Atomic Inputs to Calculate Radiative Forces in Stellar Models

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1 Introduction

Photoabsorption processes imply momentum transfer from the radiation flux to the atomic absorbers in a plasma. The resulting radiative forces act selectively on different chemical species. According to the local imbalance between gravitational $\mathbf{g}$ and radiative accelerations $\mathbf{g}_{\rm rad}$ in a star, a given element can diffuse up or down in layers where mixing hydrodynamical processes are negligible. Effects of chemical stratification occurring during stellar lifetimes are observed as peculiar surface abundances. The diffusion of strongly absorbing species can ultimately influence the evolutionary path of the star and might affect its pulsational stability.

Standard stellar evolution codes assume homogeneity of chemical composition throughout the star (except in nuclear reaction zones). Rosseland opacities $\kappa_{\rm R}$ are interpolated from a grid of plasma conditions in T (temperature), ρ (density) and X, Y, Z (mass fractions of hydrogen, helium and 'metals'). The relative abundances of metals are held fixed in Z.

When including atomic diffusion in stellar models, local under- or over-abundances may develop. Because of their influence on radiative accelerations but also on the Rosseland opacity these local variations of the metallic relative abundances in Z have to be taken into account. This increases the number of free parameters and precludes the use of precalculated data. One has to turn to in-line computations. Very efficient and finely tuned methods must be found as the Rosseland opacity and the radiative accelerations for many elements must be computed at each layer and each evolutionary step of the star for several iterative steps.

2 Radiative Accelerations on an Ion

The radiative acceleration on an element A in the ionization state k at radius r in a star is given by:

$$g^k_{\rm rad}(A) = \frac{L_{\rm rad}(r)}{4\pi r^2 c}\,\frac{\kappa_{\rm R}}{X_{A,k}}\int_0^\infty \frac{\tilde{\kappa}_{A,k}(u)}{\kappa(u)}\,\mathcal{P}(u)\;{\rm d}u \tag{1}$$

where $L_{\rm rad}(r)/4\pi r^2 c$ is the total radiative momentum flux at r, $\kappa_{\rm R}$ is the Rosseland opacity, $X_{A,k}$ is the mass fraction of the ionization state, $u = \frac{h\nu}{kT}$ is the dimensionless frequency variable, $\kappa(u)$ is the total opacity at frequency u, and $\tilde{\kappa}_{A,k}(u)$ is the opacity for the ion under consideration (corrected for the fact that only that part of the photon momentum absorbed *and* transfered to the final ion is needed; see below). $\mathcal{P}(u)$ is the normalized black body flux:

$$\mathcal{P}(u) = \frac{15}{4\pi^2} \frac{u^4 \mathrm{e}^u}{(\mathrm{e}^u - 1)^2} \ . \tag{2}$$

The frequency dependent factor $\mathcal{P}(u)/\kappa(u)$ appears because the 'diffusion' approximation for the radiative flux is assumed. Hence Eq. (1) is relevant only for stellar envelopes. In atmospheres the actual flux should be used. The value of $g^k_{\mathrm{rad}}(A)$ depends on the competition for the photons between the ion and the other elements. Increasing the abundance of the element leads to saturation and may also modify the radiative acceleration on the other elements.

Total monochromatic opacities must first be computed:

$$\kappa(\nu) = \sum_A \kappa_A(\nu), \qquad \kappa_A(\nu) = \sum_k \kappa_{A,k}(\nu), \qquad \rho\kappa_{A,k}(\nu) = \sum_{\substack{\text{transitions} \\ \text{i}\rightarrow\text{j}}} N_i \sigma_{ij}(\nu) \ . \tag{3}$$

where N_i is the population density of the absorbing state i (of the ion A, k), and $\sigma_{ij}(\nu)$ the cross section for the transition. This requires data for energy levels, oscillator strengths and line profiles for bound-bound absorptions, as well as photoionization cross sections for bound-free absorptions. All these data for all main contributors to the Rosseland opacity are now available or can be derived from recent large atomic data banks.

