From Escape Probabilities to Exact Radiative Transfer

Ivan Hubeny

AURA/NOAO, NASA Goddard Space Flight Center, Greenbelt, MD 20771

Abstract. The physical basis and the approximations involved in the escape probability methods are discussed, with particular emphasis on their advantages and drawbacks in individual applications. Next, a brief review of the Accelerated Lambda Iteration (ALI) methods is presented and it is outlined how they can be implemented in the current photoionization codes.

1. Introduction

Most of the present-day photoionization codes (the two most widely used codes being CLOUDY - Ferland 1999, and XSTAR - Kallman 2000) are based on treating radiation transfer by means of the so-called escape probability methods. Although this approach has proved to be extremely useful in the past, it is recently becoming more and more clear that for more realistic calculations one needs more exact radiative transfer techniques. Another motivation for implementing exact radiative transfer into the photoionization codes follows from recent great advances in efficient numerical methods, in particular the so-called Accelerated Lambda Iteration (ALI); it is now feasible to develop a treatment that will replace the traditional escape probability methods in the photoionization codes while using a reasonable amount of computer resources.

This paper has several goals. First, I will briefly discuss the physical basis and the approximations involved in the escape probability methods, and show what are their advantages and, in particular, their drawbacks. Second, I will explain the basis of the ALI methods, and to outline how they can be implemented in the photoionization codes.

The paper is organized as follows. In Section 2, I will summarize the basic physics and equations of radiative transfer in photoionized media. In Section 3, I will outline the nature of the line transfer problem, while in Section 4 I list some simple possibilities how to avoid considering radiative transfer. Section 5 contains a brief review of the escape probability methods, understood as a tool to simplify radiative transfer for practical applications. I also compare results obtained using the escape probabilities and exact radiative transfer. Section 6 is devoted to an introductory overview of the ALI methods, while Sections 7 and 8 are discuss some details of implementation and application of ALI in actual applications.
2. Basic Physics

We consider a medium, typically a plane-parallel slab or a spherical shell, irradiated by an external source. Generally, the external radiation interacts with the material of the slab, leading to a complex interplay of a number of atomic transition processes, such as photoionization and photo-excitation, and their inverse processes of radiative recombination and de-excitation. All these processes have their collisional counterparts. The basic physics of photoionized media is described in several excellent textbooks (e.g., Osterbrock 1989 for specifically photoionized media; or Mihalas 1978 for general aspects of interaction of radiation and matter).

The ionization and excitation state of matter is dominated by radiation. Because the radiation field is generally far from its equilibrium (Planckian) distribution, the ionization/excitation balance cannot be described by the equilibrium, Saha-Boltzmann distribution. Assuming this description is usually referred to in astrophysics as Local Thermodynamic Equilibrium, or LTE. (Strictly speaking, the definition of LTE also involves the condition that the velocity distribution of all particles are Maxwellian, with the same kinetic temperature, referred to electron temperature, or simply temperature.) Instead, the atomic level populations have to be determined by solving a set of statistical equilibrium equations (also called rate equations). For a certain level $i$ we have

$$n_i \sum_{j \neq i} (R_{ij} + C_{ij}) = \sum_{j \neq i} n_j (R_{ji} + C_{ji}),$$

where $n_i$ is the population (number density) of level $i$, $R_{ij}$ and $C_{ij}$ are the radiative and collisional rates, respectively, for a transition $i \rightarrow j$. The set of rate equations for all levels of an atom would form a linearly dependent system. Therefore, one equation of the set has to be replaced by another equation. Usually, this is the total number conservation equation (or abundance definition equation), $\sum_i n_i = N_{\text{atom}}$, where the summation extends over all levels of all ions of a given species.

Collisional rates are relatively “easy” to handle because they are functions of electron density, $n_e$, temperature, $T$, and atomic parameters, and are therefore local quantities. The radiative rates are given by

$$R_{ij} = \int_0^\infty d\nu \frac{4\pi}{h\nu} \sigma_{ij}(\nu) J_\nu,$$

$$R_{ji} = (n_i/n_j)^* \int_0^\infty d\nu \frac{4\pi}{h\nu} \sigma_{ij}(\nu) \left( \frac{2h\nu^3}{c^2} + J_\nu \right) \exp(-h\nu/kT),$$

where $\sigma_{ij}(\nu)$ is the cross-section, and $J_\nu$ the mean intensity of radiation. Quantity $(n_i/n_j)^*$ is the LTE (Boltzmann) ratio of populations. Equations (2) and (3) apply for both bound-bound and bound-free transitions.

Specifying the radiative rates for bound-bound transitions (lines), the relevant cross-sections are given by

$$\sigma_{ij}(\nu) = \frac{\pi e^2}{m_e c^2} f_{ij} \phi_{ij}(\nu)$$
where the quantity \( \pi e^2/(m_e c^2) \) is the classical value of the total cross-section, \( f_{ij} \) the oscillator strength, and \( \phi_{ij}(\nu) \) is (normalized) absorption profile coefficient (such that \( \int_0^\infty d\nu \phi_{ij}(\nu) = 1 \)). Introducing the usual Einstein coefficients for absorption, stimulated emission, and spontaneous emission, viz.,

\[
B_{ij} = \frac{4\pi}{h \nu} \frac{\pi e^2}{m_e c^2} f_{ij}, \quad B_{ji} = (g_i/g_j) B_{ij}, \quad A_{ji} = (2h\nu^3/c^2) B_{ji},
\]

the radiative rates for lines can be written as

\[
R_{ij} = B_{ij} \tilde{J}_{ij} \quad R_{ji} = A_{ji} + B_{ji} \tilde{J}_{ij},
\]

where \( A \) and \( B \) are Einstein coefficients, and

\[
\tilde{J}_{ij} = \int_0^\infty d\nu J_\nu \phi_{ij}(\nu),
\]

which is sometimes called the frequency-averaged mean intensity of radiation.

The radiative rates are “difficult”. This is because they explicitly depend on the radiation field, which has to be determined by solving the radiative transfer equation, viz.,

\[
\frac{dI_\nu}{ds} = \nu_\nu I_\nu - \eta_\nu,
\]

where \( I \) is the specific intensity of radiation, \( s \) measures the pathlength along the direction of propagation, and \( \nu_\nu \) and \( \eta_\nu \) are the absorption and emission coefficients, respectively. This equation looks deceivingly simple. It would indeed be simple had the absorption and emission coefficients been known. However, these coefficients depend explicitly on atomic level populations, so we are faced with a coupled problem to solve the transfer equation together with the set of statistical equilibrium equations. But it is not the end of the story. The most serious complication follows from the fact that the mean free path of photons is typically much larger than the mean free path of particles. The radiation field thus introduces a long-range interaction problem; in other words, radiation couples vastly distant regions of physical space. The general problem is thus a non-linear and non-local coupled problem, which is numerically more difficult than, for instance, simple hydrodynamics, where one deals with several coupled, but essentially local, equations.

