g_{i,0}^{\text{rad}}$ corresponds to the radiative acceleration acting on one given ion (with charge i) in the limit of unsaturated lines, when the concentration C_i is vanishing. The quantity $C_{i,0}$ may be interpreted as a critical value of the concentration above which lines become saturated. Following Alecian (1985) (see also Michaud et al., 1976), the expression of $g_{i,0}^{\text{rad}}$, (in cgs units) can be written as:

$$g_{i,0}^{\text{rad}} = 5.574 \times 10^{-5} \frac{T_{\text{eff}}^4}{T} \left(\frac{R}{r} \right)^2 \frac{1}{A} \Phi_i \tag{2}$$

where T_{eff} is the effective temperature of the star, T is the local temperature, R and r represent the total and local radius of the star respectively. A, is the number of nucleons of the considered element. The quantity, Φ_i, is one of the two parameters depending on atomic properties. Its explicit form is given later on.

When the concentration C_i is larger than the critical value $C_{i,0}$, saturation of lines takes place and the radiative acceleration becomes less efficient. The concentration $C_{i,0}$ has been approximated by Alecian (1985) as

$$C_{i,0} = 9.83 \times 10^{-23} \, \bar{\kappa} N_e T^{-1/2} \Psi_i^2 \tag{3}$$

where $\bar{\kappa}$ is the Rossland mean opacity, N_e the number density of electrons. Ψ_i is the second atomic parameter introducing the line broadening effects (the profiles are assumed to be lorentzian).

The expression (1), together with expressions (2) and (3), of the radiative acceleration differs from Eq. (30) of Michaud et al. (1976) in three main features: (i) the atomic properties of individual ions are here considered in detail, (ii) these properties have been

gathered into two parameters, Φ_i and Ψ_i, which can be tabulated independently from the local plasma conditions, (iii) the lines profile has been assumed to be lorentzian.

The expressions (1), (2), and (3) correspond to the same approximations for the radiative acceleration as given by Alecian (1985) in his Eqs. (5), (6), (7), and (9). These approximations consist in assuming that, for the considered lines, the opacity of the continuum is equal to $\bar{\kappa}$, on average, and that the lorentzian component of the line profile dominates in the calculation of $g_{i,0}^{\text{rad}}$. The effect of blends is neglected. The formal differences between the expressions presented here and those of Alecian (1985) arise from the fact that the atomic parameters Φ_i and Ψ_i are expressed here in a different way. In the present work, they are defined as follows:

$$\Phi_i = \sum_l P_l f_l \frac{N_{i,l}}{N_i} = \sum_l \Phi_{i,l} \tag{4}$$

and

$$\Psi_i = \frac{\sum_l \left(\dfrac{\gamma_{i,l}}{f_{i,l} \dfrac{N_{i,l}}{N_i}} \right)^{1/2} \Phi_{i,l}}{\sum_l \Phi_{i,l}} \tag{5}$$

where f_l is the absorption oscillator strength of the bound-bound transition number l, $N_{i,l}$ the population of the initial level of the transition and N_i the population of the ion. The coefficient γ_l is the factor of the line broadening parameter depending on the specific atomic transition, the full line width at half maximum resulting from collisional broadening being expressed as $\Gamma_l = \gamma_l N_e T^{-1/2}$ (see for instance Griem, 1974).

The function, P_l, which introduces the spectral dependence of the incident radiation flux, was first defined by Michaud et al. (1976) as:

$$P_l(u) = u^4 \frac{e^u}{(e^u - 1)^2} \tag{6}$$

with the undimensioned quantity u

$$u = h\nu_l / kT \tag{7}$$

where $h\nu_l$ is the photon energy, and kT the local thermal energy.

Alecian (1985) has taken P_l as a constant ($P_l \approx 3$ or .3 for ions with rare-gas configuration). Hereafter Eq. (6) has not been approximated for the computation of Φ_i and Ψ_i in order to improve the accuracy.

3. The atomic parameters and their trends towards high ionization stages

3.1. Method of investigation

The atomic parameters Φ_i and Ψ_i defined by Eqs. (4) and (5) depend on the spectroscopic data of the absorbing ion (wavelengths, f-values and line widths) and also on the local plasma conditions T and N_e, only through P_l and $N_{i,l}$. In the following study, which is made for a star with $T_{\text{eff}} = 12\,000$ K, the values of these parameters have been considered at the depth where the ion is dominant (according to the Saha equilibrium) over the other ions of the same atom. This is justified a posteriori since Φ_i and Ψ_i

vary smoothly around this depth (T_i^* is defined as the temperature of this depth). These approximated quantities will be designated by the notation Φ_i^* and Ψ_i^*.

The extensive data of Kurucz and Peytremann (1975) were used to compute Φ_i^* and Ψ_i^* for many ions, as will be described below (Sect. 4). These data are well suited for systematic numerical computations, but they are limited to lower ionization stages ($i < 5$) and are not very accurate for ions with charge larger than 3 (the data have been corrected when errors or missing lines have been found). In this section the behavior of Φ_i^* and Ψ_i^* is analyzed with respect to the ionization degree, in order to determine how they could be extrapolated for highly charged ions. The value $i = 30$ has been chosen as a standard upper limit. Note that relativistic effects are not considered here and the limit at $i = 30$ must be considered cautiously (see Paper II).

