Abstract. This review presents basic equations for the solution of the NLTE radiative transfer problem for trace elements and methods for its solution are summarized. The importance of frequency coupling in radiative transfer in stellar atmospheres is emphasized.

1 Introduction

A stellar atmosphere is the transition between the dense optically thick stellar core and the transparent interstellar medium. It is the boundary layer of a star and it is the only part of the star we can see directly. Knowledge of the stellar atmosphere is a gate to the investigation of the stellar interior, and, consequently, to stellar evolution processes. The radiation passing through it serves not only as an information tool describing what is happening there, but it also significantly modifies the stellar atmosphere itself. This makes the task of determining the emergent radiation from the star highly nonlinear and therefore also complicated.

Since the stellar atmosphere is a transition from the optically thick stellar interior to optically thin interstellar medium, the corresponding radiative transfer equation for the whole atmosphere cannot be subject to global simplifications. For the optically thick part of the atmosphere the diffusion approximation is valid. Radiation propagates forward slowly resembling the process of diffusion. This approximation greatly simplifies the radiation transfer equation. However, the diffusion approximation is unusable for the optically thin part of the atmosphere. The situation there is again simple from another point of view. Since the medium is optically thin, very little interaction with matter occurs there, which often allows us to neglect absorption and to take into account only emission. Between these two relatively simple regions there is a transitional region, where neither diffusion nor optically thin approximations are valid. We have to solve the full set of radiative transfer equations together with many constraint equations, which introduce the dependence of the absorption and emission coefficients on radiation and which make the problem to be solved highly nonlinear.
Radiation carries information about the medium where it was created. In stellar atmospheres, it has an additional role. Since the photon mean free path is much larger than the particle mean free path, radiation in stellar atmospheres influences the matter far from the place where it is formed, sometimes very significantly. It changes the population numbers of particular atomic energy levels, sometimes very far from the equilibrium values. These changes then influence spectral lines, which are observed by us. Radiation also transfers energy causing heating (or cooling) of specific parts of the stellar atmosphere. In some cases radiation has such an enormous effect on the atmospheric matter that it becomes the basic reason for a stellar wind, which is then called as ‘radiatively driven’. All these crucial effects of radiation influence the transfer of radiation, which becomes strongly nonlinear.

2 Model stellar atmosphere

Construction of a stellar atmosphere model is a standard task of stellar atmosphere physics. It may be considered as a task to determine space distribution of basic macroscopic physical quantities \( \mathbf{r} \) is the position vector and \( \nu \) is the frequency, temperature \( T(\mathbf{r}) \), electron number density \( n_e(\mathbf{r}) \), density \( \rho(\mathbf{r}) \), velocity \( \mathbf{v}(\mathbf{r}) \), radiation field \( J(\nu, \mathbf{r}) \), population numbers \( n_i(\mathbf{r}) \) of the level \( i \), and others by solving equations for energy equilibrium (which determines \( T \)), radiative transfer (\( J \)), statistical equilibrium (\( n_i \)), state equation (\( n_e \)), continuity equation (\( \rho \)), equation of motion (\( \mathbf{v} \)), and possibly also some other. For the simpler case of a static atmosphere in radiative equilibrium, equations of continuity and motion are replaced by the hydrostatic equation (which determines \( \rho \)) and the energy equation simplifies to the equation of radiative equilibrium. Even in the static case the system of equations is quite complicated and further simplifications are often used. Once the atmospheric structure is known, detailed radiation field specific intensity \( I(\nu, \mathbf{n}) \) for each direction \( \mathbf{n} \) can be calculated by a simple formal solution of the radiative transfer equation.

The final goal of stellar atmosphere modelling is straightforward. We want to compare the theoretical emergent radiation with that detected by observational instruments. In principle, it is possible to determine a detailed emergent radiation energy distribution from scratch (together with a model atmosphere). Due to the need to know many details of the emergent spectrum, both the number of variables which need to be determined and consequently the number of equations to be solved become enormous. To make the problem tractable, this task is usually not solved at once, but it is divided into particular steps. First, the model atmosphere (preferably NLTE) is calculated by taking into account all substantial contribution of both physical processes and atomic data. Minor chemical elements and weak lines need not be taken into account in a great detail providing they do not influence the atmosphere structure significantly. Then the emergent radiation is calculated for a given model atmospheric structure taking into account all details of the chemical composition and line profile structure including the weakest lines.

Alternatively, it is possible to insert an intermediate step after the model atmosphere calculation, namely we may determine the NLTE level populations of
some ions not significantly influencing the atmospheric structure (trace elements) more accurately, and to solve the coupled set of radiative transfer and statistical equilibrium equations for them. For this restricted case with a given model atmosphere (i.e. $T$ and $\rho$ are fixed) we do not solve the radiative and hydrostatic equilibrium equations and we solve only the radiative transfer and statistical equilibrium equations. This is the case of the NLTE line formation of trace elements in stellar atmospheres, which is the subject of these proceedings. In this case, we have to account for full angle and frequency dependence of radiation. In the subsequent step of emergent radiation calculation, they are considered as given. Note that in all steps the radiative transfer equation has to be solved.

3 Basic equations

3.1 Radiative transfer equation

The full radiative transfer equation for the specific intensity of radiation $I(r, n, \nu, t)$ in three dimensions reads (Mihalas, 1978, Eq. 2-24)

$$\frac{1}{c} \frac{\partial I(r, n, \nu, t)}{\partial t} + (n \cdot \nabla) I(r, n, \nu, t) = \eta(r, n, \nu, t) - \chi(r, n, \nu, t) I(r, n, \nu, t). \quad (3.1)$$

Here $\eta(r, n, \nu, t)$ is the emissivity and $\chi(r, n, \nu, t)$ is the absorption coefficient (opacity). In some mathematicians’ language this equation becomes a “7D” equation (3 spatial dimensions, 2 directional cosines, time, and frequency). However, in the following, we shall use the notation “xD” referring only to the spatial dimensions. To describe fully the stellar atmosphere with all its properties and possible features (imagine a picture of the closest star – the Sun), it is necessary to use the full 3D radiative transfer equation. This is a huge task and it may hardly give any reasonable results, even using contemporary fast computers.