Besides the radiative transfer equation and the statistical equilibrium equations, the structure of the medium may be generally governed by other equations, such as the energy balance equation, the hydrostatic equilibrium equation, and others. In the paper we will consider a simpler problem where the general structure of the medium (i.e., the temperature, density, etc.) is given, while we simultaneously solve the radiative transfer equation and the statistical equilibrium equations – the so-called restricted non-LTE (or NLTE) problem. The rationale is that the numerical methods for treating the general problem are typically just a straightforward extension of the methods that treat the restricted NLTE problem.
3. The Nature of NLTE Line Transfer Problem

Let us now consider for simplicity a plane-parallel slab; a generalization for other geometries is relatively straightforward. The transfer equation (8) is usually written as

$$
\mu \frac{dI_{\mu \nu}}{d\tau_{\nu}} = I_{\mu \nu} - S_{\nu}
$$

(9)

where $\mu$ is cosine of the angle between the direction of photon propagation and the outward-directed normal to the surface, $S$ is the source function, defined by

$$
S_{\nu} \equiv \eta_{\nu}/\kappa_{\nu},
$$

(10)

and $\tau_{\nu}$ is the optical depth, defined by

$$
d\tau_{\nu} = -\kappa_{\nu} dz,
$$

(11)

where $z$ is the geometrical coordinate, defined such that it increases outward. With this definition, optical depth increases inward.

The specific intensity, which fully specifies the radiation field (at least for the case of unpolarized radiation considered here), depends on three variables: the frequency $\nu$, the directional cosine $\mu$, and the (monochromatic) optical depth $\tau_{\nu}$. Traditionally, $\nu$ and $\mu$ are written as subscripts. The formal solution of equation (9) may be written as

$$
I_{\mu \nu} = \Lambda_{\mu \nu}[S],
$$

(12)

where $\Lambda$ operates on the quantity within $[\phantom{\text{ ]}}$]. Equation (12) represents an elementary form of the formal solution. By integrating this equation over angles and/or frequencies, one obtains other useful expressions for the mean intensity $J_\nu$ and for the frequency-averaged mean intensity $\bar{J}$, viz.

$$
J_\nu = \Lambda_\nu[S], \text{ where } J_\nu = \frac{1}{2} \int_{-1}^{1} I_{\mu \nu} d\mu \text{ and } \Lambda_\nu = \frac{1}{2} \int_{-1}^{1} \Lambda_{\mu \nu} d\mu,
$$

(13)

and

$$
\bar{J} = \bar{\Lambda}[S], \text{ where } \bar{J} = \int J_\nu \phi_\nu d\nu \text{ and } \bar{\Lambda} = \int \Lambda_{\nu \nu} \phi_\nu d\nu,
$$

(14)

For instance, an explicit form of equation (13) is called the Schwarzschild-Milne equation, and is written as (e.g., Mihalas 1978)

$$
J_\nu(\tau_\nu) = \int_{0}^{\tau_\nu} S_{\nu}(t) E_1(t - \tau_\nu) dt + \int_{\tau_\nu}^{T_\nu} S_{\nu}(t) E_1(t - \tau_\nu) dt,
$$

(15)

where $E_1$ is the first exponential integral function. The exponential integrals are defined generally as

$$
E_n(x) = \int_{1}^{\infty} e^{-xt} t^{-n} dt.
$$

(16)

Equations (12) – (14) involve $\Lambda$ written as an operator. It should be stressed that the $\Lambda$ does not have to be constructed explicitly. $\Lambda$ is normally thought of as a process of explicitly calculating the intensity from the source function.
Any method of solving the transfer equation can be used here: for instance, the familiar Feautrier (1964) difference-equation method (also see Mihalas 1978), the short-characteristics method (e.g., Olson & Kunasz 1987), or the Discontinuous Finite Element method (Castor, Dykema, & Klein 1992).

We stress that the term formal solution refers to the solution of the transfer equation with the fully specified source function. As we discussed above, the formal solution is easy because it involves a solution of a linear differential equation [or, equivalently, can be written as a simple linear operator action – equation (12)]. We repeat that what complicates the situation is the fact that the source function is generally not known in advance because it generally depends, in a complex non-linear and non-local way, on the radiation field.

Let us illustrate the phenomenon on the simplest case of the coupled problem of radiative transfer and statistical equilibrium, namely the case of a two-level atom without an overlapping continuum. In this case, the equation (1) can be rewritten to give an explicit expression for the source function (e.g., Mihalas 1978)

\[ S = (1 - \epsilon)\bar{J} + \epsilon B, \tag{17} \]

where \( B \equiv B_{\nu_0} \) is the Planck function at the line center (with frequency \( \nu_0 \)), and

\[ \epsilon = \frac{C_{ul}}{C_{ul} + A_{ul} / (1 - e^{-h\nu_0/kT})} \approx \frac{C_{ul}}{C_{ul} + A_{ul}}, \tag{18} \]

so it has an approximate meaning of the photon destruction probability. Here the indices \( l \) and \( u \) refer to the lower and upper level, respectively.

Combining equations (14) and (17), we obtain

\[ S = (1 - \epsilon)\Lambda[S] + \epsilon B. \tag{19} \]

which formally expresses the radiative transfer problem through an integral equation for the source function. Because \( \Lambda \) is a linear operator, (19) may in fact by solved in a single step. However, due to the above mentioned coupling, the matrix representing \( \Lambda \) may be large, and therefore a direct solution may be impractical. Another concern is that even if \( \Lambda \) is simple enough to warrant a direct solution in a few individual cases, it may still be too time-consuming in problems requiring the solution of (19) many times, which may easily occur in photoionization codes, or even more so in hydrodynamical simulations. For all these reasons, developing simpler, iterative methods is highly desirable.

The simplest and most straightforward iteration scheme is the notorious “ordinary” lambda iteration. Denoting the \( n \)-th iterate of the source function as \( S^{(n)} \), we may write

\[ S^{(n+1)} = (1 - \epsilon)\Lambda[S^{(n)}] + \epsilon B, \tag{20} \]

The advantage of (20) can be seen immediately: all of the coupling is treated iteratively; one performs only (cheap) formal solutions of the transfer equation, for one frequency-angle point at a time. Unfortunately, this method fails in most cases of interest (i.e., when scattering is important). The reasons for this failure are well understood (see, e.g., Mihalas 1978): the iterations correspond to successive photon scatterings in the medium. If the number of scatterings
is large, which is the usual case in astrophysical applications (i.e., small $\epsilon$ and large optical depth), an impractical number of iterations would be required to get the converged solution. Worse yet, Lambda iteration tends to stabilize, not to converge the solution, so that a smallness of relative corrections is no guarantee of convergence (for a very illustrative example, see Auer 1991; his Fig.1). An illuminating mathematical discussion is given by Olson, Auer, & Buchler (1986).

We shall return to the problem later, and first discuss other possibilities of how to avoid treating the coupling involved by the radiation field altogether.

