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THE USE OF ITERATION FACTORS IN THE SOLUTION OF THE NLTE LINE TRANSFER PROBLEM—I. TWO-LEVEL ATOM

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Abstract—From the original idea of the monochromatic variable Eddington factors and through a critical revision of the straightforward Λ iteration scheme we have developed an improved iterative method to solve the line formation problem. Our study deals with the computational aspects of the method when applied to the solution of the two-level-atom line transfer problem. At each iteration step, angle and frequency averaged depth-dependent factors defined as the ratios of the relevant intensity moments are computed form the current values of the radiation field. These factors are then used to close the system of the radiative transfer equation moments. Due to the quasi-invariance of the factors, the exact solution of the system is achieved within only a few iterations, even under physical conditions very far from LTE.

1. INTRODUCTION

The global solution of many astrophysical problems necessarily passes through the repeated solution of the NLTE line transfer problem. Therefore, the achievement of new numerical methods, fast and accurate, deserves special attention. The present paper presents an improved iterative method, which satisfies the above requirements.

It is well known that the intrinsic difficulty of the NLTE line formation problem arises from the non-local coupling between the radiation field and the excitation state of the gas. From the mathematical point of view, when the sources and sinks of photons are known, the radiative transfer (RT) equation reduces to an ordinary differential equation. However, due to the aforesaid coupling, i.e. the dependence of the transport (emission and absorption) coefficients on the intensity of the radiation field, the RT equation takes, in general, an integro-differential form.

Different forms of the dependence of the transport coefficients on the radiation field bring about different mathematical problems. When the dependence is explicit, the NLTE line transfer problem can be formulated in terms of the corresponding integro-differential equation, and solved by using either direct or iterative methods. But in many actual problems it is not possible to write explicitly the transfer coefficients (hence the source function), so that the self-consistent solution of the RT and statistical equilibrium equations has to be achieved by means of an iterative method. This is the case, for instance, of the multi-level-atom NLTE line transfer.

In the first part of our study on NLTE line radiative transfer, we shall limit ourselves to the well known case of spectral line formation under the assumption of a two-level-atom model with complete redistribution, where the sources at each point depend linearly on the density of the radiative energy, or, more generally, upon *an integral over both angles and frequencies of the specific intensity of the radiation field.* In practice the integral is replaced by a finite sum of values of the specific intensity. These values are chosen on a proper grid of discrete ordinates, so that to give an adequate representation of the dependence of the specific intensity on directions and frequencies. The radiative transfer equation will be solved only for such discrete values.

In spite of the capability of our method to deal with the general case, in the following we will consider the particular instance of a plane-parallel medium of constant physical properties, in order to check the numerical accuracy of the solution against the known analytical solution. For the sake

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of simplicity in presentation, the two-level atom case with no background continuum is considered throughout the paper with the exception of Sec. 3.3. where the method is easily extended to the case when the background opacity is present at line frequencies. In the second paper the method will be applied to a medium of variable properties, whereas its extension to a more complex case of the multi-level atom line formation problem will be treated in the third paper of this series.

2. THE TWO-LEVEL-ATOM PROBLEM

Under the aforesaid hypothesis, the radiative transfer equation takes the form

$$\mu \frac{\mathrm{d}I_{x,\mu}}{\mathrm{d}\tau} = \varphi_x [I_{x\mu}(\tau) - S(\tau)]. \tag{1}$$

According to the standard notation, $I_{x\mu}(\tau)$ is the specific intensity of the radiation field at 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 path and the outward normal; φ_x is the normalized profile function that is supposed to be depth independent. The frequency independent line source function:

$$S(\tau) = \epsilon B(\tau) + (1 - \epsilon) J_\varphi(\tau) \tag{2}$$

contains the scattering integral:

$$J_\varphi(\tau) = \int_{-\infty}^{\infty} \varphi_x J_x(\tau)\, \mathrm{d}x = \int_{-\infty}^{\infty} \varphi_x \, \mathrm{d}x \tfrac{1}{2} \int_{-1}^{1} I_{x\mu}(\tau)\, \mathrm{d}\mu, \tag{3}$$

that describes the angle and frequency coupling of the radiation field at a given depth point. The boundary conditions are the values of the incident intensity upon the surface at $\tau = 0$, and the diffusion approximation for the outgoing intensities at large depth (i.e., $\tau \gg 1$).

We have chosen a constant properties medium without continuum opacity because, due to the null gradient of the thermal source B, the features of the solution, namely the values of the variation scale, depend only on ϵ. The values of ϵ for typical NLTE problems are very small in most cases, so that numerical errors can easily blur the solution. Therefore this case is the ideal paradigm to check the numerical accuracy of any algorithm to solve the RT equation. The case with background opacity will be treated in Sec. 3.3. of this paper.

2.1. Global methods of solution

Direct differential methods[1,2] are based on a finite difference algorithm that allows one to couple, point by point, the specific mean intensity. These methods necessarily imply the storage and inversion of matrices, whose dimensions equal the number of the discrete ordinates required to describe the dependence of the radiative intensity on angles and frequencies. On the contrary, in integral methods,[3] the frequency integrated mean intensity at each depth point can be expressed as a linear function *of the values at all the other points*, by using the formal solution of the transfer equation:

$$J_\varphi(\tau) = \Lambda(\tau, \tau') S(\tau'). \tag{4}$$

The values of $J_\varphi(\tau)$ are then obtained by solving the linear system formed by Eqs. (2) and (4) (inversion of the Λ-operator), whose dimension is equal to the number of depth points necessary to describe the radiation field.

These techniques have been used by Auer and Mihalas[4] in the complete linearization method, developed to solve the non-linear problem of multi-level line formation in stellar atmosphere modelling. They linearized the set of coupled equations by expanding to the first order the relevant variables around an initial estimate. The solution consists of the simultaneous determination of the variables' increment. The rate of convergence is high but, due to the large number of points required for a proper discretization of the system, the memory storage and the computational time necessary for the inversion of big matrices is exceedingly high. Moreover, numerical instabilities can arise when the cumbersome linearization procedure requires large corrections.

2.2. *Iterative methods of solution*

With respect to the above methods, iterative ones are easier both from the theoretical and the practical point of view. Usually each iteration is split into two steps. In the first one $J_\varphi(\tau)$ is computed according to Eq. (4) by using the source function $S(\tau)$ coming from the previous iteration. Later, in the second step, this value of $J_\varphi(\tau)$ is used to update $S(\tau)$ via Eq. (2).

This simple procedure, called Λ-iteration, deals separately with the radiative transfer and the statistical equilibrium equations, avoiding in such a way the inversion of the Λ matrix corresponding to the coupling between radiative transfer and atomic population. However, in most cases of interest the rate of convergence results infinitely slow, preventing in practice the convergence to the exact solution.

