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A FORTH-AND-BACK IMPLICIT Λ-ITERATION

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ABSTRACT

In many radiative transfer (RT) problems, the sources contain a scattering term that couples all the specific RT equations, one for each frequency and direction, so that solving the problem means solving the system formed by these equations. Each of them is a first-order linear differential equation with its own initial condition assigned at a different point of the medium, which makes the solution of the system extraordinarily difficult.

One simple way to achieve a solution is with the so-called Λ-iteration: sources and sinks given as a first approximation → computation of the specific intensities from their own RT equations → computation of the scattering terms → recomputation of the sources and sinks. This scheme is straightforward, but unfortunately in practice its convergence rate is too slow to be of value in the case of optically thick systems.

The aim of this paper is to show that a *forth-and-back* approach (the natural approach to describing sequentially the two intensities propagating along the two directions of a straight line), together with an *implicit* representation of the source function in the computation of the intensities within the above iterative scheme, can dramatically accelerate the convergence of the iterative process while retaining the straightforwardness of ordinary Λ-iteration.

Subject headings: methods: numerical — radiative transfer

1. INTRODUCTION

It is well known that one intrinsic difficulty of non-LTE radiative transfer (RT) problems arises from the nonlocal coupling between the radiation field and the excitation state of the gas: the transport (absorption and emission) coefficients depend on the specific intensity of the radiation field, namely, on the solution itself of the RT problem. In turn, the specific intensity at each point of the medium depends, via the RT process, on the values of the transport coefficients over a wide range of distant points. Therefore, in general, an iterative solution must be sought in order to solve the global problem. Two alternative approaches can be envisaged. Either a sequential iterative procedure can be considered, in which the different phenomena coupled together are tackled one by one while all the others are assumed to be known, or, the different phenomena can be faced simultaneously by means of the corresponding linear formulation.

Although the transport coefficients may be assumed to be known, at least within each step of the iterative procedure, a further difficulty is introduced by the existence, within any specific RT equation (one for each pair of frequency and direction), of a scattering term that depends on the full set of the specific intensities. Therefore, all the RT equations are strongly coupled by the scattering term.

In some cases, such as in the well-known instance of the two-level atom line formation problem, the source function can be explicitly formulated in terms of a scattering integral, and the problem, in this case linear, can be solved by using either direct or iterative methods. Yet in many other physical problems it is not possible to write the source function explicitly, so the self-consistent solution of the RT and statistical equilibrium equations, which here play the role of a scattering-like process, has to be achieved by means of an iterative method. This is the case, for instance, with the multilevel atom non-LTE line transfer.

The aim of this paper is to show that the convergence of some of the iterative methods currently in use can be greatly accelerated when we treat separately, within a forth-and-back process, the natural two-stream representation of the radiation field along each line.

As with the integral methods based on the Λ-operator, we employ an implicit representation of the source function when computing the mean intensity of the radiation field. In contrast to the Λ-operator implicit scheme, which we might regard as global, we may consider the implicit scheme proposed here as local.

In the former, the operator $\Lambda(\tau, \tau')$ is equivalent to the integral form of the RT equation: one can express the specific intensities $I_{x\mu}(\tau)$, hence the frequency-integrated mean intensity $J_{\varphi}(\tau)$, through a linear combination of the unknown values of the source function $S(\tau')$ for all the values τ' of the optical depth grid.

On the contrary, the forth-and-back approach allows us to introduce an implicit local scheme: any intensity at a given point, propagating along a given direction, is expressed as a linear combination of the unknown values of the source function $S(\tau)$ and its τ-derivative $S'(\tau)$ at previous points along the same direction.

This alternative choice leads to a different way of performing the iterative scheme. The result is a very high rate of convergence.

In the first part of this study on non-LTE line RT, we limit ourselves to the well-known instance of the two-level atom line formation problem, under the assumption of complete redistribution.

The particular interest of both the problem itself and the relevant methods for its solution is due not only to its intrinsic physical relevance but also, above all, to the fact that it constitutes the veritable cornerstone of RT. Moreover, because its exact solution is known, it constitutes a very useful benchmark for testing the quality of any new algorithm.

In the second part, the method is employed to solve both the two-level atom problem, in which partial redistribution is taken into account, and the non-LTE line formation problem in the case of a multilevel atom model.

For the sake of an easier presentation, we consider in this paper the case of a plane-parallel, stationary medium. However, the conclusions of this study can be straightforwardly generalized to other systems with different geometry.

2. THE TWO-LEVEL ATOM MODEL

Let us consider a stationary medium consisting of plane-parallel layers whose physical properties vary only with the coordinate z measured along the direction $\boldsymbol{k}$ perpendicular to the layers. Let the system be bound by the planes A and B, whose intersections with the z-axis have coordinates z_A and z_B such that $z_A > z_B$.

According to physical considerations, it is customary to choose z_A as the origin of the τ-coordinates (i.e., on the upper boundary surface) and to introduce a mean optical depth scale τ, defined by

$$\tau(z) \equiv \int_z^{z_A} \chi(z')dz' , \tag{1}$$

where $\chi(z)$ [or $\chi(\tau)$] is a weighted average of the opacity, assumed to be known. Thus, for $z = z_A$ it holds that $\tau = 0$; for $z = z_B$, $\tau = T$, i.e., the total mean optical depth of the system.

Under the above assumptions, the RT equation takes the form

$$\mu \frac{dI_{x\mu}}{d\tau} = \varphi_x[I_{x\mu}(\tau) - S(\tau)] . \tag{2}$$

According to the standard notation, $I_{x\mu}(\tau)$ is the specific intensity of the radiation field at the mean optical depth τ, x is the frequency displacement from the line center in Doppler width units, and μ is the cosine of the angle between the photon's direction and the outward normal $\boldsymbol{k}$. The quantity φ_x is the absorption-line profile, normalized to unity.

In the case of an atomic model consisting of only two bound levels (two-level atom), and assuming complete redistribution (CR) in the line profile, the frequency-independent line source function is

$$S(\tau) = \varepsilon B(\tau) + (1 - \varepsilon)J_\varphi(\tau) , \tag{3}$$

where J_φ is the scattering integral,

$$J_\varphi(\tau) = \tfrac{1}{2} \int_{-1}^{1} d\mu \int_{-\infty}^{+\infty} dx \; \varphi_x I_{x\mu}(\tau) , \tag{4}$$

which accounts for the angle and frequency coupling of the specific intensities at the given depth point τ. The branching ratio between the thermal (LTE) contribution $B(\tau)$ and the scattering term J_φ is represented by the non-LTE parameter ε. The latter depends on the local properties of the medium, so that it may be a function of the optical depth τ as well. The same holds true for the absorption profile coefficient φ_x, which in some cases may also depend on the direction μ.

Finally, the specific intensities incident onto the boundary surfaces are given data of the problem. They furnish the corresponding initial conditions for equation (2), namely, the known values of the down-going intensities incident onto the upper boundary surface $\tau = 0$: $I_{x\mu}(\tau = 0)$ $(-1 \le \mu < 0)$, and the up-going intensity incident onto the lower boundary surface, $\tau = T$: $I_{x\mu}(\tau = T)$, $(0 < \mu \le 1)$. As is customary, we use the notation $I^+_{x\mu}$ and $I^-_{x\mu}$ for the up-going and down-going intensities, respectively, where μ now ranges from 0 to 1.

For the sake of simplicity, in the presentation of the new method we consider the case of a profile independent of both τ and μ. The application to the most general case is straightforward, because the difference is only in the numerical computation of the optical distance between pairs of depth points for any given frequency x and direction μ.

The numerical solution of the RT equation (2) can be directly achieved by means of either differential or integal methods (see Mihalas 1978). As is customary, the first step toward a numerical solution is to consider $I^{\pm}_{x\mu}(\tau)$ at each depth τ over a finite grid of ND directions μ_i and NF frequency points x_j. Then the integrals in the scattering term $J_\varphi(\tau)$ are replaced by the corresponding quadrature sums, with proper integration weights. Therefore, we consider equation (2) only for the discrete set of specific intensities with directions μ_i, $i = 1, ND$, and frequencies x_j, $j = 1, NF$. The numerical solution of the set of equations (2) needs the discretization of the depth variable too. Thus we evaluate all the relevant depth-dependent functions only on a finite grid of mean optical depth values τ_L, $L = 1, NL$. It holds that $\tau_1 = 0$ at the surface, and $\tau_{NL} = T$ at the bottom.

3. THE Λ-ITERATION

The most straightforward iterative procedure to solve the two-level atom problem is the so-called Λ-iteration, which solves in turn the RT equation (eq. [2]) and the statistical equilibrium equations, the latter leading in this case directly to the source function given by equation (3).