4. Simplifying a Treatment of Radiation

From what we discussed above, it is quite natural that one strives to simplify the treatment of the radiation field in order to avoid the complicated non-linear and non-local coupling described above. Recall that the statistical equilibrium equations (1) form a linear set of equations for populations if the radiation field is known. Therefore, if we can prescribe the radiation intensity somehow without solving the transfer equation, the problem would be vastly simplified.

How this can be achieved? There are several possibilities:

- **Optically thin medium.** In this case we put

$$I_\nu = I_{\nu}^{\text{inc}} e^{-\tau_\nu}.$$  \hfill (21)

where $I_{\nu}^{\text{inc}}$ is the incoming, and thus known specific intensity of radiation. We assume here that $\tau_\nu < 1$. In this case, $I_\nu$ is known (if $\tau_\nu$ is known), and consequently all radiative rates are known, so that the statistical equilibrium equations (1) form a linear set, whose solution is trivial. In general the optical depth is not known since it depends on the level populations, but these populations may be improved iteratively. This procedure is not equivalent to the Lambda iteration, and typically converges quickly. Of course, the drawback of this approach is that the approximation of optically thin medium is too restrictive, and is applicable only to a limited class of astrophysical objects.

- **Optically thick medium.** In this case we have

$$I_\nu = B_\nu,$$  \hfill (22)

(or possibly with additional terms containing derivatives of the Planck function with respect to optical depth – the so-called diffusion approximation). Again, the radiation intensity is known, so we can solve the rate equation easily.

All the above approximations are very crude. What we need is something in between the optically thin and thick limits. This is exactly what is provided by the escape probability methods, which we will discuss in the next section.
5. Escape Probability Methods

The essence of the escape probability approach is that it provides a simple approximate relation between the radiation intensity and the source function. Having this relation, one can use it to simplify the coupled problem of simultaneous radiative transfer and statistical equilibrium. Such a relation may also directly provide the emergent radiation from the medium. In many cases, the physical meaning of the escape probability methods may be hidden in the formalism, but we should always bear in mind that the heart of all escape probability approaches is an approximate relation between intensity and the source function. Beautiful reviews of the topic were given by Rybicki (1984, 1991); here I give only a brief account of the method.

5.1. Net Radiative Rates

It is very useful to express the net rate of the transition between levels \( j \) and \( i \) as the spontaneous rate times a correction factor,

\[
n_j A_{ji} + n_j B_{ji} \tilde{J} - n_i B_{ij} \tilde{J} \equiv n_j A_{ji} \rho,
\]

where the correction factor \( \rho \) is called the net radiative bracket (there are other names for this quantity, see Rybicki 1984). Noting that the line source function for the transition \( i \leftrightarrow j \) is given by

\[
S_{ij} = \frac{n_j A_{ji}}{n_i B_{ij} - n_j B_{ji}},
\]

we may rewrite the net radiative bracket as

\[
\rho = 1 - \frac{\tilde{J}}{S_{ij}} \quad \text{i.e.,} \quad \tilde{J} = (1 - \rho) S_{ij}.
\]

The net radiative bracket as such does not immediately help to solve the coupled radiative transfer problem. Indeed, it depends explicitly on the mean intensity, so it may be evaluated explicitly only when the solution of the radiative transfer problem is already given. However, the utility of the concept of the net radiative bracket lies in the following. Imagine that we are able to estimate \( \rho \) somehow, independently of the radiation field. In such case, we may solve the set of statistical equilibrium equations, obtain all the atomic level populations and thus the line source functions, and finally compute the radiation intensities by a simple formal solution of the transfer equation with a known source function. In other words, the difficulties with a treatment of the coupling of radiation and matter (i.e., atomic level populations) would be avoided.

We shall show below that this is exactly the escape probability approach that is able to provide a desired approximate form of the net radiative bracket.

5.2. Concept of Escape Probability

We adopt here a conventional definition of the escape probability to be the probability that a photon escapes the medium in a single direct flight. There are different kinds of escape probability depending on the specification of the initial photon.
(i) The elementary escape probability is defined for a photon at a specified position in the medium, with a specified frequency, and propagating in a specified direction. Let $t_\nu$ be the monochromatic optical depth along the ray from the given point to the boundary of the medium. Then the escape probability is given by
\[ p_\nu(t_\nu) = e^{-t_\nu}. \] (26)
In a plane-parallel, horizontally homogeneous slab, any ray is specified by the directional cosine $\mu$; we may then view the elementary escape probability as a frequency- and angle-dependent escape probability,
\[ p_{\nu\mu}(\tau_\nu) = e^{-\tau_\nu/\mu}, \quad \text{for } \mu > 0, \] (27)
and
\[ p_{\nu\mu}(\tau_\nu) = e^{-(T_\nu-\tau_\nu)/\mu}, \quad \text{for } \mu < 0, \] (28)
because for the opposite direction, the optical distance towards the other surface is $(T_\nu - \tau_\nu)/\mu$, where $T_\nu$ is the total optical thickness of the slab. Here $\tau_\nu$ is the monochromatic optical depth measured in the normal direction.

(ii) The angle-averaged escape probability is given by
\[ p_\nu(\tau_\nu) = \frac{1}{2} \int_{-1}^{1} p_{\nu\mu} d\mu = \frac{1}{2} \int_{-1}^{0} e^{-(T_\nu-\tau_\nu)/\mu} d\mu + \frac{1}{2} \int_{0}^{1} e^{-\tau_\nu/\mu} d\mu. \] (29)
Using the second exponential integral $E_2$, defined by equation (16), we may write
\[ p_\nu(\tau_\nu) = \frac{1}{2} [E_2(T_\nu - \tau_\nu) + E_2(\tau_\nu)] \equiv P_\nu(T_\nu - \tau_\nu) + P_\nu(\tau_\nu). \] (30)
It is sometimes convenient to introduce the one-sided escape probability, which represents the probability that a photon emitted isotropically into one hemisphere will escape through the corresponding boundary in a single flight. We denote this probability as $P_\nu(t)$. In this case, we have $P_\nu(t) = E_2(t)/2$, where $t$ is the optical distance from the corresponding boundary.

(iii) The frequency- and angle-averaged escape probability describes the averaged escape probability for an ensemble of photons in a given line. In this case, $\phi(\nu)$ is the emission profile coefficient. Let us assume, for simplicity, the case of complete frequency redistribution, in which case the emission profile coefficient is assumed to be equal to the absorption profile. We also introduce the frequency-averaged optical depth in a line through the expression $\tau_\nu = \tau \phi(\nu)$. The one-sided averaged escape probability for line photons is thus given by
\[ P_e(\tau) = \frac{1}{2} \int_{0}^{\infty} E_2[\tau \phi(\nu)] \phi(\nu) d\nu \equiv \frac{1}{2} K_2(\tau). \] (31)
The integral on the right-hand-side is denoted as $K_2$, after Avrett and Hummer (1965); an efficient method for its evaluation was developed by Hummer (1981). The total escape probability is given by
\[ P_e(\tau) = P_e(\tau) + P_e(T - \tau) = \frac{1}{2} K_2(\tau) + \frac{1}{2} K_2(T - \tau). \] (32)
5.3. First-order Escape Probability Methods

Are the escape probability and the net radiative bracket equal in all points in the medium? As we shall see below, they are indeed approximately equal. This can be understood both from the mathematical and physical standpoint. These views are complementary and each provides a different insight into the nature of the escape probability methods, so we shall briefly describe them below.