These iterative corrections to the current solution are not effective because of the numerically unfortunate treatment of the wing photons, which are the protagonists at large optical depth when defining the length of thermalization. But, according to their small probability of being absorbed locally, they are weighted by the wings of the narrow-peaked profile φ_x in the scattering term $J_\varphi = \int J_x \varphi_x \, dx$ of the source function. Therefore their contribution when numerically evaluating this integral will be negligible, compared to the contribution of the core photons that, because of the quasi-isotropy of the relevant specific intensity, play only a *passive* rôle at large optical depth. Thus the contribution of the physically most significant photons is not properly taken into account by the Λ-iteration, and the solution thermalizes generally much higher in the atmosphere.

In order to account properly for the wing photons, Rybicki[5] suggested to eliminate the passive core photons by equating the mean intensity J_x to the local isotropic source function S_x at the optically thick core frequencies. In such a way only the wing photons contribute to the correction of the current source function. The solution by the Λ-iteration of the "wing-only" transfer equation shows much better convergence properties than that of the original "full" equation. However, the accuracy and the rate of convergence depend quite a lot on the *ad hoc* parameter introduced to define the core-saturation region.

The idea of using such physical assumptions to accelerate the Λ iteration together with the operator perturbation technique introduced by Cannon[6,7] to simplify the direct solution, makes the basis of the class of methods known as ALI [Accelerated (or Approximate) Lambda Iteration]. Namely, the approximate operators were introduced as early as 1962 by Kopp[8] within the frame of so-called synthetic method developed for certain nuclear reactor calculations (see Allen and Wing[9]).

Differently from the Λ-iteration, in the first step of each iteration ALI does not evaluate $J_\varphi(\tau)$ directly from the given current value of $S(\tau)$, but computes the coefficients of a linear relationship between $J_\varphi(\tau)$ and $S(\tau)$:

$$J_\varphi(\tau) = \lambda(\tau) + \Lambda^*(\tau, \tau')S(\tau'). \tag{5}$$

This relation, where λ and Λ^* are mutually dependent, together with Eq. (2) leads to the up-to-date source function.

In other words, ALI uses certain physical or computational approximations to replace the full description of radiative transfer (the "exact" Λ operator) by a simpler approximate one (Λ^*), correcting thus obtained solution iteratively. Thus, in contrast to the classical Λ iteration, the inversion of the matrix corresponding to the Λ^* operator is now required at each iteration. We recall that in the global integral method just one inversion of the "exact" Λ-operator is necessary. Here, although each iteration requires one inversion, a certain degree of freedom is left to choose the approximate operator Λ^*.

Hence, the optimum choice of Λ^* becomes the central task. On one hand, the approximate operator Λ^* must be as close a physical approximation of the "exact" Λ operator as possible in order to ensure stable and rapid convergence, but, on the other hand, it must be much simpler for inversions than Λ. Proceeding from the Rybicki's core saturation assumption, Scharmer[10] has constructed a diagonal (local) approximate operator whose inversion is trivial. However, the disadvantage of Scharmer's Λ^* operator, as well as of all other Λ^* operators based on the core saturation methodology, is that the convergence properties depend significantly on the value of an adjustable parameter.

Olson, Auer, and Buchler[11] were the first to point out that a good choice for Λ^* is the diagonal of the exact Λ matrix. No arbitrary parameter is then needed, however, certain mathematical approximations of the source function are required for numerical derivation of the diagonal elements. However, numerical instabilities may always occur, which would prevent to warrant *a priori* the successful convergence of the algorithm.

More elaborate (upper-diagonal or multi-diagonal) approximate operators are developed, giving rise to a more stable and rapid convergence. They are free of any arbitrary parameter, however, in contrast to the diagonal ones, they are computationally more expensive due to the inevitable matrix inversions.

In this paper we formulate the Λ-iteration scheme in a way different from ALI methods. The rapid convergence to the exact solution is achieved by making use of proper quasi-invariant iteration factors, computed in the first step of each iteration, and chosen accordingly to the physics of the specific problem and the form of the relevant equations. The major advantage of this method arises from the fact that it does not require any mattrical algorithm for the solution of the RT equation. The root of the method can be found in Feautrier's[12] suggestion that model atmosphere computations would be made faster using the ratio of two moments of the radiation field intensity.

Later Auer and Mihalas[13] applied successfully this idea to the solution of the monochromatic (gray case) transfer problem, by introducing the variable (depth-dependent) Eddington factors (VEFs). These are defined as the ratio of the third to the first angular moment of the radiation field (i.e., K_ν/J_ν). As ratios, the VEFs will be closer to the exact values than the corresponding current estimates of J_ν and K_ν at each step of iteration. Therefore they will depend only slightly on the choice of the initial source function, and will change very little from one iteration to another. Because of their "quasi-invariance", the use of VEFs to close the system of μ-moments of the RT equation provides an extremely fast convergence to the exact solution.

The VEFs have been applied to the linearization method to reduce the "angular" dimension of the system under study. However the basic idea of using the good quasi-invariance properties of the ratios of homologous physical quantities was not applied to a more general class of problems till the paper by Borsenberger et al.[14] In this study on resonance line photons transfer together with transport of excited atoms, Feautrier's idea was applied to the other variables (frequencies and velocities), and two kinetic equations, coupled by their source terms, were solved by using the relevant factors.

The method of the iteration factors to compute the self-consistent temperature correction for a plane-parallel LTE stellar atmosphere model has been successfully applied in radiative equilibrium by Simonneau and Crivellari,[15] and to the case where also convective transport is present.[16] Fieldus et al[17] generalized the method to include spherically extended line-blanketed model atmospheres.

3. THE METHOD OF THE ITERATION FACTORS

Prior to the description of the iteration factors method developed to solve the line formation problem, we shall briefly remind of the method of variable Eddington factors as its analog in the monochromatic transfer problem. The consideration of this familiar example enables then an almost direct generalization of the basic idea to the multi-frequency (line formation) problem.

3.1. The monochromatic Eddington factors

In the gray case the time independent radiative transfer equation for a static plane-parallel one-dimensional medium is:

$$\mu \frac{\mathrm{d}I_\mu(\tau)}{\mathrm{d}\tau} = [I_\mu(\tau) - S(\tau)]. \tag{6}$$

Here $S(\tau)$ is the monochromatic source function:

$$S(\tau) = \epsilon B(\tau) + (1-\epsilon)J(\tau) \tag{7}$$

consisting of the thermal (local) term $B(\tau)$ and the scattering (non-local) term:

$$J(\tau) = \tfrac{1}{2}\int_{-1}^{1} I_\mu(\tau)\,\mathrm{d}\mu, \tag{8}$$

which depends on the solution $I_\mu(\tau)$. Substitution of (7) and (8) into (6) leads to an integro-differential equation for each direction μ.

For the monochromatic case in plane-parallel geometry, here considered, the solution of the above integro-differential equation can be achieved with a limited number of Λ-iterations. But, in view of more general cases, where a large number of Λ-iterations is required, it will be necessary to seek for speeding up its convergence.