However, in some situations it is possible to use various simplifying assumptions. The basic common assumption is the assumption of stationarity, which means that all $\partial/\partial t \to 0$, thus, all quantities are time independent. This assumption is used very often, however, it does not mean that it is necessarily always valid. Observational data are always averages over a certain time interval, which is usually much longer than the typical time scale for rapid changes in the atmosphere. This is, of course, true for distant objects, like most stars (where we have to collect enough light), but it fails for the closest star, our Sun. Nonetheless, in the following, we shall assume that the stationarity assumption is justified.

Fig. 1. Schematic picture of the plane-parallel stellar atmosphere. Specific intensity of radiation depends on a $z$-coordinate, on the angle cosine $\mu = \cos \theta$, and on frequency $\nu$. 

\[\text{\[\theta/\]}
\[\text{x} \]

\text{\[\text{Fig. 1. Schematic picture of the plane-parallel stellar atmosphere. Specific intensity of radiation depends on a $z$-coordinate, on the angle cosine $\mu = \cos \theta$, and on frequency $\nu$.}\]}


If the stellar atmosphere is very thin compared to the stellar radius, then its curvature may be neglected and close parallel rays stay almost nearly parallel throughout the atmosphere. Then we can assume that the atmosphere is an infinite thin horizontally homogeneous plane. Such model stellar atmosphere is called plane-parallel (Fig. 1). This is a very common assumption, which simplifies the geometry of a problem, it allows to use a 1D radiative transfer equation instead of the full 3D one. Then, the radiative transfer equation takes the form (in the following we will often use the common notation convention $I(\nu) \rightarrow I_\nu$)

$$
\mu \frac{dI_{\mu\nu}(z)}{dz} = \eta_\nu(z) - \chi_\nu(z)I_{\mu\nu}(z) = \chi_\nu[S_\nu(z) - I_{\mu\nu}(z)],
$$

(3.2)

where $\mu = \cos \theta$ is the angle cosine of the ray and $S_\nu = \eta_\nu/\chi_\nu$ is the source function. Note that the one-dimensionality of equation (3.2) means that the physical quantities depend only on one coordinate ($z$). The radiation field fills the whole space in and full angle dependence is taken into account, of course, with inherent symmetries, which allow to use only one angle cosine.

If the stellar atmosphere is not thin compared to the stellar radius, the plane-parallel assumption may become invalid (e.g. for limb radiation calculations). Then another very common simplifying assumption, which also leads to one-dimensional atmosphere, may be used. It is the assumption of spherical symmetry. This assumption is useful for the treatment of extended atmospheres. The radiative transfer equation (3.1) then takes the form

$$
\mu \frac{\partial I_{\mu\nu}(r)}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I_{\mu\nu}(r)}{\partial \mu} = \eta_\nu(r) - \chi_\nu(r)I_{\mu\nu}(r).
$$

(3.3)

Here $r$ is the radial coordinate and $\mu = \cos \theta$ is again the angle cosine of the ray, as in the plane-parallel case.

Alternatively, if we introduce the so-called variable Eddington factor $f_\nu = \frac{1}{2} \int_{-1}^{1} \mu^2 I_{\mu\nu} \, d\mu/J_\nu$ \cite{Auer & Mihalas, 1970}, we may write this equation as a 2nd-order differential equation for the first moment of the intensity $J_\nu = \frac{1}{2} \int_{-1}^{1} I_{\mu\nu} \, d\mu$ (the mean intensity),

$$
\frac{d^2[f_\nu(z)J_\nu(z)]}{d\tau_\nu^2} = J_\nu(z) - S_\nu(z),
$$

(3.4)

where $d\tau_\nu = -\chi_\nu \, dz$ is the optical depth. Opacity ($\chi_\nu$) and emissivity ($\eta_\nu$) in the radiative transfer equation depend not only on local temperature and density, but also on radiation, which may propagate much longer distances than the mean free path of particles. This makes the problem non-local and non-linear.

Equation (3.4) has to be supplemented by boundary conditions, which for the case of the stellar atmosphere may be

$$
\frac{d}{d\tau_\nu}[f_\nu(z)J_\nu(z)] = g_\nu(z) - H^-_\nu \quad \text{for the upper boundary and}
$$

(3.5a)

$$
\frac{d}{d\tau_\nu}[f_\nu(z)J_\nu(z)] = H^+_\nu + g_\nu(z) \quad \text{for the lower boundary},
$$

(3.5b)
where $g_\nu = \int_0^1 \mu (I_{\nu \mu}^+ - I_{\nu \mu}^-) \frac{d\mu}{J_\nu}$, and $H_\nu^+$, $H_\nu^-$ are incident fluxes at corresponding boundaries. It is common to assume zero incident radiation ($H_\nu^- = 0$) and diffusion approximation at the lower boundary ($H_\nu^+ = 1/3[\frac{dB_\nu}{d\tau_\nu}]$).