**Mathematical Picture.** We start with the Schwarzschild-Milne equation (15), where we observe that the kernel $E_1(t)$ has a width of the order of one optical depth unit, while the scale of depth variation of the source function $S(t)$ may be much larger. Then the source function can be taken out of the integral, setting $S_\nu(t) = S_\nu(\tau_\nu)$, so that equation (15) may be written

$$J_\nu(\tau_\nu) = \left[ 1 - \frac{1}{2} E_2(\nu) - \frac{1}{2} E_2(T_\nu - \tau_\nu) \right] S_\nu(\tau_\nu) = \left[ 1 - p_\nu(\tau_\nu) \right] S_\nu(\tau_\nu),$$

(33)

which follows from the relations between the exponential integrals (Mihalas 1978) and from equation (30). Integrating equation (33) over frequencies with weighting factor $\phi(\nu)$, and assuming that the source function is independent of frequency (i.e., the case of a single line with a complete redistribution), we obtain

$$\bar{J}(\tau) = \left[ 1 - \frac{1}{2} K_2(T_\nu - \tau) - \frac{1}{2} K_2(\tau) \right] S(\tau) = \left[ 1 - P_e(\tau) \right] S(\tau).$$

(34)

In this case, the net radiative radiative bracket is indeed equal, in all points in the medium, to the escape probability,

$$\rho(\tau) = P_e(\tau),$$

(35)

which can be seen easily by comparing equations (25) and (34).

**Physical Picture.** The above derivation is a purely mathematical one, and the only physical point is the argument concerning the scale of the variations of the source function and the kernel function. A more physically based reasoning goes as follows: Deep in the medium the escape probability is essentially zero. On the microscopic level, every downward radiative transition is immediately balanced by the upward transition. The resulting picture is the same as if every emitted photon is immediately re-absorbed at the same point in the medium. This is essentially the reason why this approximation was historically called the on-the-spot approximation; it is also sometimes called complete line saturation, or, perhaps most frequently, detailed radiative balance. In this case,

$$n_j A_{ji} + n_j B_{ji} \bar{J} - n_i B_{ij} \bar{J} = 0,$$

(36)

and thus

$$\bar{J} = S, \quad \text{so that} \quad \rho = 0.$$

(37)

Because $P_e \approx 0$, we have here again the case where $\rho \approx P_e$.

A better approximation is provided by the so-called dichotomous model. Instead of assuming that all emitted photons are re-absorbed on the spot, we
divide them into two groups. The first group of photons is indeed re-absorbed on
the spot, while the rest of photons in contrast escape the medium altogether. The
fraction of photons that do escape is obviously given by the escape probability.
The net rate in the transition, i.e., a difference between downward and upward
transition rate, and therefore a difference between the number of photons created
minus the number of those destroyed, is given by the fraction of the spontaneous
emission rate that produces the escaping photons, i.e.,

\[ n_j A_{ji} + n_j B_{ji} \dot{J} - n_i B_{ij} \dot{J} = n_j A_{ji} P_e. \]  

Comparing this equation to (23), we again see that \( \rho = P_e \) i.e., the equality of
the net radiative bracket and the escape probability is exact here. This model
is also called the normalized on-the spot approximation.

The common name for this approximation is the first-order escape probabil-
ity method. Its computational advantage is immediately seen: If we write the
statistical equilibrium equations in terms of net rates, we may replace \( \rho \) by the
escape probability \( P_e \) for all transitions. The rate equations no longer contain
an unknown radiation field, so they may be solved easily. Nevertheless, they still
must be solved by iterations, because the escape probabilities depend on optical
depths, which in turn depend on the level populations. But because these itera-
tions are not related to consecutive photon scattering, the iteration process is
quite different from the Lambda iteration scheme, and is typically much faster.

Substituting (35) into (17), we obtain the following expression for the source
function,

\[ S(\tau) = \frac{\epsilon}{\epsilon + (1 - \epsilon) P_e} B, \]  

which gives the explicit from of the source function in the first-order escape
probability approximation. It describes very well the behavior of the source
function far from the surface, but it yields for the source function at the surface
\( S(0) = 2\epsilon / (1 + \epsilon) B \), which may be quite different from the exact result, \( S(0) = \sqrt{\epsilon} B \) (Mihalas 1978). The reason for this can be easily understood: any transfer
of photons is neglected here, and the problem is reduced to just two mechanisms – a photon either escapes in a single direct flight, or is thermalized. This so-called “dichotomous” model works well deep in the atmosphere, but fails in the
outer layers of the atmosphere, where the transfer of photons is important.

Without going into any details, I will just mention that the so-called second-
order escape probability formalism, which takes into account some aspects of the
photon transport, was developed (e.g., Rybicki 1984). Its advantage is that
it provides an improved description of the source function near the boundary,
but its application is more difficult because it yields a differential equation for
the source function instead of a simple algebraic expression provided by the
first-order method.

Concluding, the escape probability approach is very useful and very pow-
erful, because it is able to provide simple approximate relations between the
source function and the mean intensity of radiation, based on simple physical
arguments. It can therefore be used in cases where detailed numerical solutions
are either too complicated and time consuming, as in the case of photoionization
codes, where the emphasis is devoted to treating as many atomic processes as
possible, or even more so in the case of radiation hydrodynamic simulations,
Figure 1. A comparison of results obtained using the first-order escape probability method (dashed lines) to the exact radiative transfer results (solid lines), for a two-level atom with depth-independent $\epsilon = 10^{-4}$ and with various values of $B$ and the total optical thickness $T$. The left panels display the source function as a function of optical depth, while the right panels display the emergent profile as a function of dimensionless frequency $x$. The upper row displays results for depth-independent $B = 1$, and for a semi-infinite slab. The middle row displays results for depth-dependent $B$, namely $B = 10$ for $\tau \leq 1000$ and $B = 1$ for $\tau > 1000$; again for a semi-infinite atmosphere. The lower row displays results for depth-independent $B = 1$, and for finite slab with the total optical thickness $T = 100$. 
where the radiative transfer equation is solved in a huge number of time steps. Other areas of applications are all situations where a high accuracy of predicted emergent radiation is not required. However, one should always keep in mind that the escape probability methods are inherently approximate, and therefore one should be always aware of their potential limitations and inaccuracies.