An alternative way to obtain an improved source function for the present case is given by using the μ-moments of the RT equation. The first- and the second-order μ-moments are defined as

$$\frac{\mathrm{d}H(\tau)}{\mathrm{d}\tau} = J(\tau) - S(\tau) \tag{9a}$$

$$\frac{\mathrm{d}K(\tau)}{\mathrm{d}\tau} = H(\tau). \tag{9b}$$

From Eqs. (9) one obtains the second-order differential equation

$$\frac{\mathrm{d}^2K(\tau)}{\mathrm{d}\tau^2} = \epsilon[J(\tau) - B(\tau)]. \tag{10}$$

One more relationship between $J(\tau)$, $H(\tau)$ and $K(\tau)$ is however necessary to close the system of Eqs. (9). The most straightforward way to do that is to generalize the Eddington approximation:

$$\frac{K(\tau)}{J(\tau)} = \frac{\tfrac{1}{2}\int I_\mu \mu^2\,\mathrm{d}\mu}{\tfrac{1}{2}\int I_\mu\,\mathrm{d}\mu} = F(\tau). \tag{11}$$

The unknown function $F(\tau)$ is determined iteratively. It must be stressed that in contrast with the Λ-iteration, where $J(\tau)$ and $S(\tau)$ are computed directly from the specific intensity $I_{x\mu}(\tau)$, the latter are used here to compute the Eddington factor $F(\tau)$. By using this current estimate of $F(\tau)$, and hence to obtain the new source function.

This procedure (see the right-hand side of Fig. 1), the analog from the operational point of view of the Λ-iteration, leads to a very fast convergence without any extra computational cost. Three iterations are enough both for plane-parallel[13] and spherical[18] geometry. This is due to the fact that $F(\tau)$ is a good quasi-invariant for this problem. As it is the ratio of two functionals of the intensity, it results nearly independent of the initial source function, and so is also insensitive to the errors in $I_\mu(\tau)$. Almost exact already at the first iteration and quickly improving, $F(\tau)$ speeds the convergence to the exact solution.

Although not necessary in this case, a more general closure relation can be introduced in order to achieve an even better convergence.

To conclude, the Eddington factors method is an example of mixed iteration, where the computation of the "iteration" factors via the RT equation and the solution of Eq. (10) are performed at separate steps.

3.2. The iteration factors for the line problem

As mentioned before, in the present paper we will study the line formation problem for a two-level-atom under the assumption of complete redistribution, in a semi-infinite medium of constant physical properties. The relevant equations are Eqs. (1)–(3) of Sec. 2. These equations can be solved by direct generalization of the procedure described in the previous section.

Starting from an initial estimate of the source function, the specific intensity $I_{x\mu}(\tau)$ at each chosen frequency x, angle μ and optical depth τ, is obtained from the solution of the RT equation (1). As the source function is given, the computation of $I_{x\mu}(\tau)$ can be easily performed at a high degree of reliability. The intensities so obtained are then used to compute the relevant iteration factors

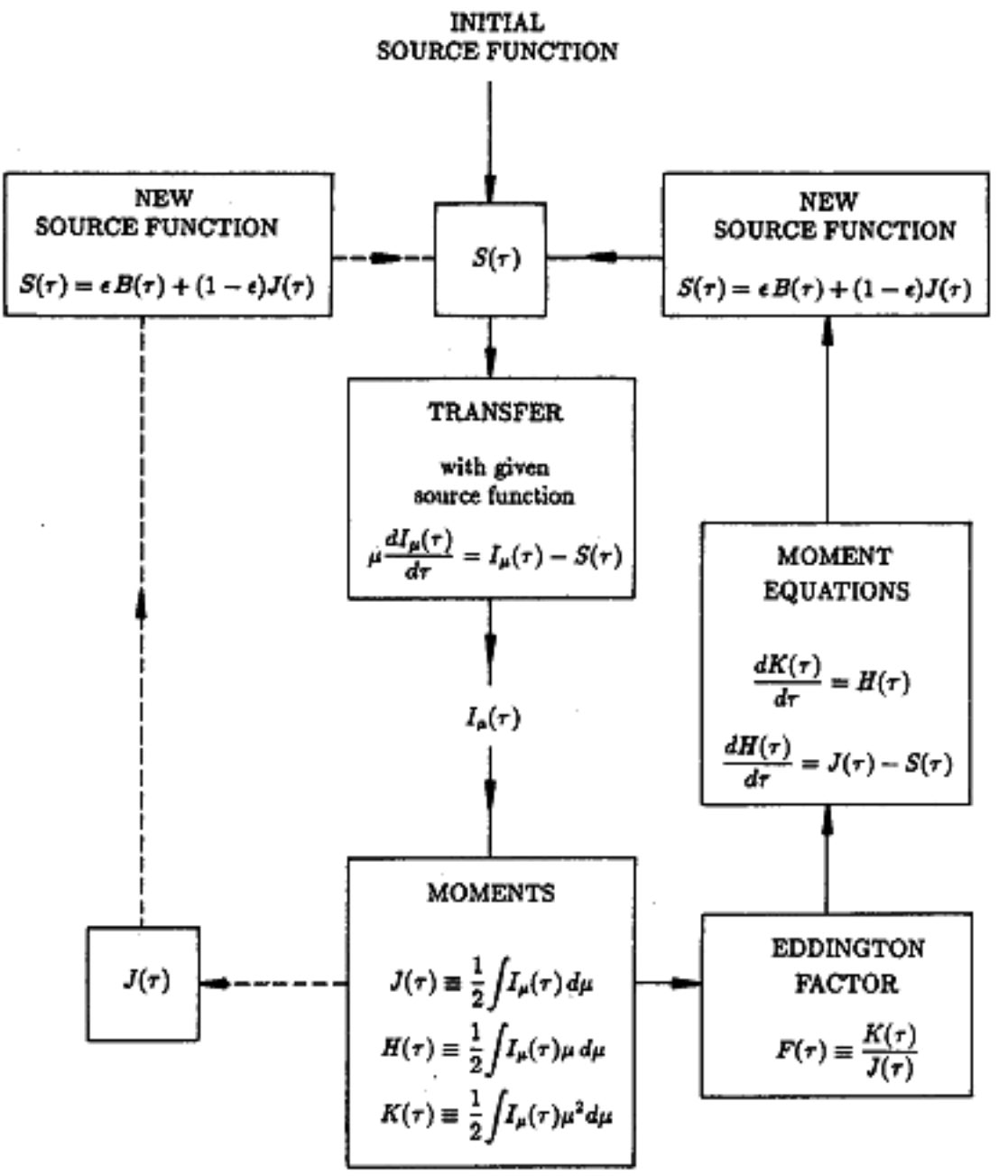

Fig. 1. Flow-chart of the variable Eddington factors method.