In the modified opacity $\tilde{\kappa}_{A,k}(\nu)$ of Eq. (1), bound-bound contributions are summed as in Eq. (3). But for bound-free absorptions two modifications occur. First, two ionization states are involved in the process. The state k for which we want the acceleration is the *final* ion. The photoionization cross sections one has to use are those of the previous $(k-1)$ state. Second, in such a process, only a part of the absorbed photon momentum is transmitted to the final ion (the rest goes away with the photoelectron). This implies the use of modified cross sections, usually written $\tilde{\sigma}_{ij}(\nu) = f_{\mathrm{ion},ij}(\nu)\, \sigma_{ij}(\nu)$. This second point applies as well to free-free absorptions. f_{ion} is an atomic parameter almost absent in the literature (more details in an accompanying contribution [1]).

3 Diffusion of an Element

For reasons of rapidity and efficiency the diffusion of an element A is treated as a whole, and not through its individual ions. The effective radiative acceleration to be used to study the diffusion of A is some average of its ion accelerations. The approach is to weight $g^k_{\mathrm{rad}}(A)$ with the ion population times its diffusion coefficient:

$$g_{\mathrm{rad}}(A) = \frac{\sum_k N_k D_k \ g^k_{\mathrm{rad}}(A)}{\sum_k N_k D_k} \ . \tag{4}$$

For an ion diffusing in a bath of protons, one roughly has $D_k \propto 1/z_k^2$, where z_k is the net charge of the ion (an estimate for neutrals ($z_k = 0$) leads to an effective approximate value $z_k \simeq 0.1$). The process of averaging enhances the weight of less ionized states.

Redistribution processes have to be taken into account too. Following a bound-bound absorption, an ion may be ionized through (electronic) collisions before being deflected (by protons). Thus the ionization state in which the ion diffuses before being deflected may differ from the one in which the photon was absorbed. As the diffusion coefficients depend on the charge of the ion, the previous average has to be modified to take this effect into account. Only rough approaches are used at the moment. Precise computations would require large sets of collisional data.

4 Calculations of Radiative Accelerations

4.1 Smoothed Background Procedure

Systematic attempts ([2], [3], [4]) to calculate radiative accelerations were performed using the TOPbase data bank [5] calculated by the Opacity Project group ([6], [7]). The method is that explained in [8]. The radiative acceleration from each transition is calculated separately and then summed. The total opacity $\kappa(u)$ is divided into two parts: the opacity of the transition under consideration and a background opacity. The latter is a constant in the frequency interval Δu that contains the natural frequency of the line. It is computed by evenly distributing other bound-bound cross sections in the interval.

The method is motivated by the fact that the background opacity has to be computed only once to get the acceleration of all the ions. It allows a good treatment of saturation. Electron recoil, averages with diffusion coefficients and redistribution can be included. However evenly distributing in an interval all lines falling in that interval artificially fills the valleys in the background opacity. Thus at low temperatures when line widths are small this method underestimates exact accelerations. It is also too time consuming to be used in-line in present evolution codes.

4.2 Opacity Sampling Procedure

In [9] and [10] another approach was used to calculate radiative accelerations. At a given temperature and density an opacity spectrum is pre-computed for each element at given points on a certain frequency grid (opacity sampling). Then Eq. (1) is directly integrated. The method is accurate in as much as the sampling is sufficient not to miss important lines in the elements. Hence the lower the temperature, the finer the grid mesh should be. Optimization of the number of grid points and use of an non-evenly spaced grid are discussed in [11].

Actual computations ([9]) were done based on the OPAL opacities for the 21 most abundant elements ([12], [13], [14], [15]). Opacities obtained from OPAL are already summed on the ionization states. Radiative acceleration on an element A is then calculated according to:

$$g_{\rm rad}(A) = \frac{L_{\rm rad}(r)}{4\pi r^2 c}\,\frac{\kappa_{\rm R}}{X_A}\int_0^\infty \frac{\kappa_A(u)}{\kappa(u)}\,\mathcal{P}(u)\ {\rm d}u\ . \tag{5}$$

This expression is simply the momemtum absorbed from the radiation. It assumes that this momentum is entirely transfered to the element A. Though the effects of electron recoil, averaging over the ions or redistribution are not included with this use of elemental opacities, the gain in computation time obtained by not treating ions individually allows one to calculate radiative accelerations in-line in stellar evolution codes for any given chemical composition ([16], [17]). A correction factor can also be pre-computed ([9]) wich is simply the ratio of the radiative accelerations of an element calculated with and without these corrections.

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