Starting from a current solution $S^0(\tau)$ of the source function, we compute the frequency-integrated mean intensity $J_\varphi(\tau)$, either by means of equations (2) and (4) within a differential approach or by means of an integral operator like that defined by equation (5) within an integral approach. Then the updated values $S^n(\tau)$ of the source function are computed via equation (3). This may be represented by the following sequence: $S^0(\tau) \to I_{x\mu}(\tau) \to J_\varphi(\tau) \to S^n(\tau)$.

The differential approach, which uses a finite-difference form of equation (2) is one of the most general and flexible methods used to solve the aforementioned problem. However, the integral formalism which employs the Λ-operator (Hopf 1934) to represent the formal solution of the transfer equation,

$$J_\varphi(\tau_L) = \Lambda(\tau_L, \tau_l) S(\tau_l) , \tag{5}$$

is also in current use (for the line formation problem see Avrett & Loeser, 1969). The aforementioned iterative sequence is named Λ-iteration after the Λ-operator, whatever the actual method employed for the solution of the RT equation.

But, irrespective of the approach chosen, the convergence of this straightforward procedure in practical computations is too slow to be useful for systems that are optically thick.

Let us now comment upon the construction of the $\Lambda(\tau_L, \tau_l)$ operator. From a prescribed functional form for $S(\tau)$, one can write, for all the values τ_L of the optical depth grid, linear relations for the specific intensities $I_{x\mu}(\tau_L)$, and consequenty for the frequency-integrated mean intensity $J_\varphi(\tau_L)$, as a function of the unknown values of the source function $S(\tau_L)$.

In order to do this in the frame of the classical product integration method (Avrett & Loeser 1969), a polynomial representation of $S(\tau)$ on each subinterval (τ_{L-1}, τ_L) must be assumed. As the RT is a typical integrodifferential, second-order problem, a piecewise quadratic approximation for $S(\tau)$ is necessary from the mathematical point of view and sufficient from the numerical point of view. Of course, it is important to ensure that the variation of the function between each two successive depth points (τ_{L-1}, τ_L) is not too abrupt. Between the last two depth points (τ_{NL-1}, τ_{NL}), it is necessary to use a linear approximation.

Although in this paper we do not employ any Λ-operator, our implicit treatment of the RT problem is based on the above functional representation of $S(\tau)$.

4. A SEMI-IMPLICIT Λ-ITERATION

This section has two purposes: to discuss an improved Λ-iteration method with results better than those of ordinary Λ-iteration by only a factor of 2, and to introduce the germ of the new method that we present in § 5.

The existence of two separate families of boundary conditions naturally suggests the separate description of the propagation of the up-going intensities $I^+_{x\mu}(\tau)$, with initial conditions at $\tau_{NL} \equiv T$, and that of the down-going intensities $I^-_{x\mu}(\tau)$, with initial conditions at $\tau = 0$. This recalls the basic idea of a forth-and-back scheme.

Consequently, we can define the corresponding mean intensities:

$$J^+_\varphi(\tau) = \int_0^1 d\mu \int_{-\infty}^{+\infty} dx\ \varphi_x I^+_{x\mu}(\tau) \tag{6a}$$

and

$$J^-_\varphi(\tau) = \int_0^1 d\mu \int_{-\infty}^{+\infty} dx\ \varphi_x I^-_{x\mu}(\tau)\ . \tag{6b}$$

Therefore, according to equation (4), we have

$$J_\varphi(\tau) = \tfrac{1}{2}[J^+_\varphi(\tau) + J^-_\varphi(\tau)]\ . \tag{7}$$

On the basis of this physical discrimination, we can seek new, more efficient iterative strategies. The first and most obvious one is a semi-implicit Λ-iteration, which works according to the following scheme.

We assume, as in ordinary Λ-iteration (cf § 3), that a current estimate of the source function, $S^0(\tau)$, is known at all the optical depths τ_L. Thus, it is straightforward to compute *explicitly* in the first part of each iteration the down-going intensities $I^-_{x\mu}(\tau_L)$ by solving the relevant RT equations with a *known* source function, either in the differential or in the integral for, and, successively, the corresponding frequency-integrated mean values $J^-_\varphi(\tau_L)$ (cf eq. [6b]).

Once $J^-_\varphi(\tau_L)$ has been explicitly evaluated at each depth, we can compute the up-going intensities in the second part through an *implicit* procedure.

From the integral form of the RT equation for the up-going intensities, we can write, for the generic layer (τ_L, τ_{L+1}),

$$I^+_{x\mu}(\tau_L) = I^+_{x\mu}(\tau_{L+1})\, e^{-\Delta\tau\varphi_x/\mu} + \int_{\tau_L}^{\tau_{L+1}} S(t)\, e^{-(t-\tau_L)\varphi_x/\mu}\, \frac{\varphi_x}{\mu}\, dt\ . \tag{8}$$

By assuming piecewise parabolic behavior for the source function, it is easy to derive the coefficients $p^{1+}_{x\mu}$, $p^{2+}_{x\mu}$, and $q^+_{x\mu}$ of the unknown values of $S(\tau_L)$, $S(\tau_{L+1})$, and $S'(\tau_{L+1})$ in the relation

$$I^+_{x\mu}(\tau_L) = I^+_{x\mu}(\tau_{L+1})\, e^{-\Delta\tau\varphi_x/\mu} + p^{1+}_{x\mu} S(\tau_L) + p^{2+}_{x\mu} S(\tau_{L+1}) + q^+_{x\mu} S'(\tau_{L+1})\ . \tag{9}$$

These coefficients, together with the exponential $\exp(-\Delta\tau\varphi_x/\mu)$, are the basic building blocks of the local implicit scheme. They depend only on the known slantout optical distances $\Delta\tau\varphi_x/\mu$, with $\Delta\tau \equiv \tau_{L+1} - \tau_L$. Here and in the following, the prime denotes derivatives with respect to τ.

We start from the bottom layer (τ_{NL-1}, τ_{NL}). The incident up-going intensities $I^+_{x\mu}(\tau_{NL})$ are given data of the problem, and consequently $J^+_\varphi(\tau_{NL})$ is also known. As $J^-_\varphi(\tau_{NL})$ has been already computed in the first part of the iteration, we obtain $J_\varphi(\tau_{NL})$ from equation (7), and hence the value of the new source function $S^n(\tau_{NL})$.

Because of the assumed linear behavior of $S(\tau)$ in the last layer (τ_{NL-1}, τ_{NL}), the derivatives at the two limiting points of this interval are given by the relation

$$S'(\tau_{NL}) = S'(\tau_{NL-1}) = [S(\tau_{NL}) - S(\tau_{NL-1})]/\Delta\tau\ . \tag{10}$$

Therefore, equation (9) particularizes into

$$I^+_{x\mu}(\tau_{NL-1}) = I^+_{x\mu}(\tau_{NL})\, e^{-\Delta\tau\varphi_x/\mu} + P^{1+}_{x\mu} S(\tau_{NL-1}) + P^{2+}_{x\mu} S(\tau_{NL})\ . \tag{11}$$

Of course, the coefficients $P^{1+}_{x\mu}$ and $P^{2+}_{x\mu}$ are easily derived from $p^{1+}_{x\mu}$, $p^{2+}_{x\mu}$, and $q^+_{x\mu}$, previously computed, by taking into account equation (10).

Because $I^+_{x\mu}(\tau_{NL})$ is a datum of the problem, and the value of $S(\tau_{NL})$ has already been computed, we can cast equation (11) in the form

$$I^+_{x\mu}(\tau_{NL-1}) = \mathscr{A}^+_{x\mu} + \mathscr{B}^+_{x\mu} S(\tau_{NL-1})\ , \tag{12}$$

where the coefficients $\mathscr{A}^+_{x\mu}$ and $\mathscr{B}^+_{x\mu}$ are easily derived. After numerical integration over all frequencies and directions (cf. eq. [6a]), we obtain the coefficients a^+ and b^+ of the expression

$$J^+_\varphi(\tau_{NL-1}) = a^+ + b^+ S(\tau_{NL-1})\ . \tag{13}$$

At this stage, $J^-_\varphi(\tau_{NL-1})$ is already known from the first part of the current iterative step, and $J^+_\varphi(\tau_{NL-1})$ is *implicitly* known in terms of the as yet unknown value of $S(\tau_{NL-1})$ (see

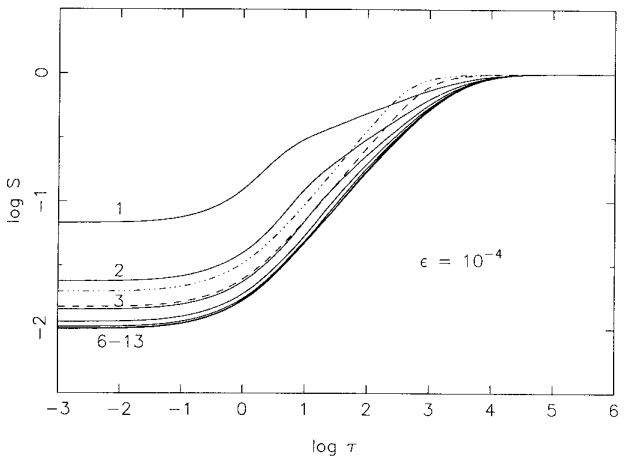

FIG. 1.—Evolution with iterations of the computed source function for a two-level atom with $\varepsilon = 10^{-4}$. The solid lines, labeled with the relevant iteration number, correspond to forth-and-back implicit Λ-iteration (see § 5). The dashed and dot-dashed lines correspond to the 1000th iteration of the semi-implicit Λ-iteration (cf § 4) and the ordinary Λ-iteration (cf. § 3), respectively.