required to close the system of the μ-moments of the RT equation. Since two families of variables now enter the problem, to obtain J_φ we must integrate the RT equations for the specific intensities over both angles and frequencies. For each frequency x, the first- and second-order μ-moments of Eq. (1) are given by integration over $\mathrm{d}\mu$ and $\mu\,\mathrm{d}\mu$, respectively:

$$\frac{\mathrm{d}H_x}{\mathrm{d}\tau} = \varphi_x(J_x - S) \tag{12a}$$

$$\frac{\mathrm{d}K_x}{\mathrm{d}\tau} = \varphi_x H_x. \tag{12b}$$

The integration over frequencies is performed applying the operators $\int \varphi_x^2[\,\cdot\,]\,\mathrm{d}x$ and $\int \varphi_x[\,\cdot\,]\,\mathrm{d}x$ to Eqs. (12a) and (12b), to obtain:

$$\frac{\mathrm{d}H_{\varphi^2}(\tau)}{\mathrm{d}\tau} = J_{\varphi^3}(\tau) - \varphi^3 S(\tau) \tag{13a}$$

$$\frac{\mathrm{d}K_\varphi(\tau)}{\mathrm{d}\tau} = H_{\varphi^2}(\tau), \tag{13b}$$

where we use the following notation for the intensity and profile moments:

$$Q_{\varphi^n}(\tau) = \int \varphi_x^n Q_x \, dx \tag{14a}$$

and

$$\varphi^n = \int \varphi_x^n \, dx. \tag{14b}$$

The system of Eqs. (13a) and (13b) can be rewritten as a second-order differential equation:

$$\frac{d^2 K_\varphi}{d\tau^2} = J_{\varphi^3}(\tau) - \varphi^3 S(\tau). \tag{15}$$

In such a way the description of the line radiative transfer process is eventually reduced to a single equation, whose terms include all the necessary information relevant to the coupling between the line photons and the two-level-atom populations.

In order to solve Eq. (15) or, equivalently, the system of Eqs. (13a) and (13b) together with Eq. (2) for the source function, two more equations are required, relating the unknown functions J_φ, K_φ, H_{φ^2} and J_{φ^3}. These equations replace the loss of information intrinsic to the double quadrature over μ and x.

As in the monochromatic case, the generalized frequency-independent Eddington factor

$$F(\tau) \equiv \frac{K_\varphi(\tau)}{J_\varphi(\tau)} \tag{16}$$

is now introduced to account for the anisotropy of the radiation field. At great optical depth the value of $F(\tau)$ tends to 1/3 because the radiation field is quasi-isotropic, whereas near the surface it departs from this equilibrium value, due to the existence of a boundary layer.

The second closure relation must involve the remaining intensity moments. Since they have been obtained by frequency quadratures, weighted by different powers of the profile φ_x, the relation required will describe the frequency distribution of the intensity over the line, taking into account the given opacity profile. Thus an efficient iterative correction towards the exact solution, throughout the whole medium and especially at great optical depth, will necessarily require a description as good as possible of the distribution of the radiation field over the line frequencies. Our aim will be to include all this information into a single *scalar* closure relationship.

In the following three different closure relations, at different degrees of sophistication, will be introduced and discussed.

3.2.1. The most straightforward closure relation. The most obvious way to relate the remaining intensity moments J_{φ^3} and J_φ in Eq. (15) is by using the iteration factor:

$$f_J(\tau) \equiv \frac{J_{\varphi^3}(\tau)}{J_\varphi(\tau)}. \tag{17}$$

Since J_{φ^3} involves the profile φ_x^3, which is much more narrow than φ_x and covers mainly the line core, the factor f_J represents the ratio of the photons in the core (J_{φ^3}) to the photons (J_φ) in the whole line.

The two auxiliary relations given by Eqs. (16) and (17) enable to close the system of Eqs. (13a) and (13b), or Eq. (15). By making use of Eq. (2), one eventually obtains:

$$\frac{d^2 K_\varphi}{d\tau^2} = \frac{f_J - \varphi^3(1-\epsilon)}{F} K_\varphi - \varphi^3 \epsilon B. \tag{18}$$

The boundary conditions for Eq. (18) must be derived consistently at the same degree of approximation. By using the specific intensities obtained at the first step of each iteration, one can compute at the surface ($i = 1$), and the bottom ($i = N$) of the atmosphere, the ratios:

$$\gamma_i = \frac{H_{\varphi^2}(\tau_i)}{K_\varphi(\tau_i)} \tag{19}$$

that we will use as initial condition in the form:

$$\left(\frac{dK_\varphi}{d\tau}\right)_{\tau=\tau_l} = \gamma_l K_\varphi(\tau_l). \tag{20}$$

Given the factors $F(\tau)$, $f_J(\tau)$ and γ_l, one can now solve the moment equation (18) together with the two corresponding initial conditions (20) in order to get the mean intensity $J_\varphi(\tau)$, hence the improved source function $S(\tau)$.

Here and in the following, we have taken as convergence criterion that the relative difference between the values of the source function in two successive iterations is less than 1% at all optical depths. This value is of the same order as the precision prescribed in the computation of $I_{x\mu}(\tau)$ at a given source function, and corresponds to the relative difference between two successive iterations when the chosen initial trial source function is the "exact" solution.

The results obtained by using this first closure relation, i.e. the iteration factors F and f_J, are shown in Fig. 2 for the case $\epsilon = 10^{-4}$ and $B = 1$. The required convergence criterion is satisfied within 31 iterations and the source function is obtained with an error lesser than 1%. Good thermalization length is achieved already in the first iteration. This clearly shows that the corrections to the current solution are performed simultaneously throughout the whole medium.

We have just seen that the use of this most straightforward closure relation in the solution of the problem for typical non-LTE conditions $\epsilon = 10^{-4}$ has proved good computational properties of our method. However, for more extreme non-LTE situations ($\epsilon \leqslant 10^{-6}$), the instabilities occur and solution diverges. The attempt to suppress the oscilatory behaviour of the solution by means of the relaxation technique:

$$S^{i+1} = (1-r)^{i+1} + rS^i, \quad (0 \leqslant r \leqslant 1) \tag{21}$$

fails.

The instabilities primarily arise at great optical depths and are due to the errors introduced on the iteration factor $f_J(\tau)$. The latter, although it can give a qualitatively correct explanation of the behaviour of the radiation field, is not accurate enough from the numerical point of view.