The accuracy of the first-order escape probability method (EPM) is illustrated in Fig. 1, where we display a comparison between the source function and the emergent profile obtained with the escape probability and with the exact solution. We display here representative results for a simple case of a two-level atom without continuum, i.e., with the source function given by equation (17), where we use a simple parametrization for $\epsilon$ and $B$. The upper row shows the results for depth-independent $\epsilon$ and $B$. As we have discussed before, the EPM yields a good agreement with the exact solution far from the boundary, while the surface value of the source function is incorrect. Nevertheless, the line profile predicted by EPM does not differ substantially from the exact profile because in the line center, where the differences would be expected to be largest, the line profile is essentially saturated.

However, in the case of a sharp variation of the Planck function (middle panel), or in the case of finite slabs (lower panel), the EPM is quite inaccurate. This demonstrates our previous conclusions that the EPM works well far from the boundaries, and for a smooth source function variations. Since the latter two cases are of particular interest in the photoionization-dominated media, we should indeed strive to replace the EPM treatment by exact radiative transfer. In the rest of the paper we will outline how one can achieve this.

6. Accelerated Lambda Iteration to the Rescue

In this section we will explain the basis of one of the most important numerical methods of the modern radiative transfer theory: the Accelerated Lambda Iteration, or ALI, method. It is no exaggeration to say that this method made it possible to reach fundamentally more advanced stages of astrophysical quantitative spectroscopy by allowing us to construct theoretical models of unprecedented realism and complexity.

The basic philosophy of the method is as follows. We have already explained that the radiative transfer problem is complicated due to the presence of the non-linear, non-local coupling of level populations to the radiation field. Mathematically, to deal with this coupling in a straightforward way, it is necessary to invert relatively large matrices. However, one should realize that any method that describes a coupling of various quantities by means of a direct matrix inversion is fundamentally limited in that the computer time scales as the cube of the number of quantities (i.e., the number of frequency points in our case).

Therefore, one needs faster schemes. How can this be accomplished? The clue is to realize that some part of the physical coupling is more important than the rest. In other words, not all parts of the coupling should necessarily be treated on the same footing; it is more or less a numerical overkill to do so. So, this hints that the “important part” of the coupling should be treated exactly, while the rest may be treated iteratively.
Below, I demonstrate the method on an example of a two-level atom. We first recall that the two-level problem may be formulated as an integral equation for the source function, equation (19),

\[ S = (1 - \epsilon)\hat{\Lambda}[S] + \epsilon B, \quad (40) \]

Because \( \Lambda \) is a linear operator, Eq. 40 may in fact be solved in a single step (but notice, this applies only for a two-level atom!). However, due to the above mentioned angle-frequency coupling, the matrix representing \( \Lambda \) may be enormous, and therefore a direct solution may be impractical.

Mathematically, the ideas to handle these types of problems iteratively date back to the mid-nineteenth century, to the work of Jacobi. The first who applied the idea in the context of astrophysical radiative transfer was Cannon (1973), who in this seminal paper introduced the method of deferred corrections, also called, somewhat inaccurately, operator splitting. The idea consists of writing

\[ \Lambda = \Lambda^* + (\Lambda - \Lambda^*), \quad (41) \]

where \( \Lambda^* \) is an appropriately chosen approximate lambda operator. The iteration scheme for solving Eq. 40 may then be written as

\[ S^{(n+1)} = (1 - \epsilon)\Lambda^*[S^{(n+1)}] + (1 - \epsilon)(\Lambda - \Lambda^*)[S^{(n)}] + \epsilon B. \quad (42) \]

The action of the exact \( \Lambda \) operator is thus split into two contributions: an approximate \( \Lambda^* \) operator that acts on the new iterate of the source function, and the difference between the exact and approximate operator, \( \Lambda - \Lambda^* \), acting on the previous, old (and thus known) source function. The latter contribution may be easily evaluated by the formal solution.

We emphasize that although we use an approximate operator, equation (40) is solved exactly, i.e., it is exact at the convergence limit. If we choose \( \Lambda^* = 0 \), we recover the "ordinary" lambda iteration, which is straightforward, but is known to converge very slowly – see, e.g. Mihalas (1978); for a very illustrative example, see Auer (1991; his Fig.1), and an illuminating mathematical discussion is given by Olson, Auer, & Buchler (1986 – hereafter referred to as OAB). On the other hand, the choice \( \Lambda^* = \Lambda \) represents the exact method, which is done without any iteration, but an inversion of the exact \( \Lambda \) operator may be costly. So, in order that \( \Lambda^* \) brings an essential improvement over both methods, it has to incorporate all the essential properties of the exact \( \Lambda \) operator (in order to obtain a fast convergence rate of the iteration process), but at the same time it must be easy (and cheap) to invert. These requirements are generally incompatible; therefore, the construction of the optimum \( \Lambda^* \) is a delicate matter. Cannon (1973) used a special variant of the \( \Lambda^* \) operator so that the advantages of the ALI method were not fully realized by most workers in the most workers in the field. This realization came about a decade later, when Scharmer (1981) has reformulated in idea of ALI in a more physical way, and motivated an intensive development of the ALI-based approaches. An interesting history of the quest for the optimum \( \Lambda^* \) operator is summarized by Hubeny (1992).

We may write equation (42) in a slightly different form. First, we introduce an "intermediate" source function, namely that obtained from the old source function by the mere formal solution,

\[ S^{FS} = (1 - \epsilon)\Lambda[S^{(n)}] + \epsilon B. \quad (43) \]
(superscript FS stand for Formal Solution). Using this definition, equation (42) can be rewritten as

\[ S^{(n+1)} - S^{(n)} = [1 - (1 - \epsilon)\Lambda^*]^{-1}[S^{FS} - S^{(n)}]. \]  

(44)

This equation is particularly instructive. To put it in a better perspective, let us rewrite the equation (20) that governs the traditional Lambda iteration, using equation (43),

\[ S^{(n+1)} - S^{(n)} = S^{FS} - S^{(n)}. \]  

(45)

These equations show that the ALI iteration process is driven, similarly as the ordinary lambda iteration, by the difference between the old source function and the newer source function obtained by formal solution. However, unlike the ordinary lambda iteration, this difference is amplified by the “acceleration operator”, \([1 - (1 - \epsilon)\Lambda^*]^{-1}\).

To gain more insight, let us consider a diagonal (i.e., local) \(\Lambda^*\) operator. The appropriate \(\Lambda^*\) has to be chosen such that \(\Lambda^*(\tau) \to 1\) for large \(\tau\) (see below). Because in typical cases \(\epsilon \ll 1\), the acceleration operator indeed acts as a large amplification factor. This interpretation was first introduced by Hamann (1985) and Werner & Husfeld (1985), who also coined the term “Accelerated Lambda Iteration” (ALI). The acronym ALI is also sometimes understood to mean “Approximate Lambda Iteration”.