Opacity and emissivity (and then the source function $S_\nu$) in stellar atmospheres can be calculated using the expressions (see Mihalas, 1978, Eqs. 7-1 and 7-2)

\[
\chi_\nu = \sum_i \sum_{l > l} \left[ n_l - \frac{g_i}{g_l} n_l \right] \alpha_{il}(\nu) + \sum_i \left( n_i - n_i^* e^{-\frac{h\nu}{kT}} \right) \alpha_{ik}(\nu) + \sum_k n_e n_k \alpha_{kk}(\nu, T) \left( 1 - e^{-\frac{\nu}{kT}} \right) + n_e \sigma_e \quad (3.6)
\]

\[
\eta_\nu = \frac{2 h \nu^3}{c^2} \left[ \sum_i \sum_{l > l} m_i \frac{g_i}{g_l} \alpha_{il}(\nu) + \sum_i n_i^* \alpha_{ik}(\nu) e^{\frac{\nu}{kT}} + \sum_k n_e n_k \alpha_{kk}(\nu, T) e^{-\frac{\nu}{kT}} \right]. \quad (3.7)
\]

The first term on the right hand sides of both equations (3.6) and (3.7) corresponds to line opacity (bound-bound transitions), the second one to bound-free transitions, the third one to free-free transitions, and the last one (only in 3.6) to electron scattering. In these equations, $n_i$, $n_l$, and $n_k$ are level populations ($n_i^*$ is the equilibrium value defined with respect to the ground level of the next higher ion), $g_i$ and $g_l$ are statistical weights, $\alpha$ denotes the cross section for the corresponding transition, $n_e$ is the electron number density, and $\sigma_e$ is the Thomson scattering cross section. Note that all level population may be heavily influenced by the radiation field.

For the case where we can use the equilibrium values of population numbers (the so-called ‘local thermodynamic equilibrium – LTE’), quantities $n_i$ can be replaced by their equilibrium values $n_i^*$, which depend only on local values of temperature $T$ and electron density $n_e$ through the Saha ionization and Boltzmann excitation equilibrium laws. This greatly simplifies the problem, because both opacity and emissivity then depend only on local temperature and density, and are independent of radiation. Then the radiative transfer equation (3.4) is linear in $J_\nu$.

### 3.2 Equations of statistical equilibrium

However, such a simplified description is not generally valid. In stellar atmospheres, the conditions may be far from thermodynamic equilibrium and Saha-Boltzmann equations for level population numbers cannot be used. In this case, level populations are determined using the equations of statistical equilibrium,

\[
\sum_{i \neq i} [n_i (R_{li} + C_{li}) - n_i (R_{il} + C_{il})] = 0, \quad i = 1, \ldots, NL \quad (3.8)
\]
This is the set of NL equations for each explicitly considered level. Since these equations are linearly dependent, an additional equation has to be used. Usually the charge or particle conservation equations are used. In the case of trace elements the equation which defines the abundance of the element with respect to some reference element (usually hydrogen, but not necessarily) may be used.

The quantities $R_{il}$ and $C_{il}$ in the equation (3.8) are radiative and collisional rates, respectively, for transitions between energy levels $i$ and $l$. Collisional rates,

$$n_i C_{il} = n_i n_e q_{il}(T),$$

(3.9)

where $q_{il}$ is a function of temperature only, do not depend on the radiation field (note that $n_i C_{il} = n_i C_{il}$). On the other hand, both upward ($R_{il}$) and downward ($R_{li}$) radiative rates,

$$n_i R_{il} = n_i 4\pi \int \frac{\alpha_{il}(\nu)}{h\nu} J_\nu \, d\nu, \quad (3.10a)$$

$$n_l R_{li} = n_l g_i 4\pi \int \frac{\alpha_{il}(\nu)}{h\nu} \left( \frac{2h\nu^3}{c^2} + J_\nu \right) \, d\nu, \quad (3.10b)$$

depend explicitly on the mean radiation intensity $J_\nu$. Detailed expressions for radiative rates can be found in the next chapter (Kubát, 2010, these proceedings).

### 3.2.1 Two-level atom

The basic principles are usually best shown using very simple, so called textbook cases. The concept of a two-level atom falls within them. Let us assume an atom having only two levels (see Mihalas, 1978). In this case the equations of statistical equilibrium (3.8) reduce to

$$n_2 (R_{21} + C_{21}) - n_1 (R_{12} + C_{12}) = 0 \quad (3.11)$$

For this case it may be derived that the source function

$$S_\nu = (1 - \varepsilon) \int \phi_\nu J_\nu \, d\nu + \varepsilon B_\nu, \quad (3.12)$$

where $\phi_\nu$ is the line profile function, $B_\nu$ is the Planck function, and $\varepsilon = \varepsilon'/(1 + \varepsilon')$, and $\varepsilon' = C_{21} \left[ 1 - \exp (-h\nu/kT) \right] / A_{21}$. Equation (3.12) clearly shows that the physical processes can be separated into the scattering ones, which depend on the radiation field $J_\nu$, and to the thermal ones, which depend on the local Planck function. The lower the value of $\varepsilon$, the less the LTE assumption is acceptable.

### 3.3 Final radiative transfer equation with a constraint of statistical equilibrium

If we explicitly emphasize the quantity dependences in the equation (3.2), it then takes the form

$$\frac{d}{d\tau_\nu} \left[ f_\nu(z) J_\nu(z) \right] = J_\nu(z) - S_\nu(z, J_\nu) \quad (3.13)$$
which shows its nonlinearity in the specific radiation intensity $J$. Using $\nu'$ instead of $\nu$ indicates that the radiative transfer in a particular frequency generally depends on the radiation field at all other frequencies.

Equation (3.13) with the boundary conditions (3.5) has to be solved using opacity (3.6) and emissivity (3.7), together with the statistical equilibrium equations (3.8) using both radiative (3.10) and collisional (3.9) rates. These equations together describe the basic NLTE radiative transfer problem which has to be solved in stellar atmospheres.