At great optical depths were f_J approaches the value of φ^3 and F tends to 1/3, Eq. (18) should reduce to the following diffusion equation:

$$\frac{1}{3}\frac{d^2J}{d\tau^2} = \epsilon\varphi^3(J-B). \tag{22}$$

However, the numerical errors affecting the computation of f_J, when of the order of ϵ, may prevent to meet the above condition. The spurious contribution to the computation of the J_φ and J_{φ^3} moments, brought about by the numerical errors, may overcome the contribution of the wing

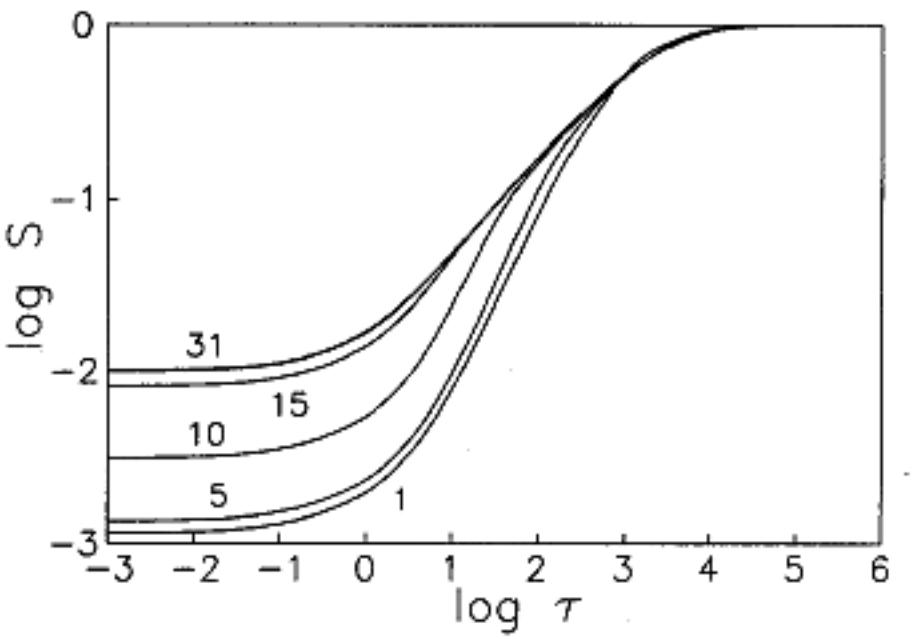

Fig. 2. The convergence of the $S(\tau)$ using the factors $F(\tau)$ and $f_J(\tau)$ for the case $\epsilon = 10^{-4}$ and $B = 1$.

Table 1. Results obtained using two line regions: core and wings ($\varphi_{x_c} = \sqrt{\epsilon}/10$); $B = 1$; r-relaxation factor

ϵ	r	$S(\tau = 0)$	No. iter.
10^{-2}	0	0.100170	5
10^{-4}	0.5	0.010049	9
10^{-6}	0.75	0.001003	23

photons. Thus the iteration factor f_J, defined by Eq. (17), cannot transmit correctly the information carried by the wing photons.

Such a statement can be easily verified by separating the line into two regions: core and wings. By choosing some critical frequency x_c dividing these two regions, and performing the integration of Eqs. (12a) and (12b) over the frequencies within the line core $(0, x_c)$ and the line wings (x_c, ∞) separately we obtain a twofold number of intensity moments and corresponding iteration factors. Finally, we are left with two second-order moment equations, one for each line region:

$$\frac{d^2K^{c,w}}{d\tau^2} = J^{c,w}_{\varphi^3} - \varphi^3_{c,w}S, \tag{23}$$

coupled by the source function:

$$S = \epsilon B + (1-\epsilon)(J^c_\varphi + J^w_\varphi). \tag{24}$$

The above system is solved using the same above described mixed iteration. The solutions obtained for different non-LTE conditions are given in Table 1.

With respect to the results of the previous case, where a single equation was written for the line as a whole, the above results are significantly better, to confirm our hypothesis about the origin of the instabilities. Nevertheless, some instabilities still appear in the case of very large departures from LTE (a great relaxation factor, i.e., $r = 0.75$, is necessary for $\epsilon = 10^{-6}$).

However, our aim is to find out the proper iteration factors to deal with the line as a whole (which would imply just one second-order moment equation), that allow to get rid of the afore mentioned difficulties.

3.2.2. A general closure relationship. As discussed above, the most straightforward closure relation via the iteration factor, given by Eq. (17), provides a fast and accurate solution. But it does not satisfy completely the requirement of stability.

An improved closure relation can be derived from what is the best numerical simulation of the transfer process. The formal solution of the RT equation, that describes the evolution of the specific intensity at each frequency x along any direction μ, can be written in the form:

$$I^+_{x\mu}(\tau) = \int_\tau^\infty S(t)\exp(-(t-\tau)\varphi_x/\mu)\frac{dt\varphi_x}{\mu}, \quad 0 \leqslant \mu \leqslant 1 \tag{25a}$$

$$I^-_{x\mu}(\tau) = \int_0^\tau S(t)\exp((\tau-t)\varphi_x/\mu)\frac{dt\varphi_x}{\mu}, \quad -1 \leqslant \mu \leqslant 0. \tag{25b}$$

In this way one takes into accout separately two streams: $I^+_{x\mu}(\tau)$ and $I^-_{x\mu}(\tau)$, namely the outgoing and incoming radiation field defined on the μ-intervals [0, 1] and [−1, 0], respectively. All the moments appearing in the systems of Eqs. (13a) and (13b) can be easily computed in terms of the above intensities. By integrating Eqs. (25a) and (25b) over angles and frequencies, we can write the relations between any pair of two-stream moments and the relevant "full" moment:

$$J_\varphi = \tfrac{1}{2}(J^+_\varphi + J^-_\varphi), \qquad J_{\varphi^3} = \tfrac{1}{2}(J^+_{\varphi^3} + J^-_{\varphi^3}),$$
$$H_{\varphi^2} = \tfrac{1}{2}(H^+_{\varphi^2} - H^-_{\varphi^2}), \quad K_\varphi = \tfrac{1}{2}(K^+_\varphi + K^-_\varphi). \tag{26}$$

We can now rewrite Eqs. (25a) and (25b) in the form:

$$I^{+}_{x\mu}(\tau) = S(\tau) + \int_{\tau}^{\infty} \left(\frac{\mathrm{d}S}{\mathrm{d}t}\right) \mathrm{e}^{-(t-\tau)\varphi_x/\mu}\, \mathrm{d}t \tag{27a}$$

$$I^{-}_{x\mu}(\tau) = S(\tau)(1 - \mathrm{e}^{-\tau\varphi_x/\mu}) - \int_{0}^{\tau} \left(\frac{\mathrm{d}S}{\mathrm{d}t}\right) \mathrm{e}^{-(\tau-t)\varphi_x/\mu}\, \mathrm{d}t. \tag{27b}$$

In the above expressions the first term in the right-hand side represents the contribution of the local source function to the radiation field at any given depth point. The integrals involving the first-order (and higher) derivative account for the non-local character of the transfer problem.

We can define the local contribution as the "passive" component of the two streams:

$$I^{0+}_{x\mu}(\tau) = S(\tau) \tag{28a}$$

$$I^{0-}_{x\mu}(\tau) = S(\tau)(1 - \mathrm{e}^{-\tau\varphi_x/\mu}) \tag{28b}$$

In both cases the "passive" term consists of the source function, multiplied by a specific coefficient that introduces the main scale length of the transfer problem, namely the exponential decay due to the escape of the photons through the boundary surface.

Accordingly we can introduce the "active-transfer" term, corresponding to the non-local contribution:

$$\tilde{I}^{+}_{x\mu}(\tau) = I^{+}_{x\mu}(\tau) - S(\tau) \tag{29a}$$

$$\tilde{I}^{-}_{x\mu}(\tau) = I^{-}_{x\mu}(\tau) - S(\tau)(1 - \mathrm{e}^{-\tau\varphi_x/\mu}). \tag{29b}$$

Only these terms will take part in the definition of the iteration factors, necessary to the iterative correction.