How do we know that \(\Lambda^*\) should approach unity at large depths? Here comes the intimate relation between the escape probability and the ALI methods. Recall the central role escape probability formalism gives a relation between the mean intensity and the source function, namely \(J = (1 - \rho_e)S\). This is exactly what we need here – a local approximate relation between \(J\) and \(S\). We may thus put, as a reasonable choice, \(\Lambda^* = 1 - \rho_e\), which indeed shows that \(\Lambda^*\) approaches unity for large \(\tau\). This escape-probability form of \(\Lambda^*\) may be used for numerical work, but modern approaches provided more efficient and robust ways to construct the approximate \(\Lambda^*\) operator.

Equation (44) can be also derived using a different, but related, procedure. Let us assume that we have a current estimate of the source function, \(S_0\). We write the correct source function as \(S = S_0 + \delta S\). We further write the exact \(\Lambda\) operator as \(\Lambda = \Lambda^* + \delta\Lambda\), i.e. as an approximate operator \(\Lambda^*\) plus a “perturbation” \(\delta\Lambda\). We require that the source function satisfies equation (40), i.e.,

\[ S = (1 - \epsilon)\Lambda[S] + \epsilon B. \]

By substituting the perturbation expansions for \(S\) and \(\Lambda\) we obtain

\[ S_0 + \delta S = (1 - \epsilon)\Lambda^*[S_0] + (1 - \epsilon)\Lambda^*[\delta S] + (1 - \epsilon)\delta\Lambda[S_0] + \epsilon B, \]

where we dropped the first-order contribution \(\delta\Lambda[\delta S]\). By rearranging the terms we obtain

\[ [1 - (1 - \epsilon)\Lambda^*][\delta S] = (1 - \epsilon)\Lambda[S_0] + \epsilon B - S_0 \equiv S^{FS} - S_0, \]

(46)

where the term \((1 - \epsilon)\Lambda[S_0] + \epsilon B \equiv S^{FS}\) is the updated source function obtained by performing the formal solution with the current source function \(S_0\).
(46) is easily seen to be equivalent to equation (44). This procedure explains why the approach is sometimes called the “Operator Perturbation”.

The iteration proceeds as follows:

(a) For a given \( S^{(n)} \) (with the initial estimate \( S^{(0)} = B \), or some other suitable value), we perform a formal solution, for one frequency and angle at a time. We obtain new values of the specific intensity \( I_{\nu \mu} \).

(b) We calculate the new source function \( S^{FS} \) from equations (43), (13), and (14), using the new values of the specific intensity.

(c) We then apply equation (42) or (44) to evaluate a new iterate of the source function, \( S^{(n+1)} \).

(d) Because the source function found in step (c) differs from that used in step (a), we iterate steps (a) through (c) to convergence.

7. Implementation of ALI

7.1. Evaluation of the \( \Lambda^* \) operator

Construction of the optimum approximate \( \Lambda^* \)-operator is the very gist of the method. As pointed out above, it has to satisfy two dichotomous conditions, namely it should be easy and cheap to invert, and it has to describe well the basic physics of the problem. Again, by the terms “constructing” and “inverting” the \( \Lambda^* \) operator we generally understand a process of solving the transfer equation in some approximate, though judicious, way.

We will not discuss here all possible variants of \( \Lambda^* \) operator; the interested reader is referred to Hubeny (1992). We will mention here only those forms that have survived the test of time, and which are being presently used in actual applications. There are several categories of the \( \Lambda^* \) operator, each category offers certain advantages and suffers from certain drawbacks.

Diagonal Operators. In one of the seminal papers of the astrophysical radiative transfer, OAB showed that a nearly optimum \( \Lambda^* \) operator is in fact a diagonal part of the exact \( \Lambda \) operator,

\[
\Lambda^* = \Lambda^*(\tau) I,
\]

where \( I \) is the unit diagonal matrix, and we understand \( \Lambda^*(\tau) \) as a simple scalar function of \( \tau \). This variant of ALI is sometimes called the Jacobi method (e.g., Trujillo Bueno & Fabiani Bendicho 1995). A diagonal operator is indeed the easiest one to use because its inversion is a simple scalar division. However, how to evaluate the diagonal part of exact \( \Lambda \) efficiently? There are several possibilities, depending on exactly what formal solver for the transfer equation is used.

- Quite generally, the diagonal part can be evaluated as

\[
\Lambda_{dd} = \Lambda_{\tau_d}[\delta(\tau_d - \tau)].
\]
In other words, the diagonal element of the $\Lambda$ matrix at depth point $d$ is equal to the mean intensity (or the specific intensity, in the case of elementary, frequency- and angle-dependent $\Lambda_{\mu v}$) computed for the source function having the zero value everywhere but in the point $d$, i.e., $S_d = 1$, and $S_i = 0$, $(i \neq d)$. As follows from equation (48), to evaluate the diagonal operator at $\tau_d$, we merely have to take the coefficient that multiplies $S(\tau_d)$. This method can be used with many formal solvers, including the short characteristics method (in one or more dimensions), or the Discontinuous Finite Element Method (Castor et al. 1992).

- Olson & Kunasz (1987) were the first to suggest the use of the method of short characteristics to evaluate the $\Lambda^*$ operator. In this case, one can either use the approach from the previous item, or one can also write down explicit expressions for $\Lambda^*$. For instance, using the linear form of the short characteristics method, one obtains for the approximate operator corresponding to the mean intensity of radiation, $\Lambda^*_{\nu}$, namely

$$\Lambda^*_{\nu} = 1 - \frac{1}{2} \int_0^1 \left( \frac{1 - e^{-\Delta \tau_{d-1/2}}}{\Delta \tau_{d-1/2}} + \frac{1 - e^{-\Delta \tau_{d+1/2}}}{\Delta \tau_{d+1/2}} \right) d\mu.$$  \hspace{1cm} (49)

where $\Delta \tau_{d-1/2} = \tau_d - \tau_{d-1}$ and analogously for $\Delta \tau_{d+1/2}$.

- Rybicki & Hummer (1991) used a formalism based on the Feautrier scheme, employing a very efficient algorithm for inverting a tridiagonal matrix, and demonstrated that the entire set of the diagonal elements of $\Lambda$ can be found with an order of $ND$ operations. Thus, if one uses the Feautrier method as a formal solver, the Rybicki-Hummer method of evaluation of $\Lambda^*$ is the method of choice.

A drawback of the diagonal operator is that the convergence speed decreases with increasing spatial resolution, which was first demonstrated by OAB. In other words, the higher the depth resolution, the lower the convergence speed. This is easily understood. Roughly speaking, in a finer grid, the information must go through more points in order to propagate the same distance in the optical depth space, and therefore the iteration is slower. However, in many applications one needs a high spatial resolution. A possible cure is an application of the non-linear multigrid methods (see sect. 7.3.).

**Higher multi-band operators**  Olson & Kunasz (1987) suggested the use of a tridiagonal part of the exact $\Lambda$-operator as an even better approximate $\Lambda^*$ operator. They presented expressions for off-diagonal elements based on the short characteristic method, which are analogous to, but more complicated than, equation (49). The off-diagonal elements may also be easily evaluated in the context of the Rybicki-Hummer scheme.