4 Frequency coupling of radiation

Let us turn our attention to another aspect of the radiative transfer problem, namely radiation coupling. One of the most striking features of radiation is the coupling of distant places, which would otherwise remain uncoupled. This coupling may occur over very long distances within stellar atmospheres. This long-distance coupling is described by the radiative transfer equation (3.1, 3.2, 3.3). Besides long distance coupling, scattering causes coupling between different radiation propagation directions.

An important aspect of radiation is the frequency coupling, which is crucial in stellar atmospheres. Although we succeeded to reduce the geometry complexity of the problem significantly, we have to retain full frequency dependence of the equations (3.2) and (3.3), since the radiative transfer in individual frequencies influences transfer in many other frequencies. Each of the equations (3.2) or (3.3) represents a set of frequency coupled equations.

The trivial case is that of no interaction of radiation with matter. Then the specific intensity $I$ remains constant and there is no frequency coupling. The simplest case is that of pure coherent scattering, either continuum (like electron scattering) or in lines. In this case, photons may change direction, but not frequency and the radiative transfer equation has the form

$$\mu \frac{dI_\mu}{d\tau} = I_\mu - \frac{1}{2} \int_{-1}^{1} \sigma_{\mu \mu'} I_{\mu'} d\mu',$$

(4.1)

where $\sigma_{\mu \mu'}$ is the scattering cross-section. This kind of radiative transfer problem forms a significant part of the Chandrasekhar’s Radiative Transfer book (Chandrasekhar 1950). In this case the radiative transfer at individual frequencies may be solved independently of other frequencies.

4.1 Frequency coupling within spectral lines

In a spectral line, frequencies of absorbed and emitted photon may differ within the line profile, which for the case of pure natural broadening (Lorentz profile) is

$$\varphi_\nu = \frac{\Gamma}{4\pi^2} \left( \frac{\Gamma}{4\pi} \right)^2 \frac{1}{(\nu - \nu_0)^2 + \left( \frac{\Gamma}{4\pi} \right)^2},$$

(4.2)
where $\nu_0$ is the central line frequency and $\Gamma$ is the damping parameter. For the case of complete or partial frequency redistribution there is a coupling between them via the redistribution process.

Thanks to thermal motions the spectral lines are subject to Doppler broadening. As a consequence, even in the case of coherent scattering (which takes place in the atomic frame), thermal motions may cause the difference between absorbing and emitting frequency. The broadened line profile for the case of atomic frame coherent scattering (Doppler profile) is

$$\varphi_\nu = \frac{1}{\Delta \nu_D \sqrt{\pi}} \exp \left( \frac{\nu - \nu_0}{\Delta \nu_D} \right)$$

where the Doppler half-width $\Delta \nu_D = (\nu_0/c) \sqrt{2kT/m}$. For the case of a naturally broadened line the profile is (Voigt profile)

$$\varphi_\nu = \frac{1}{\Delta \nu_D \sqrt{\pi}} H(a,v),$$

where $H(a,v)$ is the Voigt function (see Mihalas, 1978, Eq. 9-34). Thermal broadening is dominant in stellar atmospheres, which strongly couples frequencies within each line. In addition other additional broadening mechanisms, line Stark or collisional broadening, may introduce further frequency coupling.

To further illustrate the effect of lines on frequency coupling, we use the example of a two-level atom with partial frequency redistribution. The radiative transfer equation for this case is

$$\mu \frac{dI_\nu}{dz} = \frac{h\nu}{4\pi} \left[ -n_l \varphi_\nu B_{lu} I_\nu + n_u \psi_\nu (A_{ul} + B_{ul} I_\nu) \right],$$

where the emission profile $\psi_\nu = \int r(\nu',\nu) \varphi_\nu(\nu') d\nu'$, $r(\nu',\nu)$ is the redistribution function, $n_l$ and $n_u$ are the occupation numbers of the lower ($l$) and upper ($u$) levels, and $A_{ul}$, $B_{ul}$ and $B_{lu}$ are the Einstein coefficients. All line frequencies, which are coupled via Equation (4.3), have to be solved together.

### 4.2 Frequency coupling across lines

A photon after being absorbed, may be then re-emitted in the same line (this option was already mentioned in the preceding Section), or it may be emitted in a different line (or continuum transition), or it may be destroyed by collisional transition. In the latter case the photon’s energy is converted to heat. As a reverse process, photons may be emitted after collisional excitation, which causes cooling.

Each absorption or emission changes the distribution of atomic excitation states, which causes the change in the opacity. The changes are reflected by the set of statistical equilibrium equations. However, the radiative rates depend on radiation field. Consequently, we have to solve the equations simultaneously.
This coupling, which causes absorption of radiation in one part of the spectrum and its subsequent emission in a different spectral part, peaks in the effect usually referred to as line-blanketing. Spectral lines are not distributed across the frequency spectrum evenly. There appears a huge amount of lines in the UV spectral region. In addition, the radiative flux in this region is large. As a consequence, the radiation is absorbed in UV and re-emitted in the visual and infrared regions, where the opacity is lower. It is caused mostly by metallic lines dominated by Fe and Ni. The effect of line blanketing has been studied by a number of authors (e.g. Kurucz, 1979; Carbon, 1984; Dreizler & Werner, 1993; Hillier & Miller, 1998; Hubeny & Lanz, 1993; Lanz & Hubeny, 2003, 2007, and references therein).