We shall stress here that the elimination of the *known* "passive" term of the radiation field is already possible at the beginning of each iteration, when the formal solution is performed. *There is no need of any arbitrary definition of the line core.*

The non-local terms of the two-stream moments can be written in the form:

$$\begin{aligned} \tilde{J}^{+}_{\varphi} &= J^{+}_{\varphi} - S & \tilde{J}^{-}_{\varphi} &= J^{-}_{\varphi} - S(1 - M_{01}) \\ \tilde{J}^{+}_{\varphi^3} &= J^{+}_{\varphi^3} - S\varphi^3 & \tilde{J}^{-}_{\varphi^3} &= J^{-}_{\varphi^3} - S(\varphi^3 - M_{03}) \\ \tilde{H}^{+}_{\varphi^2} &= H^{+}_{\varphi^2} - \tfrac{1}{2}\varphi^2 S & \tilde{H}^{-}_{\varphi^2} &= H^{-}_{\varphi^2} - S(\tfrac{1}{2}\varphi^2 - M_{11}). \end{aligned} \tag{30}$$

For the "full" moments there holds:

$$\begin{aligned} \tilde{J}_{\varphi} &= J_{\varphi} - S(1 - \tfrac{1}{2}M_{01}) \\ \tilde{J}_{\varphi^3} &= J_{\varphi^3} - S(\varphi^3 - \tfrac{1}{2}M_{03}) \\ \tilde{H}_{\varphi^2} &= H_{\varphi^2} - \tfrac{1}{2}M_{12}S. \end{aligned} \tag{31}$$

Here, the $M_{mn}(\tau)$s are the frequency integrated integro-exponential functions:

$$M_{mn}(\tau) \equiv \int \varphi_x^n \,\mathrm{d}x \int_0^1 \mathrm{d}\mu\, \mu^m \,\mathrm{e}^{-\tau\varphi_x/\mu} = \int \varphi_x^n E_{m+2}(\varphi_x \tau)\,\mathrm{d}x. \tag{32}$$

Since the basic idea is to isolate the "passive" photons, and to iterate only on the ratios of the above non-local contribution of the intensity moments, we are led to define the iteration factors as

$$\alpha^{\pm} = \frac{\tilde{J}^{\pm}_{\varphi^3}}{\tilde{J}^{\pm}_{\varphi}} \quad \theta^{\pm} = \frac{\tilde{H}^{\pm}_{\varphi^2}}{\tilde{J}^{\pm}_{\varphi}}. \tag{33}$$

They will be directly computed from Eqs. (27a) and (27b) at the first step of each iteration, known as the source function. The factors $\alpha^{\pm}$ and $\theta^{\pm}$ account separately for the behaviour of the non-local parts of the radiation field, both outgoing and incoming. The factor $\alpha^{\pm}$ accounts for the frequency

redistribution between the line core and the wings. The factor $\theta^{\pm}$ represents the redistribution over directions and, to some extent, also over frequencies. Both are considered as "form factors".

Once the $\alpha^{\pm}$s and $\theta^{\pm}$s are computed at each optical depth, we can use their definition

$$\alpha^{+} \equiv \frac{J^{+}_{\varphi^3} - S\varphi^3}{J^{+}_{\varphi} - S} \qquad \alpha^{-} \equiv \frac{J^{-}_{\varphi^3} - S(\varphi^3 - M_{03})}{J^{-}_{\varphi} - S(1 - M_{01})}$$

$$\theta^{+} \equiv \frac{H^{+}_{\varphi^2} - S\varphi^2/2}{J^{+}_{\varphi} - S} \qquad \theta^{-} \equiv \frac{H^{-}_{\varphi^2} - S(\varphi^2/2 - M_{11})}{J^{-}_{\varphi} - S(1 - M_{01})} \tag{34}$$

to obtain, after some algebra, the second closure relation for the system of Eqs. (13a) and (13b) or Eq. (15):

$$J_{\varphi^3} - \varphi^3 S = f_J(J_\varphi - S) + f_H H_{\varphi^2} + f_S S. \tag{35}$$

The coefficients f_J, f_H and f_S are simply related to the iteration factors by the relationships:

$$f_J = \frac{\alpha^{+}\theta^{-} + \alpha^{-}\theta^{+}}{\theta^{+} + \theta^{-}}$$

$$f_H = \frac{\alpha^{+} - \alpha^{-}}{\theta^{+} + \theta^{-}}$$

$$f_S = \tfrac{1}{2}(f_J M_{01} - M_{03} - f_H M_{12}). \tag{36}$$

In the frame of the "two-stream" model, the coefficient f_H is a measure of the anisotropy of the radiation field. The anisotropy is explicitly taken into account by a separate treatment of the outward and inward intensity moments. The coefficient f_J still plays the rôle of a diffusion coefficient. The coefficient f_S contains the frequency integrated integro-exponential functions which reproduce the kinetic behaviour of the transfer process. As we have already said, the main scale length to describe the radiation field is introduced explicitly in the definition of the iteration factors, so that they carry on only second-order properties from one iteration to another. The correct behaviour of the solution at great optical depths is provided by the corresponding differences of the intensity moments and the local source function. Therefore we might expect a higher quality procedure, namely a better solution of the second-order equation:

$$\frac{\mathrm{d}^2 K_\varphi}{\mathrm{d}\tau^2} = f_J(J_\varphi - S) + f_H H_{\varphi^2} + f_S S. \tag{37}$$

For the sake of further discussion, we will rewrite Eq. (37) into the form:

$$\frac{\mathrm{d}^2 K_\varphi}{\mathrm{d}\tau^2} - f_H(\tau)\frac{\mathrm{d}K_\varphi}{\mathrm{d}\tau} - \frac{\epsilon f_J(\tau) + (1-\epsilon) f_S(\tau)}{F(\tau)} K_\varphi(\tau) = -[f_J(\tau) - f_S(\tau)]\epsilon B. \tag{38}$$

Equation (38) is an ordinary second-order linear differential equation with two-point boundary conditions. In order to solve it we use a conventional implicit forward elimination–back substitution method.

We will remember that f_J is always of the order of φ^3 (see Fig. 7). When the radiation field is almost isotropic ($\tau \gtrsim 1$), f_H becomes zero. On the other hand, $F(\tau)$ is of the order of 1/3 and f_S decreases with an angle-frequency integrated exponential decay, which defines the thermalization length L_T. Thus, when $\tau < L_T$ it will be $\epsilon f_J < (1-\epsilon) f_S$, and Eq. (38) will represent the kinetic-transfer regime. When $\tau > L_T$, it will be $\epsilon f_J > (1-\epsilon) f_S$, and the diffusion regime with its characteristic length $1/\sqrt{(\varphi^3 \epsilon)}$ will be recovered. Any error on the factors f_J, f_H and f_S can only slightly modify these characteristic scale heights, therefore they will not severly affect the results.