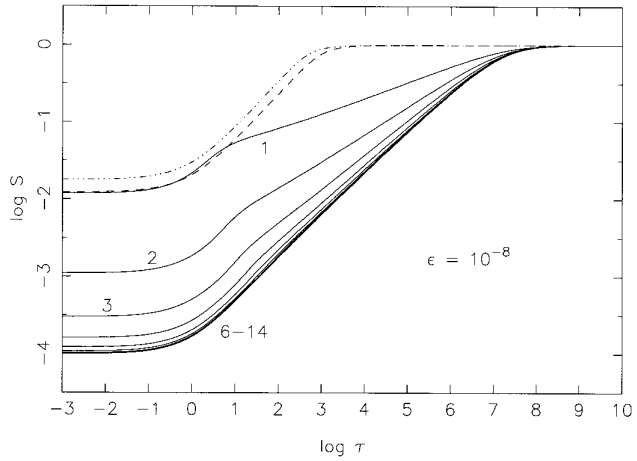

FIG. 2.—Same as Fig. 1, but for the case with $\varepsilon = 10^{-8}$

eq. [13]). By using equation (7), we can express $J_\varphi(\tau_{NL-1})$ in the form

$$J_\varphi(\tau_{NL-1}) = \alpha_{NL-1} + \beta_{NL-1} S(\tau_{NL-1}) . \quad (14)$$

Again, the numerical values of the coefficients α_{NL-1} and β_{NL-1} are easily derived. This relation, together with the definition of $S(\tau_{NL-1})$, as in equation (3), lead to the new numerical value of $S^n(\tau_{NL-1})$.

Once the values of $S^n(\tau_{NL})$ and $S^n(\tau_{NL-1})$ are known, the derivatives at τ_{NL-1} and τ_{NL} are given by equation (10). The values of $I^+_{x\mu}(\tau_{NL-1})$ are straightforwardly obtained by means of equation (12).

Then the previous elimination scheme can be repeated for all the successive layers (τ_L, τ_{L+1}), sweeping upward from $L = NL - 2$ up to $L = 1$. The *known* output from the previous layer (τ_{L+1}, τ_{L+2}), i.e., $I^+_{x\mu}(\tau_{L+1})$, $S(\tau_{L+1})$, and $S'(\tau_{L+1})$, is the necessary and sufficient input for the treatment of the succeeding layer (τ_L, τ_{L+1}), where, via equation (9), we can derive the coefficients $\mathscr{A}^+_{x\mu}$ and $\mathscr{B}^+_{x\mu}$ of an equation like equation (12) at any τ_L, and eventually obtain the values of the coefficients α_L and β_L of a linear relation like equation (14):

$$J_\varphi(\tau_L) = \alpha_L + \beta_L S(\tau_L) . \quad (15)$$

By now taking into account equation (3), we obtain the new value $S^n(\tau_L)$ of the source function at τ_L.

Just a minor difference arises in the way of computing $S'^n(\tau_L)$. Equation (10) must be replaced by

$$S'(\tau_L) = 2[S(\tau_{L+1}) - S(\tau_L)]/\Delta\tau - S'(\tau_{L+1}) , \quad (16)$$

which follows from the assumed piecewise parabolic behavior of $S(\tau)$.

In the above scheme, we assumed that both $I^-_{x\mu}(\tau = 0)$ and $I^+_{x\mu}(\tau = \tau_{NL})$ were known data of the problem. This does not hold true, however, in some cases, e.g., in the important one of a semi-infinite atmosphere. In this instance, the intensities incident on the last layer are not explicitly known. However, at large optical depth the so-called diffusion approximation holds for the specific intensity. Namely, $I^+_{x\mu}(\tau_{NL})$ can be expressed as a linear combination of $S(\tau_{NL})$ and $S'(\tau_{NL})$. Thus, $J_\varphi(\tau_{NL})$ results as a linear combination of $S(\tau_{NL})$ and $S(\tau_{NL-1})$, after we have eliminated $S'(\tau_{NL})$ by means of equation (10). A similar linear form for $J_\varphi(\tau_{NL-1})$ is derived by starting from equation (11). The values of $S^n(\tau_{NL-1})$ and $S^n(\tau_{NL})$ are straightforwardly derived from equation (3).

It is self-evident that the ease of use of this semi-implicit Λ-iteration is the same as that of the classical one. The distinctive difference is brought about by the fact that the former uses the updated values of the source function in order to compute the up-going intensities.

This approach is similar to that of the Gauss-Seidel method discussed by Trujillo Bueno & Fabiani Bendicho (1995). However, the way of computing the values of $I^+_{x\mu}(\tau_L)$ is different. There, the intensities were computed by means of a differential operator expressed by a three-point difference formula, which may introduce minor numerical difficulties, since such a formula needs the value of $S(\tau_{L+1})$ that has just been recomputed, that of $S(\tau_L)$ which is actually computed, and that of $S(\tau_{L-1})$, whose removal requires a global treatment of all the values of $\{S(\tau_L)\}$.

On the contrary, the integral method proposed here is a two-point algorithm that works by taking into account the values of both the source function and its first derivative on pairs of successive depth points.

However, the improvement in terms of rate of convergence brought about by this "half" Λ-iteration is not substantial. With respect to classical Λ-iteration, only a factor of about 2 is gained, which is, of course, not enough (See Figs. 1 and 2.)

5. IMPLICIT Λ-ITERATION

The conclusion of § 4 is that although better than that of the ordinary Λ-iteration by a factor of 2, the rate of convergence of semi-implicit Λ-iteration is still exceedingly slow. Therefore, we must explore the possibility of further acceleration.

In their work already mentioned in § 4, Trujillo Bueno & Fabiani Bendicho (1995) introduce a successive overrelaxation (SOR) method in order to achieve a faster iterative

procedure. However, the value of the relaxation parameter ω that optimizes the iterative procedure is known for a few structured problems only. In more complicated problems, a fairly sophisticated eigenvalue analysis may be necessary in order to determine, case by case, the optimum value of ω (cf. Golub & Van Loan 1983, § 10.1).

On the contrary, we achieve here a substantial improvement of the rate of convergence by fully exploiting the idea of an implicit representation of the source function in the computation of both the up-going and the down-going intensities.

In semi-implicit Λ-iteration, we store the numerical values of the down-going mean intensities $J_\varphi^-(\tau)$, computed from the known values $S^0(\tau)$ of the current estimate of the source function. Alternatively, in forth-and-back implicit Λ-iteration, we shall use the old values of the source function to compute and store, for each L ($L = 1, NL$), the coefficients b_L^- and c_L^- of the linear relation

$$J_\varphi^-(\tau_L) = b_L^- S(\tau_L) + c_L^- S'(\tau_L) , \tag{17}$$

which represent *implicitly* the values of the down-going mean intensities. The way of computing the coefficients of equation (17) is straightforward and will be described in § 5.1. These coefficients are used later in the succeeding backward process.

We show in what follows that the results lead to a new method whose rate of convergence is extremely high. Perhaps it is worth stressing that the implementation of this new method comes from physical considerations, not from a previous spectral analysis of the mathematical properties of the problem.

The operative scheme of the new method is essentially the same as that of semi-implicit Λ-iteration, which in turn is the same as that of ordinary Λ-iteration. *The fundamental improvement is the way of storing the information relevant to* $J_\varphi^-(\tau)$ (cf. eq. [17]) *in the first part of each iterative step.*

5.1. *The Forward Process*

We start at the upper boundary surface $L = 1$, where the values of $I_{x\mu}^-(0)$ are given data of the problem. Then we obtain directly from equation (6b) the corresponding known value

$$J_\varphi^-(\tau_1) = a_1^- . \tag{18}$$

Usually it holds that $a_1^- = 0$.