Analogously, one may use a higher multi-band part of the exact $\Lambda$ operator. As can be expected, using penta-diagonal and higher-order multiband operators will increase a speed of convergence, but this gain is somewhat outweighed by increasing numerical work to evaluate the corresponding matrix elements. A systematic study of the effects of the number of bands on the properties of the ALI iteration process is given by Hauschildt (1992), and MacFarlane (1992).
Gauss-Seidel approximate operator In a very interesting and important paper, Trujillo Bueno & Fabiani Bendichco (1995) suggested a different form of the $\Lambda^*$ operator, namely an upper-triangular part of the exact $\Lambda$ operator. Although inverting an upper triangular matrix looks at first sight almost as costly as inverting a full matrix corresponding to the exact $\Lambda$, they suggested an ingenious trick to invert the upper triangular $\Lambda^*$ operator, in the context of the short characteristic method, with essentially the same computational effort as with the diagonal $\Lambda^*$.

In conclusion, for most applications, using a diagonal $\Lambda^*$ operator is a safe bet. Moreover, it is the only practical choice for multi-dimensional geometries. Although a tridiagonal or higher-order band operators yield a faster convergence for 1-D problems, their application for multilevel transfer problems is more difficult for coding and are thus more prone to coding errors. A beginner is thus encouraged to start with a diagonal operator, and after gaining enough experience, and if the problem requires larger computational speed, the code may be upgraded to more complex operators.

7.2. Acceleration of Convergence

This is a highly technical topic, but is mentioned here because it has recently become an important ingredient of the ALI methods. As it is well known from linear algebra, any iteration method where the $(n+1)$-th iterate is solely evaluated by means of the previous one will converge only linearly. However, taking into account information from the earlier iterates, one may find faster schemes. I will not discuss these methods in any detail here, and the interested reader is referred to the review papers by Auer (1987, 1991), or to the original papers cited therein. I just briefly mention that for the most popular scheme, the Ng (1974) acceleration, the general expression for the accelerated estimate of the solution in the $n$-th iteration is written

$$x^{acc} = \left(1 - \sum_{m=1}^{M} \alpha_m\right)x^{(n)} + \sum_{m=1}^{M} \alpha_m x^{(n-m)}, \quad (50)$$

where the coefficients $\alpha$ are determined by a residual minimization. Practical expressions are given by OAB, Auer (1987, 1991), or Hubeny & Lanz (1992).

Other acceleration techniques are the ORTHOMIN (orthogonal minimization) acceleration (Klein et al. 1989; for detailed expressions, see Auer 1991), and the Successive Overrelaxation (SOR) method, first used in the context of the ALI method (with the Gauss-Seidel $\Lambda^*$) by Trujillo Bueno & Fabiani Bendichco (1995).

7.3. Multigrid Methods

This is a very recent upgrade of the ALI methods, pioneered by Fabiani Bendichco, Trujillo Bueno & Auer (1997). They have worked out application of the non-linear multigrid method (see, e.g., Hackbusch 1985) into multi-level radiative transfer. The essence of the method consist of composing the overall multigrid iteration process of two basic parts: (i) a smoothing one where a small number of iterations is performed on the desired fine grid (i.e., with a high spatial resolution), and (ii) a coarser grid correction. The greatest advantage of the
multigrid approach is that its convergence speed does not decrease when using finer spatial resolution. For details, the reader is referred to the original paper.

7.4. Some Representative Results

In order to test the performance of various variants of the $\Lambda^*$ operator and the effects of the acceleration techniques, we have computed a series of test examples. We display here representative results for a simple case of a two-level atom without continuum, i.e. with the source function given by equation (17), where we use a simple parametrization for $\epsilon$ and $B$, namely depth-independent $\epsilon = 10^{-4}$ and $B = 1$. The results are obtained by a pedagogically-oriented program ALIRTE, (Hubeny 1994), which may be provided to the interested user upon request.

Figure 2 illustrates the behavior of the ALI iteration process when using different variants of the $\Lambda^*$ operator, together with the effects of the Ng acceleration. The simplest ALI variant, a diagonal $\Lambda^*$ with no acceleration, converges relatively slowly, although still much faster than the traditional Lambda iteration. The tridiagonal operator yields much faster convergence. However, the most interesting result is that using Ng acceleration with a diagonal operator
yields faster convergence than the tridiagonal operator! This is a good news, because as we discussed above, the diagonal operator is the easiest to implement in any geometry. As expected, an application of tridiagonal $\Lambda^*$ with Ng acceleration is even faster.

8. Real-life Applications of ALI: Beyond a Two-level Atom

The academic case of the two-level atom without an overlapping continuum is a beautiful pedagogical tool to demonstrate the basic features of line transfer, but reality is usually more complicated. In this section, we outline the strategy of how to deal with more complicated situations.

Inspecting the case of two-level atom, one realizes that the ease with which the idea of ALI was applied follows from the fact that the radiation intensity enters the expression for the total source function only through a single frequency- and angle-integrated quantity, $\bar{J}$. In all the situations where this is not the case (we shall show some such situations below), the basic strategy is to find a quantity which is frequency- and angle-integrated, and through which the total source function can be expressed.

8.1. Two-level atom with continuum

The simplest such case is provided by the two-level atom with a background continuum. In this case the total source function is given by (Mihalas 1978)

$$S^\text{tot}_\nu = \frac{\phi_\nu}{\phi_\nu + r} S^L + \frac{r}{\phi_\nu + r} S^C.$$  \hspace{1cm} (51)

where $S^L$ is a frequency-independent line source function, given by equation (17); $S^C$ is the source function in the continuum, and $r = \kappa^C / \kappa^L$ is the ratio of the continuum to the frequency-averaged line opacity. Here the choice of the frequency- and angle-integrated quantity is obvious – it is essentially the line source function.