To extrapolate the Φ_i^* and Ψ_i^* values, one can consider either series of successive ions for a given element, or an "isoelectronic sequence" of ions from successive elements (increasing Z) with the same number of electrons ($Z_e = Z - i$). The second method has been chosen here to benefit from the similarities between the spectra of ions having the same electronic structure, which should lead to smooth variations of the atomic parameters Φ_i^* and Ψ_i^*.

In a first step the parameters Φ_i^* and Ψ_i^* have been determined for a sample of ions belonging to two isoelectronic sequences. The sequences of C-like and Mg-like ions have been chosen with, respectively 6 and 12 electrons. A limited number of transitions has been introduced by selecting those which contribute strongly to the radiative acceleration and the atomic data which seem adequate for the present approach have been collected. The purpose is first to interpret these partial results with the help of the known regularities of atomic data with increasing ionization and then to predict the general isoelectronic trends of Φ_i^* and Ψ_i^*.

Due to the similarities of isoelectronic ions, these parameters are expected to show slow variations along each sequence. As an application, a simple method has been derived and detailed in Paper II, in order to estimate approximately Φ_i^* and Ψ_i^*, at high ionization, in any isoelectronic sequence.

3.2. The atomic data and their trends

Most of the spectroscopic data (level energies, wavelengths, f-values, etc. . .) vary regularly along each isoelectronic sequence, when the ionic charge i and the atomic number Z increase together ($Z_e = Z - i$ being constant). Systematic trends of energy levels and wavelengths are currently exploited in spectroscopic analyses (e.g. Edlen, 1964 and Martinson, 1977). The recent compilation of Kelly (1987) provides convenient access to up-to-date data on energy levels, wavelengths and ionization energies for almost all ions of every element below $Z = 36$. The isoelectronic behavior of oscillator strengths against Z has been extensively studied by Smith and Wiese (1971) and their useful graphs provide f-values for many important transitions in highly ionized atoms. Extrapolation formulae at high Z are also given by Mewe (1977).

At high values of the ionic charge, the general spectroscopic properties of ions can simply be predicted from the fact that their electronic structure approaches the hydrogenic limit, scaled according to the core charge $Z_c = i + 1$. In particular all the electronic configurations with the same set of quantum numbers n, but with different values of the quantum number l, become

relatively close in energy and tend to degenerate into a "complex" when i increases (Layser, 1959; see also Cowan, 1981). For example, in the Mg isoelectronic sequence (with a ground term $3s^2\ ^1S_0$) the same $3p^2\ ^1D$ level of P IV and Fe XV occurs respectively at 38% and 15% of the ionization limit. More generally, energies of the levels belonging to the ground complex increase less rapidly than the ionization limit: they vary roughly as Z_c instead of Z_c^2.

Therefore, by using isoelectronic extrapolation and simple hydrogenic approximations, it is possible to determine some wavelengths and gf-values of highly charged ions, with a sufficient accuracy for this approach.

Ionization stages up to about $i = 30$ are considered. This allows to study stellar plasmas as hot as $T = 10^6$ K. At still higher ionizations ($i > 40$) the relativistic effects would dominate the electronic structure and introduce other trends that are ignored here (e.g. Farag et al., 1980).

In what follows, the isoelectronic properties will be used either to supply the lack of detailed atomic data at high ionization, or to analyze the general behavior of the parameters Φ_i and Ψ_i at high ionization.

3.3. The plasma conditions

For the typical star model considered here ($T_{\text{eff}} = 12\,000$ K), the Saha equilibrium has been solved for each studied element and the temperature T_i^* of maximum population has been determined for each intermediate ion. This temperature may be replaced by the dimensionless ratio $\theta_i^* = kT_i^*/\chi_i$ relative to the corresponding ionization energy χ_i. For lower ions ($i < 5$), partition functions derived from extensive atomic data are used, as described in Sect. 4. Independent calculations are performed to include all possible ionization stages of heavy elements, up to iron. Ionization energies are taken from Moore (1970) or Kelly (1987). They are also available for all ions of molybdenum up to $i = 41$ (Sugar and Musgrove, 1988). This element has been chosen to show the trend of θ_i^* at high ionizations. The partition functions of highly charged ions have been approximated by an empirical function of T which takes into account the progressive population of the two lower configurations. In order to test how the calculation of θ_i^* is sensitive to the choice of the partition function, different calculations have been made, using various crude approximations, ranging from the weight of the ground term to the total weight of the ground complex: the discrepancies between the different estimates of θ_i^* remain smaller than 15%, except for the H-like ions. The values of θ_i^* calculated for Fe, Kr and Mo ions are plotted in Fig. 1. vs. the charge i. The scattering of the points shows little dependence on the electronic structure, except when a rare-gas structure is met (this is due to their large χ_i energy). In particular, strong variations of θ_i^* occur for the last three ions (Li-like, He-like and H-like) which appear for iron at $i = 24$ and 25 (see Fig. 1). The population of a given ion is dominant over a limited range of temperature which corresponds to a variation of θ_i^* of about 20% (except for ions with noble gas structure which are populated over larger regions).