At all successive optical depths τ_L, with $L > 1$, the formal solution of the RT equation for the down-going intensities reads:

$$I_{x\mu}^-(\tau_L) = I_{x\mu}^-(\tau_{L-1})\, e^{-\Delta\tau\varphi_x/\mu} + \int_{\tau_{L-1}}^{\tau_L} S(t)\, e^{-(t_L - t)\varphi_x/\mu}\, \frac{\varphi_x}{\mu}\, dt . \tag{19}$$

As in § 4, the assumption of parabolic behavior for $S(\tau)$ in the interval (τ_{L-1}, τ_L) allows us to write

$$I_{x\mu}^-(\tau_L) = I_{x\mu}^-(\tau_{L-1})\, e^{-\Delta\tau\varphi_x/\mu} + p_{x\mu}^{1-} S(\tau_{L-1}) + p_{x\mu}^{2-} S(\tau_L) + q_{x\mu}^- S'(\tau_L) . \tag{20}$$

The coefficients $p_{x\mu}^{1-}$, $p_{x\mu}^{2-}$, and $q_{x\mu}^-$, another set of basic building blocks of the scheme, are easily derived.

The explicit numerical value of $I_{x\mu}^-(\tau_{L-1})$ is the result of the previous recursive application, from the layer (τ_1, τ_2) down to the layer (τ_{L-2}, τ_{L-1}), of equation (20), in which we have used the known values of the set $\{S^0(\tau_l);\ l = 1, L-1\}$ as well as those of the derivatives $\{S'^0(\tau_l);\ l = 1, L-1\}$. Likewise, we use the values $S^0(\tau_{L-1})$ for $S(\tau_{L-1})$ in equation (20). Consequently, by grouping together the known terms we can rewrite equation (20) in the form

$$I_{x\mu}^-(\tau_L) = \mathscr{A}_{x\mu}^- + \mathscr{B}_{x\mu}^- S(\tau_L) + \mathscr{C}_{x\mu}^- S'(\tau_L) , \tag{21}$$

where the coefficients $\mathscr{B}_{x\mu}^-$ and $\mathscr{C}_{x\mu}^-$ replace $p_{x\mu}^{2-}$ and $q_{x\mu}^-$, respectively, and it holds that

$$\mathscr{A}_{x\mu}^- = I_{x\mu}^-(\tau_{L-1})\, e^{-\Delta\tau\varphi_x/\mu} + p_{x\mu}^{1-} S^0(\tau_{L-1}) . \tag{22}$$

By integrating over frequencies and directions, we obtain the relation

$$J_\varphi^-(\tau_L) = \hat{a}_L^- + \hat{b}_L^- S(\tau_L) + \hat{c}_L^- S'(\tau_L) . \tag{23}$$

We wish to stress that the coefficients $p_{x\mu}^{1-}$, $p_{x\mu}^{2-}$, and $q_{x\mu}^-$ in equation (20), and consequently $\mathscr{B}_{x\mu}^-$ and $\mathscr{C}_{x\mu}^-$ in equation (21), hence $\hat{b}_L^-$ and $\hat{c}_L^-$ in equation (23), do not depend on the values of $S^0(\tau)$. They depend only on the optical distance $\Delta\tau(L-1, L)$. On the contrary, the coefficient $\hat{a}_L^-$ depends linearly on the values of $S^0(\tau)$ for all the optical depths with $\tau < \tau_L$. Because numerically the set of derivatives $\{S'^0(\tau_l)\}$ depends linearly on the set $\{S^0(\tau_l)\}$, one easily realizes that $I_{x\mu}^-(\tau_{L-1})$, and consequently the coefficient $\hat{a}_L^-$, are linear combinations of the set $\{S^0(\tau_l);\ l = 1, L-1\}$. In principle, we could store the coefficients $\hat{a}_L^-$, $\hat{b}_L^-$, and $\hat{c}_L^-$, evaluated at each depth point τ_L, for further use in the backward process of computation of the new values of $S(\tau_L)$.

But, in the recomputation of the new values $S^n(\tau_L)$ and $S'^n(\tau_L)$, a mismatch might occur at τ_L: the curve $S^0(\tau)$ for $\tau \le \tau_L$, used to compute $\hat{a}_L^-$, and the updated curve $S^n(\tau)$ for $\tau \ge \tau_L$, might have different values at τ_L. Thus, a more correct computation of $\hat{a}_L^-$ in accordance with this updated value of $S^n(\tau_L)$ can be reached by scaling the function $S^0(\tau)$ for $\tau \le \tau_L$ by the factor $S^n(\tau_L)/S^0(\tau_L)$. This will be automatically performed in the backward process, provided we store in the forward process, instead of the coefficients $\hat{a}_L^-$, $\hat{b}_L^-$, and $\hat{c}_L^-$, the new ones b_L^- and c_L^- of the revised relationship anticipated in equation (17):

$$J_\varphi^-(\tau_L) = b_L^- S(\tau_L) + c_L^- S'(\tau_L) ,$$

namely, the relationship that carries on the information relevant to $J_\varphi^-(\tau_L)$. It holds that

$$b_L^- = \hat{b}_L^- + \hat{a}_L^-/S^0(\tau_L) , \tag{24a}$$

$$c_L^- = \hat{c}_L^- . \tag{24b}$$

The procedure is repeated until $L = NL$.

5.2. *The Backward Process*

The backward process is, in practice, the same as in § 4. At the bottom, $J_\varphi^+(\tau_{NL})$ is directly known from the corresponding boundary conditions. By taking into account equation (17) for $J_\varphi^-(\tau_{NL})$, we obtain a similar relation for $J_\varphi(\tau_{NL})$, from which, after we have eliminated the derivative $S'(\tau_{NL})$ by means of equation (10), we can easily derive the coefficients a_{NL}, b_{NL}, and c_{NL} of the relationship

$$J_\varphi(\tau_{NL}) = a_{NL} + b_{NL} S(\tau_{NL}) + c_{NL} S(\tau_{NL-1}) . \tag{25}$$

Equation (11), i.e., the RT equation for the out-going intensity between τ_{NL-1} and τ_{NL}, allows us to express $J_\varphi^+(\tau_{NL-1})$

as a linear combination of $S(\tau_{NL})$ and $S(\tau_{NL-1})$, whose coefficients are known. On the other hand, equation (17) together with equation (10), allows us to express $J_\varphi^-(\tau_{NL-1})$ also as a linear combination of $S(\tau_{NL})$ and $S(\tau_{NL-1})$. Consequently $J_\varphi(\tau_{NL-1})$ can be expressed in the same form as equation (25):

$$J_\varphi(\tau_{NL-1}) = a_{NL-1} + b_{NL-1}\, S(\tau_{NL}) + c_{NL-1}\, S(\tau_{NL-1})\ . \tag{26}$$

By substituting equations (25) and (26) in the definition of the source function (see eq. [3]) at τ_{NL} and τ_{NL-1}, respectively, we are left with a system of two linear algebraic equations in the two unknowns $S(\tau_{NL})$ and $S(\tau_{NL-1})$, from which we easily derive the updated values of $S^n(\tau_{NL})$ and $S^n(\tau_{NL-1})$.

The values of the derivatives $S'(\tau_{NL})$ and $S'(\tau_{NL-1})$ are trivially derived from equation (10). It is straightforward to compute $I_{x\mu}^+(\tau_{NL-1})$ from equation (11).

The continuation of the backward process from τ_{NL-1} through τ_1 is obvious. For each layer (τ_L, τ_{L+1}), the numerical values of $S(\tau_{L+1})$, $S'(\tau_{L+1})$, and $I_{x\mu}^+(\tau_{L+1})$ are known from the treatment of the previous layer.

The coefficients b_L^- and c_L^- for $J^-(\tau_L)$ in equation (17) are known from the forward process. By using equation (16) to express $S'(\tau_L)$ in terms of the thus far unknown value of $S(\tau_L)$ and the known values of $S(\tau_{L+1})$ and $S'(\tau_{L+1})$, we can write $J_\varphi^-(\tau_L)$ as a linear function of $S(\tau_L)$ only.

By integration of the formal solution for $I_{x\mu}^+(\tau_L)$, as given by equation (9), and by taking into account the fact that all the terms except $S(\tau_L)$ are known, a similar expression for $J_\varphi^+(\tau_L)$ is easily derived.