The specific intensity is expressed through the elementary lambda operator acting on the total source function,

$$I_{\nu\mu} = \Lambda_{\nu\mu} \left[ S^\text{tot}_\nu \right] = \Lambda_{\nu\mu} \left[ \frac{\phi_\nu}{\phi_\nu + r} S^L + \frac{r}{\phi_\nu + r} S^C \right].$$  \hspace{1cm} (52)

Substituting this to equation (17), we obtain for the line source function

$$S^L = (1 - \epsilon) \bar{\Lambda}[S^L] + S_0 ,$$

where

$$\bar{\Lambda}[\ldots] = \frac{1}{2} \int_{-1}^1 d\mu \int_0^\infty d\nu \phi_\nu \Lambda_{\nu\mu} \left[ \frac{\phi_\nu}{\phi_\nu + r} \ldots \right] ,$$

and

$$S_0 = (1 - \epsilon) \frac{1}{2} \int_{-1}^1 d\mu \int_0^\infty d\nu \phi_\nu \Lambda_{\nu\mu} \left[ \frac{r}{\phi_\nu + r} S^C \right] + \epsilon B ,$$

so $S_0$ is a known function.
Equation (53) is completely analogous to the expression for the (line) source function without the background continuum. We may therefore use exactly the same iterative scheme as described above, where the only difference is that the integrated approximate \( \Lambda^* \) operator is given by

\[
\tilde{\Lambda}^*[\ldots] = \frac{1}{2} \int_{-1}^{1} d\mu \int_{0}^{\infty} d\nu \phi_{\nu} \Lambda^*_\nu \mu \left[ \frac{\phi_{\nu}}{\phi_{\nu} + r} \right]. \tag{56}
\]

Again, in the case of diagonal approximate operator, \( \tilde{\Lambda}^* \) is a scalar function of \( r \), and is given by

\[
\tilde{\Lambda}^*(r) = \frac{1}{2} \int_{-1}^{1} d\mu \int_{0}^{\infty} d\nu \phi^{2}_{\nu} \Lambda^*_\nu \mu(r). \tag{57}
\]

### 8.2. Multilevel Atoms

To illustrate the basic problem of applying ALI in multilevel problems, let us first write down the expression for the radiative rates. For simplicity, let us consider only lines; the treatment of continua is analogous. The net transition rate for any line \( i \to j \) (\( i \) and \( j \neq i \) represent any states of an atom), is

\[
R_{ji}^{\text{net}} = n_{j}A_{ji} - (n_{i}B_{ij} - n_{j}B_{ji}) \tilde{J}_{ij}, \tag{58}
\]

The basic ALI equation gives for \( \tilde{J}_{ij} \)

\[
\tilde{J}_{ij} = \Lambda^*[S^{\text{new}}] + (\Lambda - \Lambda^*)[S^{\text{old}}]. \tag{59}
\]

Here the second term, which may be written as \( \Delta \tilde{J}_{ij}^{\text{old}} \), is known from the previous iteration. However, the first term contains \( S^{\text{new}} \), which is a complicated and generally non-linear function of the “new” populations.

This complicates the situation. By applying the ALI idea, we have successfully eliminated the radiation intensity from the rate equations, but at the expense of ending with a set of non-linear equations for the populations. We cope with this problem by one of the possible two ways:

1. **Linearization.** The usual way of solving the set of non-linear equations is by applying the Newton–Raphson method. Each such iteration requires to set up and to invert the Jacobi matrix of the system.

2. **Preconditioning.** This is an ingenious way to analytically remove inactive (scattering) parts of radiative rates from the rate equations, and to recover a linearity of the ALI form of the rate equations.

Let us demonstrate the idea of preconditioning on a simple case, where the total source function is given by the line source function \( S_{ij} = n_{j}A_{ji}/(n_{i}B_{ij} - n_{j}B_{ji}) \) (i.e., the case of non-overlapping lines and no background continuum). Let us further assume that we have a local (diagonal) approximate \( \Lambda^* \) operator (\( \Lambda^* \) is then a real number). The net rate (58) may be written, after some algebra,

\[
R_{ji}^{\text{net}} = n_{j}A_{ji}(1 - \Lambda_{ji}^*) - (n_{i}B_{ij} - n_{j}B_{ji})\Delta \tilde{J}_{ij}^{\text{old}}, \tag{60}
\]
which is indeed *linear* in the populations.

This is a very interesting expression. Notice first that the original net rate, (58), is represented by a subtraction of two large contributions, *all* emission minus all absorptions, while the result, the net rate, is rather small. Physically, this follows from the fact that most emissions (i.e., radiative transitions \( j \to i \)) are those that immediately follow a previous absorption of a photon (transitions \( i \to j \)), i.e., they are the part of a *scattering* process. In order to improve the numerical conditioning of the system of rate equations, we have to somehow eliminate the scattering contributions, i.e., to “precondition” the rates. An illuminating discussion of this topic is presented by Rybicki (1984).

In the ALI form of the net rate, (60), we see that deep in the atmosphere, \( \Lambda^* \to 1 \), so that the first term is indeed very small. Similarly, the second term is also small because \( \Delta_j \) is small. In other words, the radiative rates are indeed preconditioned. In the context of the ALI approach, this idea was first used by Werner & Husfeld (1985); a systematic study was presented by Rybicki & Hummer (1991, 1992), who have extended it to the case of general overlap of lines and continua.

Both approaches outlined above seem at first sight to be quite different. Indeed, their original formulations differ quite substantially. However, in a very interesting paper, Socas-Navarro & Trujillo Bueno (1997) showed that both approaches, linearization and preconditioning, are essentially equivalent from the mathematical point of view. These authors showed that linearization takes into account (in an approximate way) the linear response of the radiation field to the perturbations in the source function and in opacity, while preconditioning takes into account the response to the source function perturbations. In a different variant of these approaches, they can actually both take into account (in an approximate way) the linear response of the radiation field to the perturbations in both the source function and in the opacity. The interested reader is referred to the original paper for more details.

### 8.3. Velocity Fields

Practically any ALI variant mentioned in the previous sections, developed for static problems, may include velocity fields using an observer’s frame formulation; several of them mention this extension explicitly (e.g., Scharmer 1981; Rybicki & Hummer 1991).

However, the observer’s frame formalism becomes impractical for velocities larger than few times thermal velocity, which is the case for instance in stellar winds. In such situations, where the ratio of the expansion to thermal velocity is of the order of hundreds, the comoving-frame (CMF) formalism is traditionally used (Mihalas 1978). Its basic drawback is that it may only be used for monotonic velocity fields; all the following approaches thus possess this limitation. The application of ALI to the CMF transfer problem was pioneered by Hamann (1985). Later, Puls (1991) has developed a parameter-free \( \Lambda^* \) operator for expanding atmospheres in the CMF formulation, which represent an extension of OAB to moving and spherical atmospheres. Hauschildt (1992) has extended the ALI CMF formulation to consider relativistic velocities, and Buchholtz et al. (1994) have further extended this approach for atmospheres with shocks. A
related, but somewhat different approach, called Approximate Newton-Raphson Method, was developed by Hillier (1990).

9. Conclusions

I have demonstrated that the escape probability method, which is presently the standard means of approximating radiative transfer in current photoionization codes, is prone to significant inaccuracies, in particular for slabs of finite optical thickness, and for media that exhibit sharp variations of the structural parameters with position. But these are the very conditions that are often met in photoionization-dominated media. Therefore, the time has come that one will have to think about implementing exact radiative transfer into the photoionization codes.

Fortunately, in the last decade we have witnessed great advances in efficient numerical methods for treating exact radiative transfer. I claim that it is now feasible to develop a treatment that will replace the traditional escape probability methods in the photoionization codes while using a reasonable amount of computer resources.

I have suggested that the method of choice is the Accelerated Lambda Iteration method. I have given a brief review of this method, and outlined how it can be implemented in actual applications, including the photoionization codes.

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