In the context of the OPACITY project, Mihalas et al. (1989) have recently computed a very large number of ionization equilibria for stellar plasmas, by achieving a thorough study of the equation of state and using a tremendous amount of refined atomic data. Their detailed results have not been used, but the
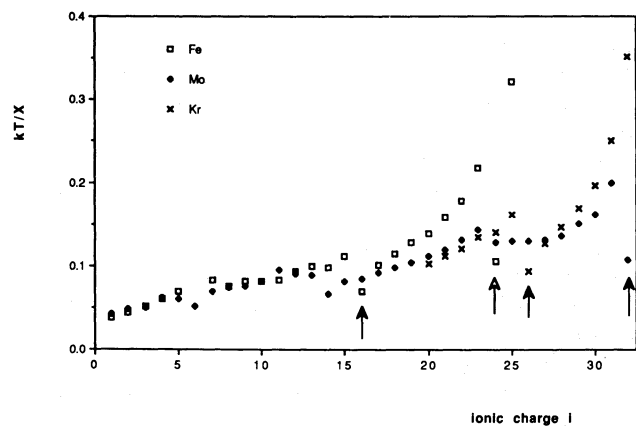
Fig. 1. Ratios $\theta_i^* = kT_i^*/\chi_i$ calculated for the ions of iron, krypton and molybdenum, versus the charge i (see Sect. 3.3). The arrows indicate He-like or Ne-like ions
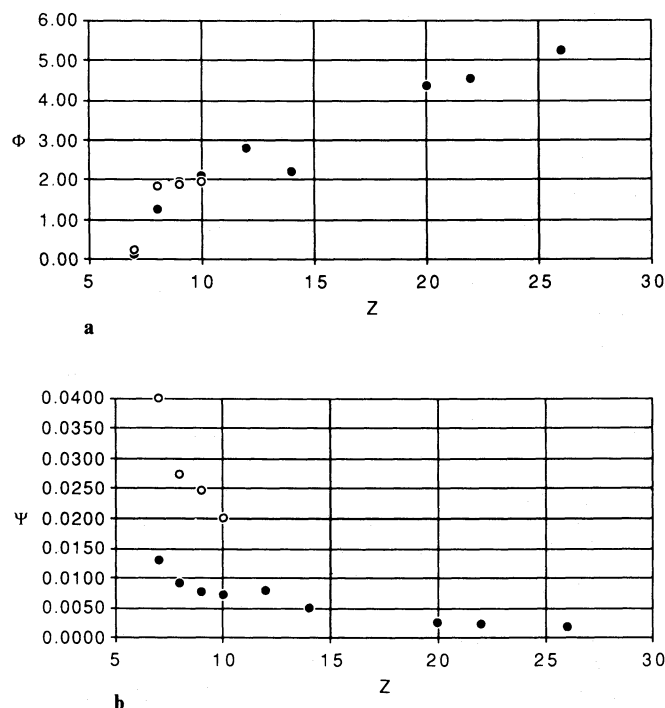
Fig. 2. a The Φ_i^* values vs. the atomic number, for the C-like isoelectronic sequence. The closed dots correspond to the detailed computations of Sect. 3. The open dots correspond to those obtained by the extensive computation of Sect. 4. **b** The Ψ_i^* values (same legend as **a**)

present evaluation of θ_i^* is in general agreement (to within 20%) with the values that can be read on their graphs (their Fig. 2).

3.4. The parameter Φ_i^*

The Φ_i^* parameter is the sum of many terms [Eq. (4)], each one giving the partial contribution of an individual transition to the radiative force, in the unsaturated case. Recall that Φ_i^* is evaluated for each ion at a specific temperature T_i^* (defined above in Sect. 3.3) which increases along the sequence.

Approximate values of Φ_i^* have been determined for a sample of highly ionized atoms by means of the following approxima-

tions. Only a few lines are considered in the sum [Eq. (4)], assuming that the main contribution to the total Φ_i^* value corresponds to a small number of low-excitation transitions of the ion. This simplification will be justified below by the comparison with the complete calculation (described in Sect. 4) at least for the first ions. Each selected multiplet (and sometimes a set of close multiplets of the same transition array) has been also treated as a single line with the total gf-value assigned to it. In order to be consistent, each partition function needed to compute the population ratio $N_{i,l}/N_i$ is deduced from the few levels which appear as lower states of the selected transitions.

To include an extra-transition in the calculation of Φ_i a term $P_l f_l g_l e^{-E_l/kT}$ has been added in the numerator and a term $g_l e^{-E_l/kT}$ in the partition function in the denominator. Therefore the resulting value is only slightly changed when adding smaller terms due to weak lines.

The atomic data were collected for several ions, up to a charge of +30, in the C-like and the Mg-like isoelectronic sequences ($Z_e = 6$ and 12 electrons). Besides the compilation of Kelly (1987), the tables of ionic energy levels is used for K, Ca, Ti, Fe (Corliss and Sugar, 1979a, b, 1982; Sugar and Corliss, 1979) and Mo (Sugar and Musgrove, 1988). When possible, oscillator strengths compiled by Wiese et al. (1966, 1969) or those derived from the graphic extrapolations of Smith and Wiese (1971) are taken. Theoretical results of Victor et al. (1976) have also been used. To complete the data (especially for transitions $\Delta n \neq 0$ in highly ionized species), the missing f-values are calculated by means of the Coulomb approximation (using the computational code described by Van Regemorter et al., 1979).