Consequently, we obtain the required linear relation between $J_\varphi(\tau_L)$ and $S(\tau_L)$, the same as equation (15), that together with equation (3), allows us to derive the new value of $S^n(\tau_L)$ and successively that of $S'^n(\tau_L)$. In such a way, the step is closed, and we can proceed upward.

6. COMPARATIVE RESULTS AND CONVERGENCE PROPERTIES

In order to test the new method proposed in § 5, we applied it to the two-level atom problem described in § 2. This represents the ideal test case for checking the numerical accuracy of any algorithm employed to solve the RT equation, because its exact solution has been known for many years. (See, e.g., Sobolev 1956; Case 1957; Avrett & Hummer 1965; Ivanov 1969.)

As at first instance, we considered a medium of constant properties, whose only opacity source is the line itself, without an overlapping continuum. In this case, due to the assumed zero gradient of the Planck function $B(\tau)$, the features of the solution, namely, the value of the source function at the surface and its characteristic scale (i.e., the depth of thermalization), depend only on the non-LTE parameter ε.

In typical non-LTE problems, the value of ε is very small ($\lesssim 10^{-4}$). For this reason numerical errors can easily blur the solution. In order to test the capability of the method and to check the accuracy of the solutions, we selected two cases with ε equal to 10^{-4} and 10^{-8}, respectively.

Figures 1 and 2 show the evolution with iterations of the source function computed. One can see at once that, in a very small number of iterations (of the order of 10–15), forth-and-back implicit Λ-iteration furnishes numerical results that practically coincide with the exact solution. For comparison's sake, we also plotted the values of the source function after 1000 iterations, obtained both with classical Λ-iteration and with semi-implicit Λ-iteration (cf. § 4). The rate of convergence of the latter is higher by a factor of 2, but in both cases the convergence is unacceptably slow.

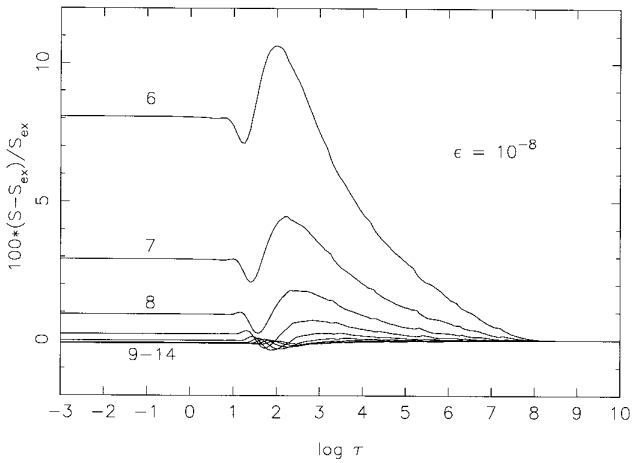

FIG. 3.—Relative error for the iterations 6–14 of the source function $S(\tau)$, shown in Fig. 2.

By comparison of our results (achieved with the same number of discrete ordinates for directions and frequencies) with the exact solution, $S_{ex}(\tau)$, by Avrett & Hummer (1965), we are in a position to plot the percent relative error on $S(\tau)$ at each iteration run.

In Figures 3 and 4 we show (on different scales on the ordinate) the errors corresponding to iterations 6–14 for the case with $\varepsilon = 10^{-8}$. For the case with $\varepsilon = 10^{-4}$, the errors are slightly smaller.

For the same two cases, we compare in Table 1 some parameters suitable for the study of the convergence properties of the method. First of all, we consider the absolute value of the *maximum relative errors* $|\Delta S^n|_M$, which corresponds to the maximum value in Figures 3 and 4, as well as the absolute value of the *maximum of the relative correction* $|\delta S^n|_M$ between two successive runs of iteration.

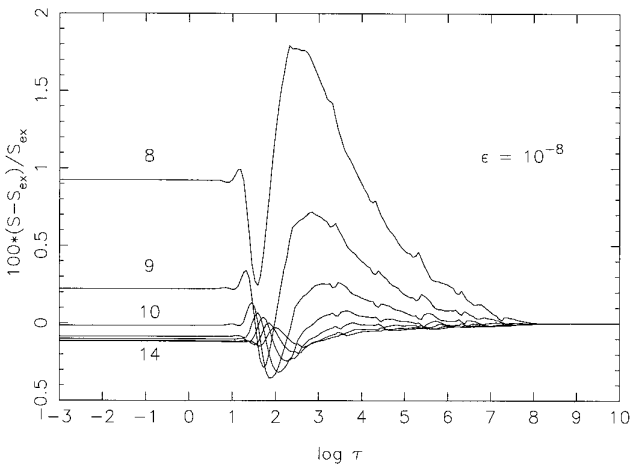

FIG. 4.—Zoom of Fig. 3, to render appreciable the evolution of the relative error along the last iterations.

TABLE 1

CONVERGENCE PROPERTIES OF THE IMPLICIT Λ-ITERATION METHOD[a]

Iteration	$\|\Delta S^n\|_M$	$\|\delta S^n\|_M$	$\|\Delta S^n\|_2$	$\|\delta S^n\|_2$	$\|E^n\|_2$
			$\varepsilon = 10^{-4}$		
1	772.944	92.412	33.242	66.228	...
2	199.491	68.386	14.084	17.453	23.698
3	69.860	46.182	6.652	7.185	12.212
4	27.422	27.208	3.241	3.370	6.347
5	11.075	14.420	1.570	1.674	3.328
6	4.359	7.058	0.734	0.847	1.716
7	1.682	3.188	0.326	0.423	0.844
8	0.969	1.385	0.134	0.210	0.419
9	0.808	0.603	**0.061**	**0.099**	0.189
10	0.541	0.485	0.043	0.047	**0.088**
11	0.344	0.369	0.036	0.025	0.053
12	0.200	0.239	0.028	0.017	0.053
13	0.124	0.141	0.021	0.013	0.051
14	0.077	**0.091**	0.016	0.009	0.038
15	0.077	0.074	0.012	0.007	0.024
16	0.075	0.057	0.010	0.005	0.017
17	0.073	0.041	0.009	0.004	0.014
18	0.067	0.025	0.009	0.003	0.012
19	0.058	0.020	0.010	0.002	0.010
20	0.055	0.016	0.010	0.001	0.007
			$\varepsilon = 10^{-8}$		
1	13587.700	98.810	28.880	76.497	...
2	1131.210	91.709	10.535	16.990	21.841
3	227.688	74.742	4.382	5.974	9.214
4	70.859	49.401	1.868	2.481	4.243
5	26.521	27.296	0.785	1.077	1.902
6	10.645	13.494	0.321	0.463	0.813
7	4.466	6.194	0.129	0.192	0.328
8	1.794	2.835	**0.050**	**0.080**	0.328
9	0.716	1.282	0.019	0.032	**0.053**
10	0.354	0.592	0.006	0.014	0.026
11	0.316	0.267	0.005	0.007	0.014
12	0.243	0.169	0.006	0.004	0.007
13	0.192	0.114	0.007	0.002	0.006
14	0.155	**0.091**	0.007	0.001	0.004
15	0.149	0.069	0.008	0.001	0.004
16	0.142	0.049	0.008	0.001	0.003
17	0.136	0.037	0.008	0.001	0.003
18	0.128	0.027	0.008	0.000	0.002
19	0.120	0.019	0.008	0.000	0.001
20	0.120	0.014	0.008	0.000	0.001

NOTE.—Col. 1: Iteration number. Col. 2: Absolute value of the maximum relative error. Col. 3: Absolute value of the maximum of the relative correction. Col. 4: Quadratic average of the relative error. Col. 5: Quadratic average of the relative correction. Col. 6: Quadratic correction ratio.

[a] All quantities are in percent.

Furthermore, we evaluate the quadratic average over the full optical depth interval of the relative error and the relative correction, respectively:

$$\|\Delta S^n\|_2 = \left\{\int_0^T [S^n(\tau) - S_{\rm ex}(\tau)]^2\, d\ln\tau \Big/ \int_0^T [S_{\rm ex}(\tau)]^2\, d\ln\tau\right\}^{1/2} \tag{27}$$

and

$$\|\delta S^n\|_2 = \left\{\int_0^T [S^n(\tau) - S^{n-1}(\tau)]^2\, d\ln\tau \Big/ \int_0^T [S^{n-1}(\tau)]^2\, d\ln\tau\right\}^{1/2}. \tag{28}$$

Finally, taking into account a previous suggestion by L. Auer (1993, private communication) also Auer, Fabiani-Bendicho, & Trujillo-Bueno 1994), we also consider the *quadratic correction ratio*:

$$\|E^n\|_2 = \frac{\|\delta S^n\|_2}{1 - \|\delta S^n\|_2/\|\delta S^{n-1}\|_2}. \tag{29}$$

From global inspection of the tabulated parameters, the excellent convergence properties of the forth-and-back implicit Λ-iteration come into view. After a comparative analysis of the run with iterations of the single parameters, we choose, as the best criterion to stop the run of iterations, the tolerance condition that the maximum value of the relative correction of $S^n(\tau)$ between two successive iterations be of the order of 0.1%.