The solutions obtained confirm our predictions about the good quality of the method. Hereinafter we show the solutions obtained assuming pure Doppler broadening. (The use of Voigt profile function does not lead to any substantial difference in convergence properties of the method.) These solutions, which on the other hand are well known (cf. Avrett and Hummer,[19] Fig. 2), are shown in Fig. 3, for different values of ϵ. For the same values, the source function at the surface as well as the number of iterations necessary to fulfill the criterion required, are given

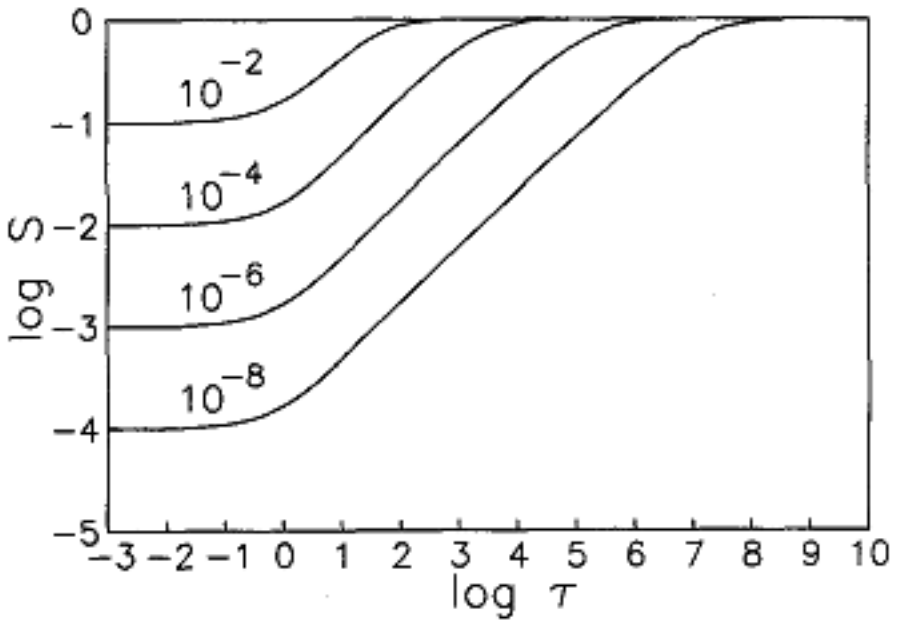

Fig. 3. $S(\tau)$ for different values of ϵ in the constant property medium $B = 1$. [The factors $\alpha^{\pm}(\tau)$, $\theta^{\pm}(\tau)$ and $F(\tau)$ are used].

in Table 2. The error of the solution is always less than 1%, even in the extreme non-LTE case with ϵ equal to 10^{-8}.

The rate of convergence is very high. Ten iterations are enough to obtain the exact solution in the case $\epsilon = 10^{-8}$. A significant stability is also achieved. For $\epsilon \geqslant 10^{-4}$, the solution is obtained without relaxation. When solving the problem for $\epsilon \leqslant 10^{-6}$ the solution oscilates (a lot) around the exact value. However, by applying the relaxation technique with $r = 0.5$ we obtained a fast and stable solution, as shown in Fig. 4.

The good convergence property of the method is also illustrated by the figures that follow. It clearly appears from Fig. 5 that even for the extreme non-LTE case $\epsilon = 10^{-8}$, the source function practically approaches its exact value already at the third iteration.

The behaviour of the four iteration factors $\alpha^{\pm}$ and $\theta^{\pm}$ is presented in Fig. 6. The iterative procedure is started with an initial estimate obtained by a simple analytical consideration on a two-stream equilibrium model. It is worthwhile to stress that the convergence is achieved with a

Table 2. Solutions at the surface of a semi-infinite medium ($B = 1$) obtained by the use of the general closure relation

ϵ	r	$S(\tau = 0)$	No. iter.
10^{-2}	0	0.996 (−1)	5
10^{-4}	0	0.997 (−2)	6
10^{-6}	0.5	0.992 (−3)	9
10^{-8}	0.5	0.989 (−4)	10

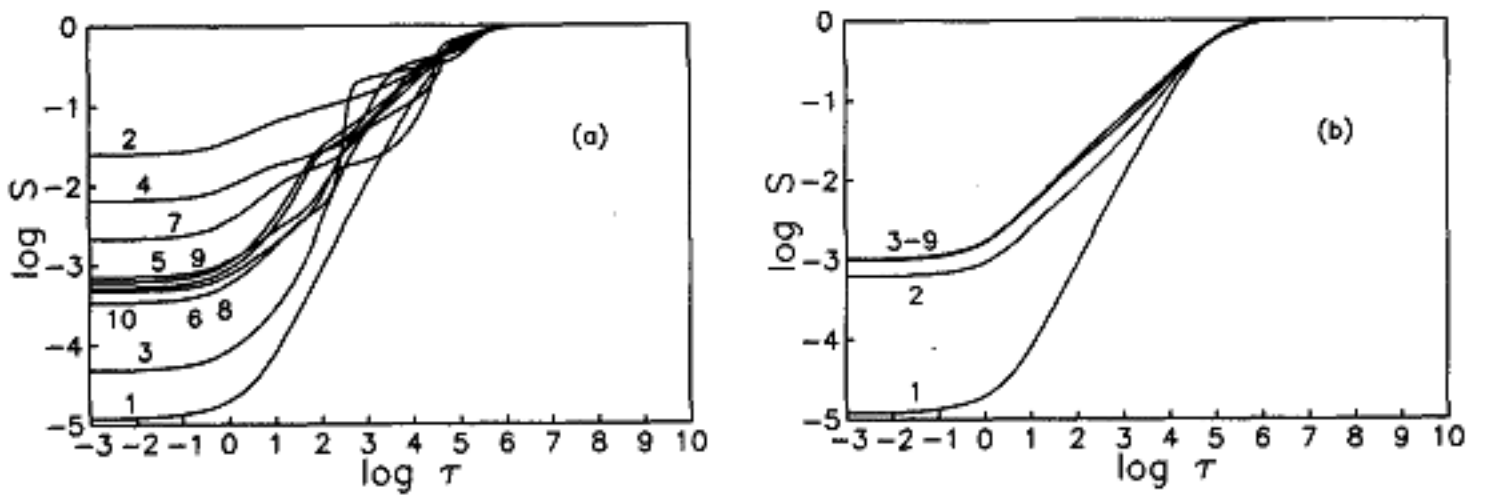

Fig. 4. The convergence of $S(\tau)$ using the factors $\alpha^{\pm}(\tau)$, $\theta^{\pm}(\tau)$ and $F(\tau)$ for the case $\epsilon = 10^{-6}$ and $B = 1$ in the labelled number of iterations: (a) without relaxation, (b) with $r = 0.5$.