In this context, it is not attempted to extract the most refined atomic results from the literature, but rather to build a coherent set of data with reasonable accuracy. The values of Φ_i^* obtained for the chosen ions in the C-like and the Mg-like sequences ($Z_e = 6$ and 12) are given in Tables 1 and 2 (column 3) and plotted in Figs. 2a and 3a.

Table 1. Sequence of carbon

Ion	Z	Tion	Φ_i^*	Ψ_i^*	$\Phi_{i,ext.}^*$	$\Psi_{i,ext.}^*$
N II	7	15100	0.14	0.0130	0.27	0.040
O III	8	35870	1.3	0.0093	1.8	0.027
F IV	9	61680	2.0	0.0078	1.9	0.025
Ne V	10	97750	2.1	0.0072	2.0	0.020
Na VI	12	199000	2.8	0.0080		
Si IX	14	358000	2.2	0.0051		
Ca XV	20	1210000	4.4	0.0027		
Ti XVII	22	1590000	4.6	0.0023		
Fe XXI	26	2720000	5.2	0.0019		
Kr XXXI	36	8070000	5.2	0.0012		

Table 2. Sequence of magnesium

Ion	Z	Tion	Φ_i^*	Ψ_i^*	$\Phi_{i,ext.}^*$	$\Psi_{i,ext.}^*$
Al II	13	8952	1.0	0.0079	1.2	0.018
Si III	14	18190	5.0	0.0065	4.8	0.014
P IV	15	33430	6.8	0.0069	6.7	0.015
S V	16	48160	6.5	0.0068	6.3	0.013
K VIII	19	127000	3.7	0.0084		
Ti XI	22	262000	2.4	0.0099		
Fe XV	26	520000	2.3	0.0085		
Mo XXXI	42	3240000	2.7	0.0032		
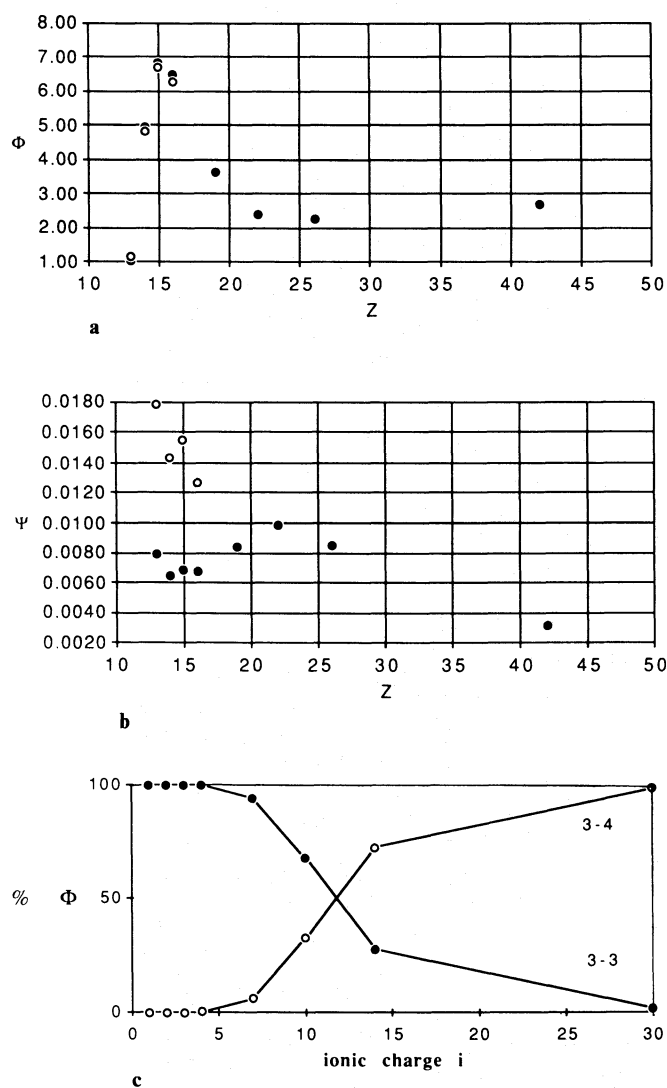
Fig. 3. a Same as Fig. 2a for the Mg-like sequence. **b** Same as Fig. 2b for the Mg-like sequence. **c** Comparison of the radiative acceleration due to the transitions $\Delta n=0\,(3\text{-}3)$ and $\Delta n\neq0$ (3-4) for Mg-like ions: the percentage of the contribution to Φ_i^* is plotted for the transitions 3-3 and 3-4, against the ionic charge i (see Sect. 3.3)

Table 3. Contribution of different transitions to the total parameter Φ_i^* in the case of Mo XXXI