Because of the nature of the method, simple precision is enough for most of the actual computations. Of course, when the value of the parameter ε is smaller than the computer's intrinsic round-off error, the use of double precision becomes necessary in order to prevent spurious contributions to the sources, as in the case of our test with $\varepsilon = 10^{-8}$.

Finally, we wish to call the reader's attention to the asymptotic behavior of the residual error $|\Delta S|_M$ with the number of iterations. Table 1 shows clearly that further iterations cannot reduce its value. This has to be ascribed to the unavoidable errors brought about by the discretization of the optical depth scale. The results displayed, obtained with 15 points per decade, show a maximum residual error of about 0.1%. With 10 points per decade, $|\Delta S|_M$ can be of the order of 0.3, and with 5 points per decade it can grow even to 1%.

7. THE PARTIAL REDISTRIBUTION PROBLEM

In this section, we apply the forth-and-back implicit Λ-iteration method to the case of the two-level atom line formation problem, in which partial redistribution is taken into account.

In this case the source function, which is not frequency dependent, takes the form

$$S_x(\tau) = \varepsilon B(\tau) + (1 - \varepsilon)\int_{-\infty}^{+\infty} dx'\; R(x', x)\, J_{x'}(\tau), \tag{30}$$

where $J_{x'}(\tau)$ is the specific mean intensity at frequency x', and $R(x', x)$ is the redistribution operator. In the discrete ordinates representation, the source function $S_k \equiv S_{x_k}$ reads:

$$S_k(\tau) = \varepsilon B(\tau) + (1 - \varepsilon)\sum_j R(j, k)\, J_j(\tau), \tag{31}$$

where the index j corresponds to x'_j, that is, to the frequency of the absorbed photon.

7.1. *The Forward Process*

Following the procedure already described in § 5.1, it is straightforward to compute and store, for each frequency x_j and each optical depth τ_L, the set of coefficients b^-_{jL} and c^-_{jL} of the relationship

$$J^-_j(\tau_L) = b^-_{jL} S_j(\tau_L) + c^-_{jL} S'_j(\tau_L). \tag{32}$$

That is, for each frequency x_j, we have a relation like equation (17).

7.2. *The Backward Process*

Likewise, exactly as in § 5.2, we know for each layer (τ_L, τ_{L+1}) the updated values of $I^+_{x\mu}(\tau_{L+1})$, and $S^n_j(\tau_{L+1})$ and

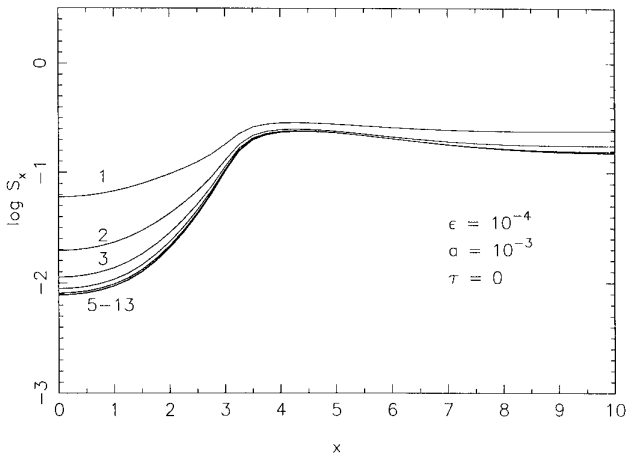

FIG. 5.—Evolution with iterations of the frequency-dependent source function $S(x)$ at optical depth $\tau = 0$, for a two-level atom line with a Voigt absorption profile $\varphi_a(x)$ and the $R_{II}(x', x)$ redistribution function. The values of ε and a are shown in the figure.

$S_j'^n(\tau_{L+1})$ for each frequency x_j. Thus, we can easily compute the coefficients of a relation like equation (9) for the outgoing intensities $I^+_{x\mu}(\tau_L)$. By integrating over μ, we obtain the coefficients $\hat{a}^+_{jL}$ and $\hat{b}^+_{jL}$ of the relation

$$J_j^+(\tau_L) = \hat{a}^+_{jL} + \hat{b}^+_{jL} S_j(\tau_L) \tag{33}$$

for all the frequencies x_j.

After removing $S_j'(\tau_L)$ in equation (32) by means of equation (16) [$S_j^n(\tau_{L+1})$ and $S_j'^n(\tau_{L+1})$ are known at this stage], we obtin the coefficients $\hat{a}^-_{jL}$ and $\hat{b}^-_{jL}$ of the relation

$$J_j^-(\tau_L) = \hat{a}^-_{jL} + \hat{b}^-_{jL} S_j(\tau_L) \, . \tag{34}$$

Equations (33) and (34) allow us to write the coefficients α_{jL} and β_{jL} of the required relationship

$$J_j(\tau_L) = \alpha_{jL} + \beta_{jL} S_j(\tau_L) \, , \tag{35}$$

which, replaced in equation (31), ensure a straightforward computation of the updated values of the source function $S_k^n(\tau_L)$ and, from equation (16), of the corresponding values $S_k'^n(\tau_L)$.

Then the process is repeated upward.

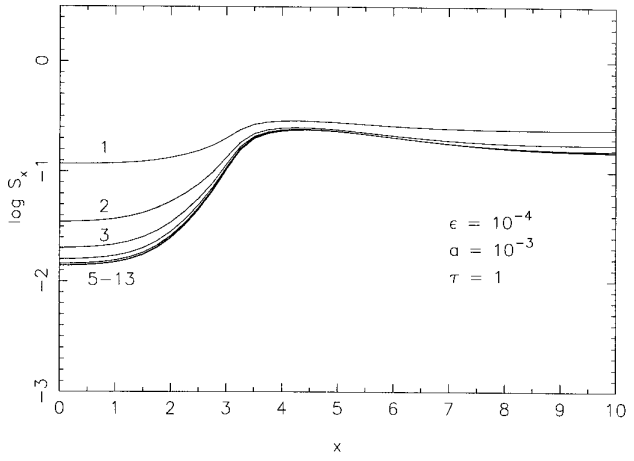

FIG. 6.—Same as Fig. 5, at optical depth $\tau = 1$

7.3. *Results*

We solved the RT equation (2) for a two-level atom with a source function as in equation (30). We used a Voigt profile $\varphi_a(x)$ with $a = 10^{-3}$ in the absorption coefficient, and the redistribution function $R_{II}(x', x)$, which corresponds to the angular mean redistribution function for the two-level atom with an infinitely narrow ground level. Again, we considered the two cases with $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-8}$, respectively.

As in the previous case of complete redistribution, a small number of iterations (13 and 15, respectively) are enough to fulfill the tolerance criterion introduced above, namely, that the greatest relative correction (for all the frequencies and optical depths) between two successive iterations be less than 0.1%.

The results reproduce the well-known ones by Hummer (1969) and Mihalas (1978). In Figures 5 and 6 we show the evolution with the iterations of $S(x)$ for the two optical depths $\tau = 0$ and $\tau = 1$, respectively.

8. THE MULTILEVEL PROBLEM

In the most general case of a multilevel atom model, we must solve an RT equation for each actual spectral line, i.e., for each allowed radiation transition between the levels considered. These radiative transitions are coupled through the level populations $\{N_j\}$, which are the solution of the statistical equilibrium (SE) equations describing the conservation of the population of each level.

In the stationary case, the SE equations are linear algebraic equations for the set of level populations $\{N_j\}$. However, some of their coefficients include the frequency-integrated means intensity of the line radiation field $J_{\varphi_{ij}}$, relevant to the radiative transition $i \to j$. For each level j, we may express the conservation of its population N_j in the form

$$\sum_{i<j} [(N_i C_{ij} - N_j C_{ji}) + (N_i B_{ij} - N_j B_{ji}) J_{\varphi_{ij}} - N_j A_{ji}] + \sum_{k>j} [(N_k C_{kj} - N_j C_{jk}) - (N_j B_{jk} - N_k B_{kj}) J_{\varphi_{jk}} + N_k A_{kj}] = 0 \, , \tag{36}$$

where B_{ij}, B_{ji}, and A_{ji} are the Einstein coefficients of the radiative transitions considered, and C_{ij} and C_{ji} are the corresponding collisional rates.