4.3 Frequency coupling in moving atmospheres

For expanding atmospheres ($v(r) \neq 0$, $dv/dr > 0$) another type of frequency coupling occurs. Since the process of atomic absorption and emission (scattering) takes place in a rest frame of an atom (i.e. in a co-moving frame), when it is observed from the reference frame connected with a star (the observer’s frame), Doppler shift changes the frequency of lines. The radiative transfer equation in the observer frame has the form (3.2), but the opacity ($\chi_{\mu\nu}(z)$) and emissivity ($\eta_{\mu\nu}(z)$) coefficients are angle dependent. The angle dependence is caused by the Doppler shift $\nu' = \nu (1 - \mathbf{n} \cdot \mathbf{v}/c) = \nu (1 - \mu \nu/c)$. Equivalently, we may write the radiative transfer equation in the co-moving frame (we change the notation $\mu' \rightarrow \mu$, $\nu' \rightarrow \nu$)

$$\mu \frac{\partial I_{\mu\nu}(z)}{\partial z} - \left[ \frac{\mu^2 \nu}{c} \frac{\partial v}{\partial z} \right] \frac{\partial I_{\mu\nu}(z)}{\partial \nu} = \eta_{\nu}(z) - \chi_{\nu}(z)I_{\mu\nu}(z).$$

The second term on the left hand side clearly shows the frequency coupling caused by a derivative $\partial I_{\mu\nu}(z)/\partial \nu$. If we can neglect this term, we obtain the static radiative transfer equation. On the other hand, if we can neglect the first term, we obtain the so-called Sobolev approximation (see Castor, 2004).

5 Discretization

Since the solution of the combined equations of radiative transfer and statistical equilibrium is performed numerically, we have to switch from continuous independent variables to a discrete set of representative points. Instead of the depth variable $z$ we use depth points indexed by $d$. Since the density in stellar atmospheres varies by several orders of magnitude, the advantageous choice is to space the depth points equidistantly in log $m$ ($m$ is the column mass depth, $dm = -\rho \, dz$) or log $\tau$, where $\tau$ is some suitable optical depth, e.g. Rosseland mean optical depth or an optical depth at some representative wavelength. The discretization of frequency $\nu \rightarrow n$ has to be done to resolve all spectral lines and continuum edges, consequently, it cannot be equidistant. On the other hand, for plane-parallel atmospheres it is advantageous to use Gaussian quadrature for angle integration, which then defines the rays along which the radiative transfer equation is solved.
Discretized radiative transfer equation  Discretizing the radiative transfer equation (3.4) for the frequency point \(n\) we obtain (see also Feautrier, 1964)

\[
\begin{align*}
    a_d f_d^{d-1} J_d^{d-1} + (b_d f_d + 1) J_d + c_d f_{d+1} J_{d+1} &= S_d \quad \text{for } d = 2, \ldots, ND - 1, \quad (5.1a) \\
    (b_1 f_1 + g_1 + 1) J_1 + c_1 f_2 J_2 &= H^- + S_1, \quad \text{and} \\
    a_{ND} f_{ND-1} J_{ND-1} + (b_{ND} f_{ND} + g_{ND} + 1) J_{ND} &= H^+ + S_{ND}. \quad (5.1c)
\end{align*}
\]

In these equations,

\[
\begin{align*}
    a_d &= -\left[\frac{1}{2} \left(\Delta \tau_d - \frac{1}{2} + \Delta \tau_d + \frac{1}{2}\right) \Delta \tau_d - \frac{1}{2}\right]^{-1} \quad (5.2a) \\
    c_d &= -\left[\frac{1}{2} \left(\Delta \tau_d - \frac{1}{2} + \Delta \tau_d + \frac{1}{2}\right) \Delta \tau_d + \frac{1}{2}\right]^{-1} \quad (5.2b) \\
    b_d &= -a_d - c_d, \quad (5.2c) \\
    c_1 &= -\left(\Delta \tau_1\right)^{-1}, \quad b_1 = -c_1, \quad (5.2d) \\
    a_{ND} &= -\left(\Delta \tau_{ND-\frac{1}{2}}\right)^{-1}, \quad \text{and} \quad b_{ND} = -a_{ND}, \quad (5.2e)
\end{align*}
\]

where \(\Delta \tau_d = \tau_d - \tau_{d-1}\). The above equations refer to the case of 2nd-order differences, which is the most stable way of discretizing the differential radiative transfer equation. We may also use either splines or Hermite differences (see Auer, 1976), which are more accurate, but sometimes we run into troubles since they are less stable and oscillatory behaviour occasionally occurs.

Discretized frequency integration  The integral both across the line profile and over continuum frequencies is replaced by a quadrature sum

\[
\int J(\nu) \, d\nu \to \sum_{n=1}^{NF} w_n J_n. \quad (5.3)
\]

For lines, it is necessary to ensure that \(\int \phi(\nu) \, d\nu = \sum_{n=1}^{NF} w_n \phi_n = 1\). If this condition is not fulfilled, it is obligatory to renormalize \(w_n\). Otherwise, an artificial unphysical source or sink of photons appears, which may dramatically change results.

To ensure correct treatment of ionization edges, it is advantageous to use two close frequency points which differ only by machine accuracy, one before and one after the ionization edge (Rauch, private communication). This ensures exact treatment of all contributions to the particular ionization rate and also to other rates where the continuum edge is a standard continuum frequency point.

Discretized angle integration  The integral over the angles in the calculation of the intensity moments is also replaced by quadrature sums,

\[
\int I(\mu) \, d\mu \to \sum_{m=1}^{NF} w_m I_m. \quad (5.4)
\]
Usually, 3 points are sufficient if Gaussian angle quadrature (see Chandrasekhar, 1950, Section 22) is used. Also in this case the check of correct normalisation is crucial.