		I	II
$3s^2\,^1S$	- 3s 3p ^1P	0.01	-
	- 3s 4p ^1P	0.21	0.29
$3s\,3p\,^3P$	- $3p^2\,^3P$	0.01	-
	- 3s 3d ^3D	0.02	-
	- 3s 4d ^3D	0.88	1.67
	- 3p 4p $^3S\,^3P\,^3D$	-	1.31
$3s\,3p\,^1P$	- 3s 4d ^1D	-	0.43
	- 3p 4p $^1S,^1P,^1D$	-	0.56
$3p^2\,^3P$	- 3p 3d $^3P\,^3D$	0.01	-
	- 3p 4d $^3P\,^3D$	1.55	-
Transitions: n=3 to n=5		-	1.1
Total Φ_i^*		2.7	5.4

Column I: The partial sums corresponding to the detailed calculation mainly based on known levels (reported in Table 2).
Column II: The a priori estimation of Paper II, based on rough hydrogenic approximations.

the considered sequences). As an example their relative contribution for Mg-like ions is plotted in Fig. 3c. The first type of transition ($\Delta n = 0$) is predominant at the beginning of the sequence, then its contribution decreases while transitions of the second type ($\Delta n\neq0$) become efficient higher in the sequence ($i>9$). This different behavior when Z increases is explained by the trend towards the hydrogenic limit: the values of u decreases rapidly towards zero for the first transitions ($\Delta n=0$), while it has a finite limit for the other ones ($\Delta n\neq0$) since the photon energy is exactly $\chi_i(1-n^2/(n+1)^2)$ in an hydrogenic ion. Moreover the f-value also tends to zero in the former case, instead of approaching the hydrogenic value as in the latter case (see Smith and Wiese, 1971). The above two different trends are also expected to occur in other sequences and it can be stated, as a general rule, that only the second type of transitions ($\Delta n\neq0$) are important at large i.

The previous considerations were used in Paper II to derive a simple method allowing to predict the value of Φ_i^* at about $i=30$. It was applied to all isoelectronic sequences up to $Z_e=22$ electrons (Table 2 of Paper II). For the C-like and Mg-like ions, the predicted values of Φ_i^* (13.4 and 5.4) appear larger than those obtained here for Kr XXXI and Mo XXXI (5.2 and 2.7). This discrepancy can be explained by strong transitions which have not been included in the present calculation. This is illustrated in Table 3 which compares for Mo XXXI, the partial contributions to Φ_i^* from different possible transitions. The larger value of Φ_i^* appears more realistic, although it was derived from rough hydrogenic approximations. The detailed calculations underestimate Φ_i^* because the structure of such highly charged ions is poorly known.

In spite of the remaining uncertainty on the real value of Φ_i^* at $i=30$, it appears well established that this parameter tends to increase towards high ionization. At lower ionization the behavior of Φ_i^* is different in the two sequences, namely a maximum is found for P IV in the Mg sequence. This is due to the different electronic structures: in this case some important resonance transitions with $\Delta n=0$ appears near the peak of the $P(u)$ function.

In the Mg-like isoelectronic sequence, seven multiplets which produce dominant lines in the spectra are considered: the two resonance multiplets ($3s^2\,^1S-3s3p\,^1P$ and $3s^2\,^1S-3s4p\,^1P$) and four low-excitation transitions (issued from the lower states $3s3p\,^3P$ and $3p^2\,^3P$). The data concerning the carbon sequence include eleven multiplets (the resonance triplets from $2p^2\,^3P$ to $2p^3$, $2p3s$ and $2p3d$, and the singulets issued from $2p^2\,^1D$).

The previous study has led to determine, the way in which the different transitions contribute to the total value of Φ_i^*. It can be stressed that the main cause of variation of the different terms is the factor $P(u)$ which shows a pronounced maximum around $u=4$ and decreases rapidly outside the interval $u=1-10$ (Michaud et al., 1976). Two types of transitions can be distinguished: the first ones ($\Delta n=0$) with no change in the principal quantum number of the jumping electron ($3s-3p$ or $2s-2p$ in Mg-like or C-like ions), and the other ones ($\Delta n\neq0$) especially those corresponding to a jump of n towards $n+1$ (3-4 or 2-3, in

3.5. The parameter Ψ_i

The parameter Ψ_i was introduced to take into account the progressive saturation of the lines at increasing concentration (Ψ_i determines the value of the critical density $C_{i,0}$). It has been defined [Eq. (5)] as a weighted mean of the ratios $(\gamma_{i,l}/f_l N_l)^{1/2}$ concerning individual lines. It is assumed that the line profiles are Lorentzian and that the dominant cause of line broadening in the stellar plasma conditions is the statistical quadratic Stark effect due to electron collisions (excluding the special case of H-like ions).

The collisional impact width, in energy unit, has been expressed as

$$\Gamma = \gamma_{i,l} N_e T^{-1/2}. \tag{8}$$

This variation with the temperature T and with the electron density N_e generally occurs for most of the low excitation transitions and remains valid for the considered plasma conditions (see, for example, Griem, 1974).

Systematic isoelectronic trends of line broadening constants are expected (see for example Wiese and Konjevic, 1982) but they have not been studied extensively enough in the case of high ionizations because of the lack of available data.