In turn, each of the integrated mean intensities $J_{\varphi_{ij}}$ depends, via the corresponding RT equation, on the source function S_{ij}, i.e., on the level populations:

$$S_{ij} = \frac{\eta_{ji}}{\chi_{ij}} = \frac{N_j A_{ji}}{N_i B_{ij} - N_j B_{ji}} \, . \tag{37}$$

In this way, the RT equation together with equations (36) and (37) represent a strong nonlinear and nonlocal problem. An iterative procedure becomes necessary. The straightforward Λ-iteration method, which solves the problem by following the scheme $\{N_j^0\} \to \{S_{ij}\} \to \{I_{x\mu}(i, j)\} \to \{J_{\varphi_{ij}}\} \to \{N_j^n\}$, has an impractically slow convergence. Alternatively, the iteration method proposed in this paper can accelerate it without any difficulty.

8.1. *Forth-and Back Implicit Λ-Interaction*

The operative procedure for this problem is exactly the same as in §§ 5 and 7. We start with a known set of popu-

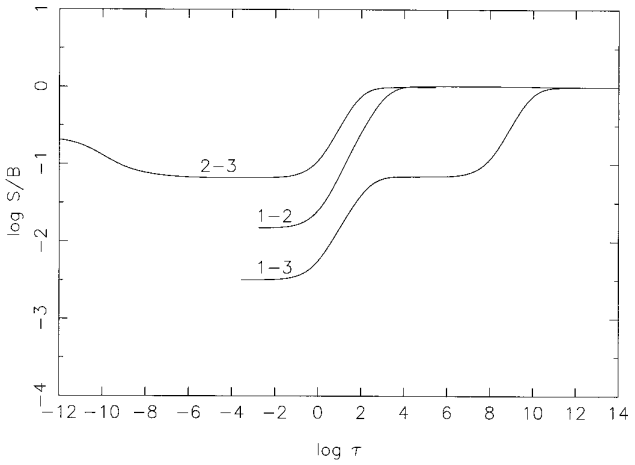

FIG. 7.—Normalized source functions S_{jk}/B_{jk}, corresponding to the three lines of a three-level hydrogen atom within an isothermal atmosphere. The log τ scale on the abscissa has to be read, case by case, as the mean line optical depth relevant to the transition considered.

lations $\{N_j^0\}$, i.e., with a set of known source functions $\{S_{ij}^0(\tau)\}$ (eq. [37]) and the corresponding first derivatives $\{S'^0(\tau)\}$ for all the transitions $i \rightarrow j$. As in the previous cases, we repeat for each transition $i \rightarrow j$ the entire forward process and the backward process layer by layer up to τ_L, in order to obtain the coefficients α_{ij} and β_{ij} of the required relation:

$$J_{\varphi ij} = \alpha_{ij} + \beta_{ij} S_{ij} \, . \tag{38}$$

By replacing $J_{\varphi_{ij}}$ in equation (36) with the expression given by equation (38) and taking into account equation (37), we can rewrite the generic SE equation for level j in the form

$$\sum_{i>j} [(N_i C_{ij} - N_j C_{ji}) + (N_i B_{ij} - N_j B_{ji})\alpha_{ij} + N_j A_{ji} \beta_{ij} - N_j A_{ji}] + \sum_{k>j} [(N_k C_{kj} - N_j C_{jk}) - (N_j B_{jk} - N_k B_{kj})\alpha_{jk} - N_k A_{kj} \beta_{jk} + N_k A_{kj}] = 0 \tag{39}$$

That is, we recover a new linear system for the set of populations $\{N_j\}$, whose coefficients are quantities explicitly known: the radiative and collisional coefficients and the interation factors $\{\alpha_{ij}\}$ and $\{\beta_{ij}\}$. As already shown in § 5.2, the latter are easily computed layer by layer.

The system of equations (39) gives the updated values of the populations $\{N_j^n\}$. The process is iterated to convergence.

8.2. *Results*

In order to test the feasibility of the method when applied to the multilevel case, we solved the same problem, namely, a three-level hydrogen atom within an isothermal atmosphere, as in Avrett & Loeser (1987). Our results, shown in Figure 7, coincide with those from Avrett & Loeser within an absolute error never greater than 3%. The existing differences are due to the unavoidable residual errors brought about by the discretization in depth. In both cases, three discrete optical depth points per decade were used.

The implicit Λ-iteration method requires only nine iterations to fulfill the usual tolerance criterion that the relative difference (for the three source functions at all the optical depths) between two successive iterations be less than 0.1%.

9. RECAPITULATIVE REMARKS

In this section we wish to comment upon the distinctive features of forth-and-back implicit Λ-iteration. Let us look back to the two-level atom problem (cf. § 2). It is well known that the straightforward Λ-iteration procedure—$S^0(\tau) \rightarrow I_{x\mu}(\tau) \rightarrow J_\varphi(\tau) \rightarrow S^n(\tau)$, has an exceedingly slow rate of convergence in optically thick media.

However, one easily realizes that this direct iterative scheme holds, from the previous iteration, more information than necessary when dealing with the current iteration, because it does not take full advantage of the linear components of the problem. That is, in order to obtain the updated values of the source function, $S^n(\tau)$, ordinary Λ-iteration computes the whole mean intensity $J_\varphi(\tau)$ from the old values of $S^0(\tau)$.

Semi-implicit Λ-iteration, thanks to the forth-and-back approach, computes from $S^0(\tau)$ only one-half of $J_\varphi(\tau)$, namely, the down-going component $J_\varphi^-(\tau)$. As already said, the improvement is not substantial. Yet, there is another way of separating the part of $J_\varphi(\tau)$ that is computed from $S^0(\tau)$ from that which is treated implicitly. Operatively, we can split $J_\varphi(\tau_L)$ into a local and nonlocal component:

$$J_\varphi(\tau_L) = J_\varphi^{\rm loc}(\tau_L) + J_\varphi^{\rm nloc}(\tau_L) \, . \tag{40}$$

We choose the local term $J_\varphi^{\rm loc}(\tau_L)$ so that it depends linearly on the unknown local values of $S(\tau_L)$ and $S'(\tau_L)$, through a functional form like

$$J_\varphi^{\rm loc}(\tau_L) = \beta_L^{\rm loc} S(\tau_L) + \gamma_L^{\rm loc} S'(\tau_L) \, , \tag{41}$$

whose coefficients $\beta_L^{\rm loc}$ and $\gamma_L^{\rm loc}$ are directly derived from the integral form of the RT equation, thanks to the assumed functional representation of $S(\tau)$. (See § 5.) They depend only on the known optical distances $\Delta\tau(L-1, L)$ and $\Delta\tau(L, L+1)$. Above all, they are independent of the trial values $S^0(\tau)$. On the contrary, the nonlocal term $J_\varphi^{\rm nloc}(\tau_L)$ depends on (and is to be computed from) the trial values of $S^0(\tau)$.

Therefore, the values of the coefficients $\beta_L^{\rm loc}$ and $\gamma_L^{\rm loc}$ are known a priori for all the τ_L. Then, at a first stage we can compute $J_\varphi^{\rm nloc}(\tau_L)$ from $S^0(\tau_L)$, i.e., the source function computed in the previous step of iteration. Successively, by taking into account the definition of the source function (cf. eq. [3], equations (40) and (41), and equation (16), in order to eliminate $S'(\tau_L)$, we obtain straightforwardly the updated source function $S^n(\tau_L)$.

However, the introduction of the forth-and-back approach—and the consequent split into a forward step and a backward step—provides a further improvement, which comes from the fact that only half of the nonlocal part of $J_\varphi(\tau)$, namely, the nonlocal part of $J_\varphi^-(\tau)$, is computed from the old values $S^0(\tau)$ when dealing with the down-going directions in the forward step. Later, when dealing with the up-going directions in the backward step, the nonlocal part of $J_\varphi^+(\tau)$ is computed from the updated values $S^n(\tau)$. In this way, a further reduction of the information carried from the previous iteration over to the next one is achieved.

We have reason to believe that the extremely good convergence properties of forth-and-back implicit Λ-iteration must be ascribed to the fact that the only quantity com-

puted from the old values $S^0(\tau)$ of the source function, and only for $\tau \leq \tau_L$, is the nonlocal part of $J_\varphi^-(\tau_L)$. The nonlocal part of $J_\varphi^+(\tau_L)$ as well as the local part of both $J_\varphi^+(\tau_L)$ and $J_\varphi^-(\tau_L)$ are computed at each depth τ_L from the updated values of $S^n(\tau)$.