Discretized equations of statistical equilibrium For all $d = 1, \ldots, ND, \ i = 1, \ldots, NL$ we may write

$$
\sum_{l \neq i} \{(n_i)_d [(R_{li})_d + (C_{li})_d] - (n_l)_d [(R_{il})_d + (C_{il})_d]\} = 0,
$$

(5.5)

where the radiative rates are given by

$$
(n_i)_d(R_{il})_d = (n_i)_d 4\pi \sum_{n=1}^{NF} w_n \frac{\alpha_{il}}{h\nu_n} J_{dn},
$$

(5.6a)

and

$$
(n_l)_d(R_{li})_d = (n_l)_d \frac{g_l}{g_i} 4\pi \sum_{n=1}^{NF} w_n \frac{\alpha_{il}}{h\nu_n} \left(\frac{2h\nu_n^3}{c^2} + J_{dn}\right).
$$

(5.6b)

6 Formal solution of the radiative transfer equation

Formal solution of the RTE is the next step after calculation of the model atmosphere and the occupation numbers. It is any radiative transfer solution for given $\chi_\nu$ and $\eta_\nu$ (given $S_\nu$) and it is relatively simple. In this step the equation (3.2) is directly solved, or it is sometimes rewritten to the 2nd-order form. The latter possibility has become more popular in one-dimensional model atmospheres. The formal solution is crucial for the total accuracy of the whole problem solution.

6.1 Feautrier solution

The most widely used radiative transfer equation solution for static plane-parallel atmospheres is the solution of the second-order system introduced by Feautrier (1964). In this scheme we combine opposite directions along a ray represented by specific intensities $I^+$ and $I^-$. Introducing “Feautrier variables”, i.e. their symmetric and anti-symmetric means,

$$
u_{\mu\nu} = \frac{1}{2} \left( I_{\mu\nu}^+ + I_{\mu\nu}^- \right)
$$

(6.1a)

and

$$\nu_{\mu\nu} = \frac{1}{2} \left( I_{\mu\nu}^- + I_{\mu\nu}^+ \right),
$$

(6.1b)

we obtain the transfer equation

$$
\frac{d^2 u_{\mu\nu}}{d\tau^2} = u_{\mu\nu} - S_\nu
$$

(6.2)

supplemented by appropriate boundary conditions.
6.2 Short characteristics

The short characteristics method is a first-order method. If we solve the radiative transfer equation for a finite slab (see Fig. 2) with an optical thickness $\tau_\nu$ along a ray with an angle $\theta$ ($\mu = \cos \theta$), then by integration of Equation (3.2) between 0 and $T_\nu$ we obtain for the outward direction

$$I^+_{\mu\nu}(\tau_\nu) = I^+_{\mu\nu}(T_\nu) e^{-(T_\nu-\tau_\nu)/\mu} + \frac{1}{\mu} \int_{\tau_\nu}^{T_\nu} S(t) e^{-\tau(t-\tau_\nu)/\mu} dt,$$

and for the inward direction

$$I^-_{\mu\nu}(\tau_\nu) = I^-_{\mu\nu}(0) e^{-\tau_\nu/\mu} + \frac{1}{(-\mu)} \int_{0}^{\tau_\nu} S(t) e^{-\tau(t-\tau_\nu)/\mu} dt.$$

The stellar atmosphere is then divided into shells (i.e. finite slabs) between particular depth points and solved by parts throughout the atmosphere.

While not being used for the solution of the one-dimensional radiative transfer equation as much as the Feautrier solution, the power of the short characteristics method emerges for multidimensional radiative transfer (see Kunasz & Auer, 1988).

7 $\Lambda$ iteration

We may formally write the formal solution of the equation (3.4), which was described in the preceding section, as an operation of an operator $\Lambda$ on the source function (see Mihalas, 1978),

$$J_\nu = \Lambda_\nu S_\nu.$$  \hfill (7.1)

Generally, the source function, $S_\nu$, depends on the radiation field intensity $J_\nu$, which makes the problem non-linear. The simplest way how to cope with the non-linearity is an iterative procedure. Let us assume some starting values for opacity and emissivity, say the LTE values based on LTE level populations $n_i^*$ (i.e. the source function $S_\nu = B_\nu$). The opacities and emissivities can be easily calculated from (3.6) and (3.7), respectively, using LTE population values. Then instead of the radiative transfer equation (3.13), equation (3.4) can be solved (for given $\eta_\nu$ and $\chi_\nu$, i.e. for given $S_\nu$), which is in fact the formal solution mentioned in the text.

![Fig. 2. Schematic representation of the short characteristics solution.](image)
preceding section. Then, the equations of statistical equilibrium are solved with radiative rates calculated for a given radiation field. New level populations \( n_i \) are determined, which are then used for calculation of new values of \( \chi\nu \) and \( \eta\nu \), and the process is iterated.

The above iteration scheme may be written as

\[
J^{(n)}\nu = \Lambda\nu S^{(n-1)}\nu,
\]

(7.2)

where \( (n) \) and \( (n-1) \) denote the iteration numbers. The occupation numbers are determined using the equation

\[
\sum_{l \neq i} \left\{ n_l^{(n)} \left[ R_{il}(J^{(n)}\nu) + C_{il} \right] - n_i^{(n)} \left[ R_{il}(J^{(n)}\nu) + C_{il} \right] \right\} = 0.
\]

(7.3)

The level populations \( n_i^{(n)} \) are used to calculate the source function \( S^{(n)}\nu \) and we follow again with solution of (7.2), now for \( J^{(n+1)}\nu \). The crucial problem of this iterative process is that, for the case of stellar atmospheres, it converges extremely slowly, it rather stabilises far from the true solution. This is caused by the fact that each iteration represents interaction over one mean free path. In the optically thick parts of the atmosphere (with a lot of scattering events) it means extremely slow propagation of information throughout the stellar atmosphere. Illustrative examples can be found in Auer (1984).

Although the lambda iteration is unusable for stellar atmospheres, for optically thin media, like planetary nebulae or circumstellar envelopes, it may work (see Dickel & Auer, 1994). However, for stellar atmospheres which are optically thick, different approaches have to be found.