To evaluate the factor γ_l which contains the dependence of the line width on the specific atomic transition, the simple semi-empirical formula has been used:

$$\gamma_{i,l} = 8\,10^{-6}(i+1)^{-2}\,\Sigma n_{\text{eff}}^4 \quad \text{(in frequency unit, } s^{-1}) \tag{9}$$

where the sum applies to the effective quantum number n_{eff} of the outer electron in the initial and final states of the transition. This approximation is basically the one introduced by Griem (1968), but the original numerical coefficient has been increased here by an empirical factor (about 2.5) as suggested by Artru and Michaud (1989) on the basis of the comparison with recent theoretical results obtained for multiple ions of carbon (C III and C IV) by Seaton (1987, 1988). This formula [Eq. (9)] is similar to that used by Michaud et al. (1976) and Alecian (1985), but these authors used a smaller numerical coefficient ($2\,10^{-6}$). For simplification they have also reduced the sum Σn_{eff}^4 to $2n^4$, where n is the quantum number of the fundamental state. The present evaluation of Ψ_i takes into account the real value of n_{eff} in the computation by hand extended to high ionization degrees. However, the approximate factor $2n^4$ has been kept in the automatic computation of Sect. 4 (n_{eff} cannot be readily derived from the line data since it depends on a correct choice of the relevant ionization limit).

The values of Ψ_i derived from the previous approximations of the Stark broadening are given in Tables 1 and 2 and displayed in Figs. 2b and 3b. For the first ions, it is possible to compare the results of the detailed calculation by hand, using a limited number of lines, with those of the automatic computation (Sect. 4): the last ones are twice or three times larger. An overestimate (by a factor of about 2) can be explained by the use of the factor $2n^4$ instead of Σn_{eff}^4 [Eq. (9)] since the effective quantum numbers n_{eff} are smaller than the n values (the difference $n - n_{\text{eff}}$ is close to unity for ns and np electrons). On the contrary the results of Ψ_i obtained from the computation by hand could be underestimated (by a factor of about 1.5) because each multiplet has been included as a whole, instead of individual lines.

Of course, only an order of magnitude of the parameter Ψ_i^* is provided here, it represents a first attempt to determine quantitat-

ively the saturation effects in the deep regions of the stellar envelope.

From the results of Tables 1 and 2, it can be verified that Ψ_i^* tends to zero at increasing ionization, proportionally to Z_c^{-1}. This was expected since all other atomic quantities in Eqs. (5) and (9), corresponding to the same levels, do not vary significantly with $Z_c = i + 1$ at high ionizations when the structure tends to be hydrogenic. This property has been used in Paper II to extend the evaluation of Ψ_i^* at high ionization to other isoelectronic sequences.

Assuming this trend for the Ψ_i^* parameter and using the fact that Z_c^2 is roughly proportional to T_i^*, the limit concentration C_0 increases roughly as $T^{1.8}$ in the deep stellar layers. This means that, for a constant concentration C, the saturation effects will become less important deeper in the envelope. This was already noted by Michaud et al. (1976) in the case of Gaussian profiles.

These two different calculations of Ψ_i^* do not consider the specific effect of the high terms of spectral series although they can have very large values of the factor Σn_{eff}^4. This is a major source of uncertainty for an accurate evaluation of Ψ_i^*, since the summation of complete series in Eq. (5) would diverge and a truncation is required (such as for a partition function). However in the present approach, the Ψ_i^* parameter is defined in such an empirical way that only its order of magnitude is interesting. Using this previous underestimated Ψ_i^* means that the saturation effects are considered only for the first transitions in spectral series, which are the strongest ones. This is a reasonable choice, except for very high concentrations which would saturate most of the lines and would then require a complete treatment of the continuum absorption. This case is not expected to occur in deeper layers since it is found that the saturation effects tend to be less important than in the atmosphere.

4. Extensive computation of Φ and Ψ

The previous analysis of Φ_i and Ψ_i considers only a few low-excitation transitions. To achieve a better estimate of Φ_i and Ψ_i at least for the first ions, all bound-bound transitions which contribute to the radiative acceleration must be taken into account, as much as possible. One must also extend these computations to other isoelectronic sequences (Paper II).

4.1. Data preparation

In order to have a set of atomic data as complete as possible, the data of Kurucz and Peytremann (1975), which are recorded on tape, have been used. In some cases, these data have been updated or corrected.

As shown in the definitions of Φ_i and Ψ_i [Eqs. (4) and (5)], one needs to gather, for each ion, the values of the oscillator strengths, the energy and the weight of the corresponding initial levels. This has been done for carbon to manganese, for neutral atom to ions $+5$ (in fact neutral atom and ion $+5$ have been used essentially for the computation of the Saha equilibrium).

Fortunately, it is not necessary to consider all the known bound-bound transitions for the computation of Φ_i and Ψ_i. A selection from the complete set of the data has been made according to the following rules:

— A line contributes to the radiative acceleration when $1 \leq u \leq 12$ (around the maximum of function $P(u)$, see Michaud et al., 1976). According to the trend shown in Fig. 1 at small ionic

charges, an ion is dominant when kT lies between 5 or 10% of χ_i. This leads to: $0.05\,\chi_i \leq h\nu \leq 1.2\,\chi_i$, where $h\nu$ is the transition energy.

— The lines involving high initial energy levels with respect to χ_i are not considered since their initial levels were not sufficiently populated in the stellar layers where the ion is dominant.

— Lines with gf-value lower than 0.001 are not considered.