Besides the latter, another substantial improvement has been introduced by the forth-and-back approach. When computing, in the forward step, the nonlocal part of $J_\varphi^-(\tau_L)$, the procedure actually employs not the old values $S^0(\tau)$ of the source function (for $\tau \leq \tau_L$) but those of a current source function $S^*(\tau)$. The latter is a replica of $S^0(\tau)$, defined so that it keeps the behavior of $S^0(\tau)$ but with values properly scaled in order to match at τ_L the value $S^n(\tau_L)$ of the updated source function (cf. § 5.2). That is to say, the current source function, actually used to compute the nonlocal part of $J_\varphi^-(\tau_L)$, includes information from both the old source function $S^0(\tau)$ (its behavior for $\tau \leq \tau_L$) and the updated source function (its value at τ_L).

In other words, in the course of each iteration step, the forth-and-back implicit Λ-iteration method retains, at each depth τ_L, the value of a single iteration factor: the ratio of the nonlocal part of the down-going mean intensity to the current source function $S^0(\tau_L)$. This iteration factor, the only piece of information retained from the current iteration, is to be used later in the next step of iteration.

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APPENDIX

A SIMPLE EXAMPLE: THE MONOCHROMATIC TWO-STREAM SEMI-INFINITE CASE

In order to illustrate the numerical procedure of the method presented in this paper, we now consider the simplest case that still retains the basic features of the two-level atom RT problem, namely, a semi-infinite, monochromatic case in which only one outgoing intensity I^+ and one down-going intensity I^- are taken into account. (The two streams correspond to directions with $\mu = +1$ and $\mu = -1$, respectively.)

For this model, it holds that $J^+ = I^+$ and $J^- = I^-$, and consequently the source function [cf. eq. (3)] reads:

$$S = \varepsilon B + (1 - \varepsilon) \frac{I^+ + I^-}{2} . \tag{A1}$$

With no incident radiation at the surface, the down-going intensity at the second depth point is given by

$$I_2^- = \int_{\tau_1}^{\tau_2} S(t) \exp\left[-(\tau_2 - t)\right] dt , \tag{A2}$$

which reduces to

$$I_2^- = a_2^- S_1 + b_2^- S_2 + c_2^- S_2' , \tag{A3}$$

under the assumption of parabolic behavior of $S(\tau)$ over the interval (τ_1, τ_2).

The coefficients of equation (A3) are given by

$$a_2^- = \frac{2}{\Delta^2} - \exp(-\Delta)\left(1 + \frac{2}{\Delta} + \frac{2}{\Delta^2}\right) . \tag{A4a}$$

$$b_2^- = 1 - \frac{2}{\Delta^2} - \exp(-\Delta)\left(-\frac{2}{\Delta} - \frac{2}{\Delta^2}\right) , \tag{A4b}$$

$$c_2^- = -1 + \frac{2}{\Delta} - \exp(-\Delta)\left(1 + \frac{2}{\Delta}\right) , \tag{A4c}$$

with $\Delta \equiv \tau_2 - \tau_1$. (The reader should note that the notation here is different from that used in the main text of the paper.)

Successively, S_1 is replaced by the current value S_1^0, and this term is multiplied by the scaling factor S_2/S_2^0. Thus, it holds that

$$I_2^- = d_2 S_2 + c_2 S_2' , \tag{A5}$$

with $d_2 = b_2^- + (a_2^- S_1^0)/S_2^0$ and $c_2 = c_2^-$.

Next by assuming again the parabolic behavior of $S(\tau)$ between τ_2 and τ_3, we can replace S_2' by means of

$$I_3^- = I_2^- \exp\left[-(\tau_3 - \tau_2)\right] + a_3^- S_2 + b_3^- S_3 + c_3^- S_3' , \tag{A6}$$

that is,

$$I_3^- = d_3 S_3 + c_3 S_3' , \tag{A7}$$

where it holds that

$$d_3 = b_3^- + \frac{1}{S_3^0}\{a_3^- S_2^0 + I_2^- \exp[-(\tau_3 - \tau_2)]\} . \tag{A8}$$

In equation (A8), the value of I_2^- is computed from equation (A5) using the current valus S_2^0 and $S_2'^0$. This process is continued until we determine the coefficients of the relationship

$$I_{NL}^- = d_{NL} S_{NL} + c_{NL} S'_{NL} . \tag{A9}$$

In this way, at the end of the forward process we have computed and stored the two set of coefficients $\{c_L\}$ and $\{d_L\}$ ($L = 2, NL$) which are to be used later in the backward step to determine the new values of S_L, starting with S_{NL} and S_{NL-1}.

In order to compute S_{NL}, S_{NL-1}, and I_{NL}^+ we assume, as a boundary condition, that $S(\tau)$ is linear for $\tau > \tau_{NL-1}$; so that on the interval (τ_{NL-1}, τ_{NL}) it holds that

$$S'_{NL-1} = S'_{NL} = \frac{S_{NL} - S_{NL-1}}{\tau_{NL} - \tau_{NL-1}} . \tag{A10}$$

Consequently, we have

$$I_{NL-1}^+ = S_{NL-1} + S'_{NL-1} \tag{A11a}$$

and

$$I_{NL}^+ = S_{NL} + S'_{NL} . \tag{A11b}$$

By recalling equation (A1), we can derive the two relationships

$$S_{NL-1} = \varepsilon B + \frac{1-\varepsilon}{2}[(1 + d_{NL-1})S_{NL-1} + (1 + c_{NL-1})S'_{NL-1}] \tag{A12a}$$

and

$$S_{NL} = \varepsilon B + \frac{1-\varepsilon}{2}[(1 + d_{NL})S_{NL} + (1 + c_{NL})S'_{NL}] . \tag{A12b}$$

(The coefficients c_{NL-1}, d_{NL-1}, c_{NL}, and d_{NL} were computed and stored in the forward step.) Now thanks to equation (A10), we can easily derive the numerical values of S_{NL} and S_{NL-1}, and hence those of $S'_{NL} = S'_{NL-1}$, I_{NL}^+, and I_{NL-1}^+.

The next step is to compute

$$I_{NL-2}^+ = I_{NL-1}^+ \exp[-(\tau_{NL-1} - \tau_{NL-2})] + a_{NL-2}^+ S_{NL-2} + b_{NL-2}^+ S_{NL-1} + c_{NL-2}^+ S'_{NL-1} . \tag{A13}$$

Because of the parabolic approximation for $S(\tau)$, the coefficients a_{NL-2}^+, b_{NL-2}^+, and c_{NL-2}^+ are given by

$$a_{NL-2}^+ = 1 - \frac{2}{\Delta} + \frac{2}{\Delta^2} - \exp(-\Delta)\frac{2}{\Delta^2} , \tag{A14a}$$

$$b_{NL-2}^+ = \frac{2}{\Delta} - \frac{2}{\Delta^2} - \exp(-\Delta)\left(1 - \frac{2}{\Delta^2}\right) , \tag{A14b}$$

and

$$c_{NL-2}^+ = -1 + \frac{2}{\Delta} - \exp(-\Delta)\left(1 + \frac{2}{\Delta}\right) , \tag{A14c}$$

with $\Delta \equiv \tau_{NL-1} - \tau_{NL-2}$.

As the numerical values of S_{NL-1} and S'_{NL-1} are known, equation (A13) can be cast in the form

$$I_{NL-2}^+ = p_{NL-2} + q_{NL-2} S_{NL-2} . \tag{A15}$$

From the forward step we have the numerical values of coefficients c_{NL-2} and d_{NL-2} of the relationship

$$I_{NL-2}^- = d_{NL-2} S_{NL-2} + c_{NL-2} S'_{NL-2} , \tag{A16}$$

in which, according to our assumption of piecewise parabolic behavior for $S(\tau)$, it holds that

$$S'_{NL-2} = 2\frac{S_{NL-1} - S_{NL-2}}{\tau_{NL-1} - \tau_{NL-2}} - S'_{NL-1} . \tag{A17}$$

Because the values of S_{NL-1} and S'_{NL-1} are known, I_{NL-2}^- (cf. eq. [A16]) can be cast in the form

$$I_{NL-2}^- = v_{NL-2} + t_{NL-2} S_{NL-2} . \tag{A18}$$

Now equations (A15) and (A18) allow us to write:

$$J_{NL-2} = \alpha_{NL-2} + \beta_{NL-2} S_{NL-2} \,. \tag{A19}$$

By recalling the definition of the source function (see eq. [A1]), we easily derive the numerical value of S_{NL-2}, and consequently that of I^{+}_{NL-2} (see eq. [A15]).

This procedure is iterated until S_1 is computed.

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