8 Complete linearization

The complete linearization method (the Newton-Raphson method) was introduced to the theory of stellar atmospheres by Auer & Mihalas (1968) for the case of a full solution of a NLTE model plane-parallel atmosphere, which means simultaneous solution of equations of radiative transfer, statistical equilibrium, radiative equilibrium, and hydrostatic equilibrium in one spatial dimension. For the simpler task, when the equations of hydrostatic and radiative equilibrium are not solved and only common solution of the radiative transfer equation together with the statistical equilibrium equations is performed, the complete linearization was described by Auer (1973).

We have to solve the plane-parallel radiative transfer equation together with the set of equations of statistical equilibrium for radiation intensities \( J\nu \) and level populations \( n_i \). Since we cannot resolve the radiation field for infinite number of frequencies, we have to replace the continuous index \( \nu \) by a discrete one \( i \), \( J\nu \rightarrow J_i \), and solve the radiative transfer equation only for these frequency points. The variables \( J_i \) and \( n_i \) may be formally written as a vector

\[
\psi = (J_1, \ldots, J_{NF}; n_1, \ldots, n_{NL}),
\]
which has the dimension $NF + NL$. The equations to be solved may be formally written as

$$F(\psi) = 0 \tag{8.1}$$

If $\psi_0$ is the current estimate of the solution, which does not satisfy the Eq. (8.1) exactly, then the correct solution can be obtained by adding a correction $\delta\psi$,

$$\psi = \psi_0 + \delta\psi. \tag{8.2}$$

Inserting it into the equation (8.1) we obtain after expansion to the first order for the corrections

$$\delta\psi = \left[ \frac{\partial F}{\partial \psi} (\psi_0) \right]^{-1} \cdot F(\psi_0). \tag{8.3}$$

Then the new values of the vector $\psi$ are calculated using Eq. (8.2).

### 8.1 Standard formulation

After implementing the difference scheme for the Eq. (3.13), the linearized radiative transfer equation may be symbolically written as

$$A_d \delta J_{d-1} + B_d \delta J_d + C_d \delta J_{d+1} = L_d, \tag{8.4}$$

where the vector $\delta J_d = (\delta J_{d,1}, \ldots, \delta J_{d,NF})$ for each $d = 1, \ldots, ND$. $A_d$, $B_d$, and $C_d$ are matrices, $A_1 = 0$, and $C_{ND} = 0$. The right hand side $L_d$ contains the source function $S_d$.

The dependence of the source function on the occupation numbers may be expressed with the help of the derivative

$$\delta S_{nd} = \sum_{l=1}^{NL} \frac{\partial S_n}{\partial n_l} (\delta n_l)_d.\tag{8.5}$$

The combined equation may be then written as

$$A_{d} \delta J_{n,d-1} + B_{d} \delta J_{n,d} + C_{d} \delta J_{n,d+1} + D_{d} \delta n_d = M_{n,d}. \tag{8.6}$$

If we formally write the statistical equilibrium equations (3.13) as $A \cdot n = b$, where $A$ is the rate matrix, $n = (n_1, \ldots, n_{NL})$, we may then, for the changes of populations numbers $\delta n_d$, write

$$\left[ \frac{\partial A}{\partial n} \delta n + \frac{\partial b}{\partial n} + A \right]_d \delta n_d + \left[ \frac{\partial A}{\partial J} \delta n + \frac{\partial b}{\partial J} \right]_d \delta J_d = b_d - A_d \cdot n_d, \tag{8.7}$$

which may be schematically written as

$$E_d \delta n_d + F_d \delta J_d = K_d.$$
Equations (8.5) and (8.7) schematically describe the problem, which we solve. Using the linearized equations of statistical equilibrium, we may express the level population changes as

$$\delta n_{l,d} = \frac{NF}{\sum n=1} \frac{\partial n_l}{\ partial J_n} \left( J_n \right)_{d}, \tag{8.8}$$

where

$$\frac{\partial n_l}{\ partial J_n} = \sum_{r=1}^{NL} A_{lr}^{-1} \left[ \frac{\partial b_r}{\ partial J_n} - \sum_{s=1}^{NL} A_{rs} \frac{\partial n_s}{\ partial J_n} \right]. \tag{8.9}$$

Then the combined radiative transfer + statistical equilibrium equations may be written as a set of tridiagonal matrices

$$\delta J_{d} - \frac{1}{1 + \delta R_t} \delta J_{d} + \delta J_{d+1} = L'_d, \tag{8.10}$$

where $\delta J_d = (\delta J_1, \ldots, \delta J_{NF})$, $d = 1, \ldots, ND$ and $A_{1'} = 0$, $C_{ND'} = 0$.

### 8.2 Formulation using net radiative brackets

Auer & Heasley (1976) reformulated the application of the complete linearization method with the help of net radiative brackets. For each transition $t$ between levels $i$ and $l$, we may introduce the quantity

$$Z_t = n_i R_{il} - n_l R_{li}, \tag{8.11}$$

which describes the net radiative rate. Linearizing this expression for each depth point $d$ we obtain

$$(\delta Z_t)_d = (n_i)_d (\delta R_{il})_d - (n_l)_d (\delta R_{li})_d. \tag{8.12}$$

Using $\delta n_i = \sum_t (\partial n_i / \partial Z_t) \delta Z_t$ we may eliminate the population numbers changes $\delta n_i$ and finally arrive at a system of equations

$$\left( 1 + R_t \frac{\partial n_l}{\partial Z_t} + S_t \frac{\partial n_l}{\partial Z_t} \right) \delta Z_t = L_t - R_t \sum_{t' \neq t} \frac{\partial n_l}{\partial Z_{t'}} \delta Z_{t'} - S_t \sum_{t' \neq t} \frac{\partial n_l}{\partial Z_{t'}} \delta Z_{t'}. \tag{8.13}$$

which is solved for $\delta (Z_t)_d$.