4.2. Atmosphere and envelope modelling

As mentioned above, ions with charge i from zero (neutral) up to five have been considered. Those of lowest charge ($i < 3$) are abundant in the stellar atmosphere, while the others are abundant in the envelope. A table of stellar temperatures, particle and electron densities is then used here including both a model of stellar atmosphere and envelope.

The model of stellar atmosphere is that of Borsenberger and Gros (1979).

The model of envelope has been obtained by using power laws ($\bar{\kappa} \approx aT^b$ and $N_p \approx cT^d$) with the coefficients shown in Table 4 (see Alecian, 1986). These coefficients (a, b, c, and d) are computed by means of polynomial regressions using tables kindly provided by G. Michaud.

4.3. Results

The values obtained for Φ_i^* and Ψ_i^* by these computations based on the extensive data of Kurucz and Peytremann (1975) are shown in Figs. 2a, b and 3a, b for the sequences C-like and Mg-like respectively and for ions $+1$ to $+4$ (open dots) and are compared to those obtained in Sect. 3 (see also Tables 1 and 2, columns 6 and 7 where these results are given as $\Phi_{i,\text{ext}}^*$ and $\Psi_{i,\text{ext}}^*$).

There is a close agreement for Φ_i^* although the number of transitions considered in the extensive computation is much larger. This confirms the fact that the low-excitation transitions (and mainly the resonance ones) give the dominant contribution to the radiation forces in the unsaturated limit (these transitions are taken into account in both computations). Indeed, for all the eight ions which are common to the two sets, the resonance lines contribute more than 75% to the sum Φ_i^*.

The discrepancies for the Ψ_i^* are much stronger and this is already discussed in Sect. 3.5.

5. How to use these approximations to compute accelerations of highly charged ions in stellar envelopes

Expressions (1), (2), and (3) provide the radiative acceleration of ions without the need to compute the detailed absorption of photons by each bound-bound transition.

The computation is split in two parts: the first one corresponds to the computation of Φ_i and Ψ_i, and depends mainly on

Table 4

T_{eff}	a	b	c	d
7240	65.7	3.224	2005	0.3797
10000	24.1	3.264	463	0.3215
12000	10.8	3.300	473	0.3533
14000	5.68	3.326	437	0.3703

the atomic properties of ions; the second one, which leads to the determination of radiative acceleration, depends only on the stellar model (if one excepts the use of Φ_i and Ψ_i).

5.1. The computation of Φ_i and Ψ_i

To compute the radiative acceleration of an ion i, three situations may occur:

(i) If atomic data are available, one has to compute Φ_i and Ψ_i at each stellar layer where the considered ion may contribute to the radiative acceleration, and then to compute $C_{0,i}$ and $g_{i,0}^{\text{rad}}$. This allows the determination of g_i^{rad} with very little computer time.

(ii) If atomic data are unknown (or not compiled), one has to use the extrapolated values of Φ_i^* and Ψ_i^* (as published in Paper II).

(iii) If one needs an analytical expression of the radiative acceleration, one has to assume Φ_i and Ψ_i constant around T_i^* and use the values of Φ_i and Ψ_i obtained by method (i) or Φ_i^* and Ψ_i^* by method (ii).

For ions having a rare-gas structure, the last two methods must be used with care since the temperature range for which these ions are populated may be too wide as already mentioned in Sect. 3.3 (remember that Φ_i^* and Ψ_i^* are equal to Φ_i and Ψ_i for the layer in which $T = T_i^*$).

5.2. The computation of the radiative accelerations

In order to compute the radiative acceleration of an element X in a stellar envelope, in a given range of local temperatures, the following procedure may be proposed:

(a) Tabulation of $\bar{\kappa}$, T, N_e, r

Possible approximation: one may use the coefficients of Table 4 to compute the density and mean opacity at each layer assuming $R/r \approx 1$.

(b) Determination of which ion X_i is dominant in each layer of the model.

Alternative crude approximation: one may use the trend shown in Fig. 1.

(c) Computation of Φ_i and Ψ_i and $C_{i,0}$ in each layer and for each ion X_i.

Possible approximation: use the extensive tables of Φ_i^* and Ψ_i^* of Paper II.

(d) Once the g_i^{rad} are computed, evaluation of the total radiative acceleration g^{rad} using the following approximation (generally valid in internal layers only, not in the atmosphere):

$$g^{\text{rad}} = \frac{\sum N_i D_i g_i^{\text{rad}}}{\sum N_i D_i} \tag{10}$$

where D_i is the diffusion coefficient of ion i (see for instance Alecian and Vauclair, 1983).

Possible approximation: if the Φ_i and Ψ_i are the ones of Paper II, one may take for a given layer with temperature T:

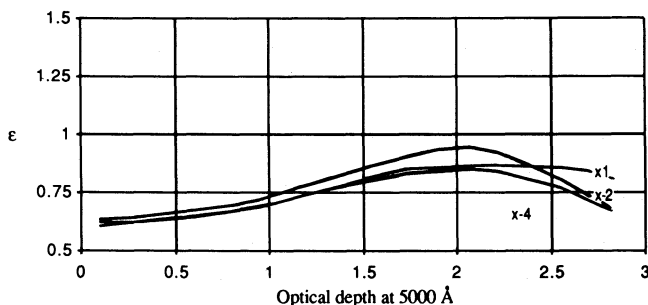$$g^{\text{rad}} \approx g_i^{\text{rad}} \quad (i \text{ being the dominant ion in the layer}). \tag{11}$$

6. Discussion

6.1. Comparison with detailed computations of radiative accelerations

In order to check the approximations (1), (2) and (3) an accurate computation of the radiative accelerations has been made for one

Fig. 4. Comparison of the radiative accelerations for Ti III, obtained by approximations of Eq. (1), (2), and (3), over those given by the complete computation with the code used for the study on gallium by Alecian and Artru (1987). The ratio ε of the two kinds of results are given vs. the logarithm of the optical depth at 5000 Å. This figure shows three curves which are labeled as follows: x 1 for the solar abundance, x-2 for 10^{-2} time underabundance, x-4 for 10^{-4} underabundance. In the three cases, the approximated method agrees to better than 25% for layers where Ti III is dominant ($1 < \log \tau_{5000} < 2.5$)

element using the same code as Alecian and Artru (1987) for their study on gallium. The radiative accelerations have been compared to those obtained by the above approximate method. One must remember that this method is intended to be used in stellar envelopes where physical conditions are very different from atmospheres. The accurate computation, with the code of Alecian and Artru (1987) just mentioned, can be done for atmospheres and for the upper envelope's layers only. One must therefore make the comparisons where both methods (the accurate one and the approximate one) are valid. The following conditions must therefore be realized.

This test must be done:

— in an optically thick region (because it is the validity domain of the present approximations), the upper envelope's layers;

— in the case of complex spectrum for which atomic data are available with many energy levels and oscillator strengths, in order to test some of the approximated sums of Eqs. (1) to (5);

— for an ion whose lines do not lie at wavelengths close to strong hydrogen absorption features, since this is typically an atmospheric effect;

— by forcing the line broadening to be Lorentzian (this is strongly inadequate in the atmosphere, however, this must be done here to compare like with like).

Ti III, which satisfies the previous constraints, has been chosen and computation has been carried out in layers with optical depths at 5000 Å from $\tau \approx 1$ to 10^3, this deeper layer corresponding to about $T = 38\,000$ K (cf. situation (i) mentioned in Sect. 5). The ratio $\varepsilon = [\text{approximation}]/[\text{accurate computation}]$ is shown in Fig. 4. The computations have been made assuming three different concentrations of Ti: x1 for solar abundance, x-2 for 10^{-2} underabundance, x-4 for 10^{-4} underabundance. These three cases correspond respectively to very saturated, slightly saturated and unsaturated lines of Ti III. One can see that for all cases, the approximation gives g_i^{rad} agreeing to within better than 25% for layers where Ti III is dominant ($1 < \log \tau_{5000} < 2.5$).

6.2. The effect of the effective temperature on Φ_i and Ψ_i

All computations described above have been made in the case of main sequence stars having $T_{\text{eff}} = 12\,000$ K. This effective tem-

perature has been chosen because it corresponds to a typical value for Ap stars, however, the effective temperature of Am and Ap stars extends from about 7000 K to 15 000 K. The first guess was that the values of Φ_i^* and Ψ_i^* will not be very sensitive to T_{eff}, because ions are dominant roughly at the same local temperature. This hypothesis is verified for about one third of the 73 ions with charge i smaller than 5 that are considered in the extensive computation of Paper II. For these ions, Φ_i^*, and Ψ_i^* are modified by less than 5% when T_{eff} is changed by about 20% around 12 000 K. However, the other two thirds of the ions are more sensitive to T_{eff}. For most of them, Φ_i^* and Ψ_i^* are changed by less than 20%. In extreme cases like Si II or P II, the change may be as strong as a factor of 5. No systematic trend has been found for this effect. The variation, with respect to T_{eff}, is mainly due to the uncertainty on the location of the layers where ions contribute strongly to the radiation force. Indeed, the relative population of an ion, close to its maximum, is flat with respect to the local temperature T, while the function $P(u)$ can be very sharp.

6.3. Estimated accuracy

Two levels of approximations have been proposed, the first one concerns the set of expressions (1), (2), and (3).

It has been verified in Sect. 6.1 that these first level approximations (Sect. 2) are accurate within about 25%. This corresponds to the internal accuracy of the method (beyond the physical hypotheses).

The second level of approximation corresponds to the extrapolations of Φ_i^* and Ψ_i^* as exposed in Paper II. The quality of this approximation, which is used in case of unknown atomic data or when analytical expression of g^{rad} is needed, is much more difficult to evaluate. However, it is based on usual methods of approximation of atomic data and its accuracy has been evaluated to better than a factor of 2.

The present results must be compared to the previous approximation proposed by Michaud et al. (1976). These authors have assumed $\overline{P(u)} \approx 3$ with $\Sigma f = 1$, except for rare-gas-like and H-like (this would give here $\Phi_i^* = \overline{P(u)} \approx 3$). For some isoelectronic sequences, the same order of magnitude is obtained for Φ_i^* (see Table 2 of Paper II). In this case, both approximations agree, at least in the unsaturated limit. However, other sequences have much larger Φ_i^* (up to 46) because of the presence of equivalent electrons increasing the total oscillator strengths.

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