### 9 Accelerated lambda iteration

Although complete linearization is a powerful method, it results in huge matrices having the dimension $NF \times NL$. On the other hand, the simple $\Lambda$-iteration suffers from convergence problems. As an alternative, Cannon (1973a) suggested an iterative method based on the operator splitting method. This method was later further developed by Scharmer (1981, 1984). Basic properties of this method, now called ‘Accelerated Lambda Iteration’ (ALI) method, were described...
by Olson, Auer, & Buchler (1986). Useful reviews of ALI methods were published by Hubeny (1992, 2003).

We can introduce an approximate operator $\Lambda^*$ representing an approximate solution of the radiative transfer equation by adding and subtracting the term $\Lambda^* S_\nu$ at the right hand side of (7.1),

$$ J_\nu = \Lambda^* S_\nu + (\Lambda_\nu - \Lambda^*_\nu) S_\nu $$

(9.1)

In analogy with (7.2), we may introduce an iteration scheme

$$ J_\nu^{(n)} = \Lambda^*_\nu S_\nu^{(n)} + (\Lambda_\nu - \Lambda^*_\nu) S_\nu^{(n-1)} + \Delta J_\nu^{(n-1)} $$

(9.2)

The basic difference with respect to the $\Lambda$-iteration is that the $\Lambda^*$-operator is now acting on $S_\nu^{(n)}$ and not on $S_\nu^{(n-1)}$ like in the case of ordinary $\Lambda$-iteration. The accurate solution of the radiative transfer equation $\Lambda_\nu S_\nu$ (the formal solution) is taken from the preceding, i.e. $(n-1)$ iteration step. In the limit of the converged solution the equation (9.2) is exact. The term $\Delta J_\nu^{(n-1)} = (\Lambda_\nu - \Lambda^*_\nu) S_\nu^{(n-1)}$ is the correction term, which describes, how the approximate solution (obtained with $\Lambda_\nu^*$) for the current estimate of the source function $S_\nu^{(n-1)}$ differs from the exact one (obtained with $\Lambda_\nu$).

The normal procedure in multilevel radiative transfer calculations with ALI is to first determine the correct source function by common solution of the equations of statistical equilibrium with a simplified expression for $J_\nu^{(n)}$ (9.2), and then to obtain the radiation intensity from the calculated source function using the formal solution. Since the source function is the ratio of emissivity and opacity, which both depend on population numbers, determination of the source function means in this case calculation of the population numbers of individual levels using the equations of statistical equilibrium. The expression (9.2) for the new estimate of the mean intensity is inserted to the expressions for the radiative rates (3.10)

$$ n_i R_{ii} = n_i R_{ii}^{(n)} + \frac{\alpha_{ii}(\nu)}{h\nu} \left[ \Lambda^*_\nu S_\nu^{(n)} + \Delta J_\nu^{(n-1)} \right] d\nu $$

(9.3a)

$$ n_i R_{il} = n_i R_{il}^{(n)} + \frac{\alpha_{il}(\nu)}{h\nu} \left( \frac{2h\nu^3}{c^2} + \left[ \Lambda^*_\nu S_\nu^{(n)} + \Delta J_\nu^{(n-1)} \right] \right) d\nu $$

(9.3b)

which are then used in the equations of statistical equilibrium (7.3). These equations may be written as

$$ \sum_{i \neq i} \left\{ n_i [ R_{ii} (n_i, n_i) + C_{ii} ] - n_i [ R_{ii} (n_i, n_i) + C_{ii} ] \right\} = 0 $$

(9.4)

and they are solved for the population numbers $n_i$. Finally, the formerly linear set of the equations of statistical equilibrium became a nonlinear one. This nonlinearity is a tax for simplifying the problem.

There are two basic possibilities how to solve this system of nonlinear equations, namely the Newton-Raphson scheme (linearization), which was used, e.g., by
Kubáš (1994), or more popular approach of pre-conditioning (Rybicki & Hummer, 1991). The linearization scheme is very similar to that described in the Section 8. However, the savings achieved are very important, since we do not solve explicitly the problem in frequencies, number of which may reach several tens of thousands or more.

9.1 Construction of the $\Lambda^*$ operator

The crucial point is the construction of the operator $\Lambda^*$. It should have two basic properties: First, it has to be simple enough to be calculated quickly, and, second, it should describe the most important interactions of the radiation field with matter as accurately as possible. Olson et al. (1986) showed that the best choice of such operator is simply the diagonal of the $\Lambda$ operator. However, also other construction methods of the approximate operator are being used. The tridiagonal operator of Olson & Kunasz (1987) was used by Werner (1989) and also by Kubáš (1994).

The approximate lambda operator has to be numerically consistent with the formal solution of the radiative transfer equation, so the Olson & Kunasz (1987) operator is suitable if we use the short characteristic solution of the radiative transfer equation. On the other hand, for Feautrier solution the approximate operator constructed after Rybicki & Hummer (1991) has to be used.

10 Summary

In this introductory part we emphasized the importance of frequency coupling of radiation (in addition to the spatial and angle coupling) for the conditions of stellar atmospheres. This frequency coupling is ensured mainly by equations of statistical equilibrium, which connect distant parts of the frequency spectrum. We also briefly summarized underlying equations for the NLTE radiative transfer problem in stellar atmospheres with a focus on the problem of its solution for the case of trace elements.

There are two basic methods of the solution of the RTE+ESE system, namely the complete linearization method, which is used by the Kiel code (see Kamp, 2010, these proceedings), and the accelerated lambda iteration method used by the DETAIL code (see Butler, 2010, these proceedings).

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