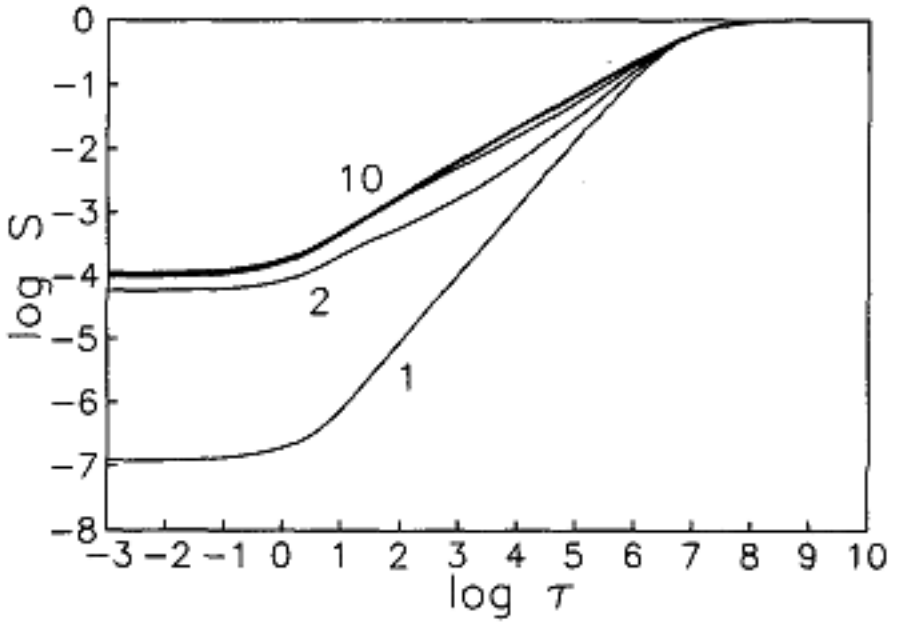

Fig. 5. The convergence of $S(\tau)$ using the factors $\alpha^{\pm}(\tau)$, $\theta^{\pm}(\tau)$ and $F(\tau)$ for the case $\epsilon = 10^{-4}$ and $B = 1$ in the labelled number of iterations ($r = 0.5$).

small number of iterations even with such initial values. Similar results would have been obtained if we had started the procedure with an equilibrium estimate for the source function.

Figure 7 shows the variation of the generalized Eddington factor $F(\tau)$ as well as that of the coefficients $f_J(\tau)$, $f_H(\tau)$ and $f_S(\tau)$ in the run of iterations. We should note here that the finite quadrature range used for the integrals over frequencies affects the behaviour of the cofficients f_S. A steep decrease of f_S at great optical depths ($\tau > 10^9$) shows up. The same occurs with the $M_{mn}(\tau)$s. In fact, all the factors containing the integrals M_{mn} are affected by the numerical properties of the quadrature formula. But, as we can see from Fig. 3, such a behaviour has no influence on the solution, since at these depths the thermalization is already achieved.

3.2.3. Further discussion on the closure relation. So far we have analysed the most general linear closure relation involving all the relevant intensity moments. This relation brings about the best

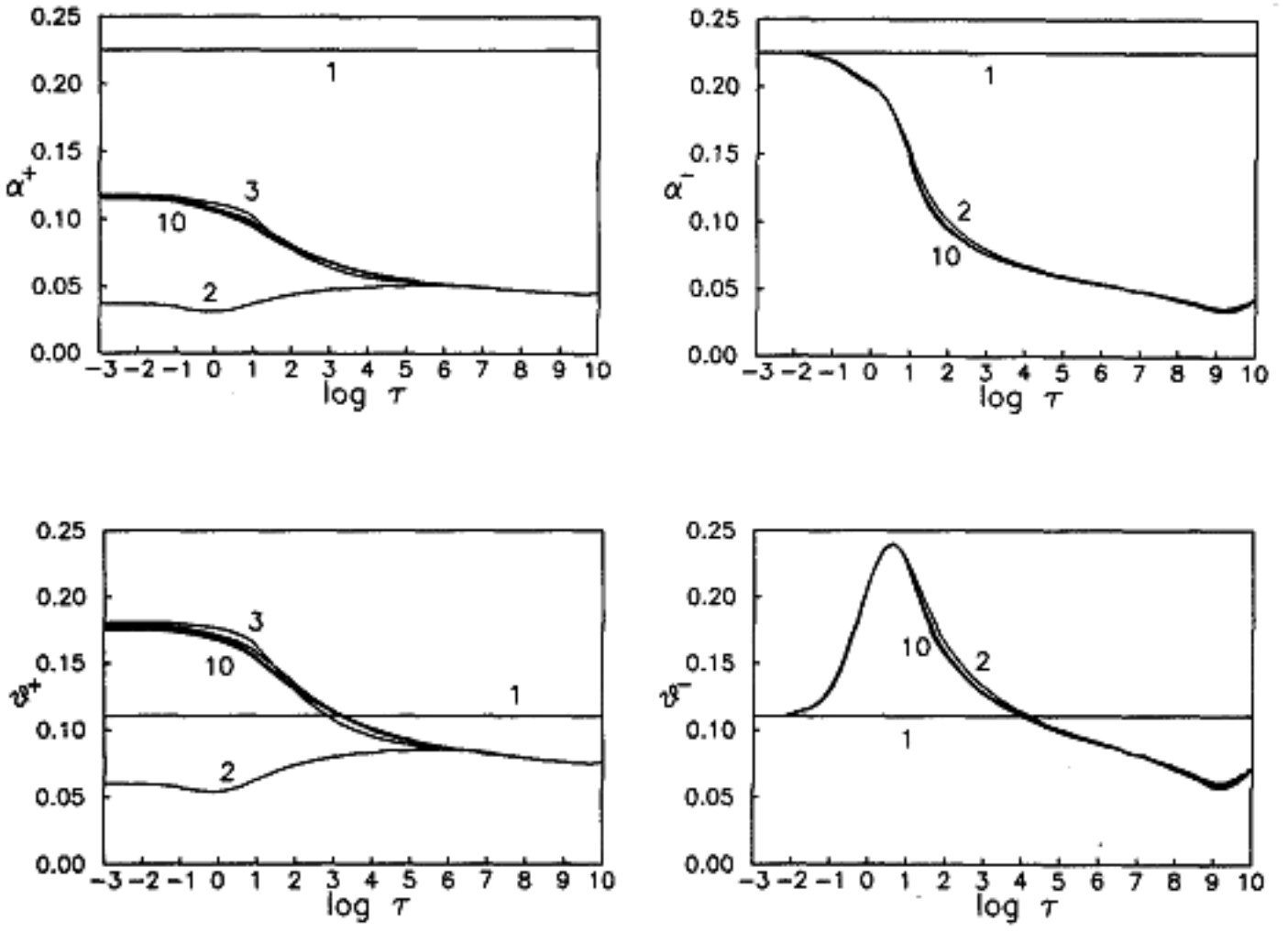

Fig. 6. The variation of the iteration factors $\alpha^{\pm}(\tau)$ and $\theta^{\pm}(\tau)$ for the case $\epsilon = 10^{-4}$ and $B = 1$ in the labelled number of iterations.

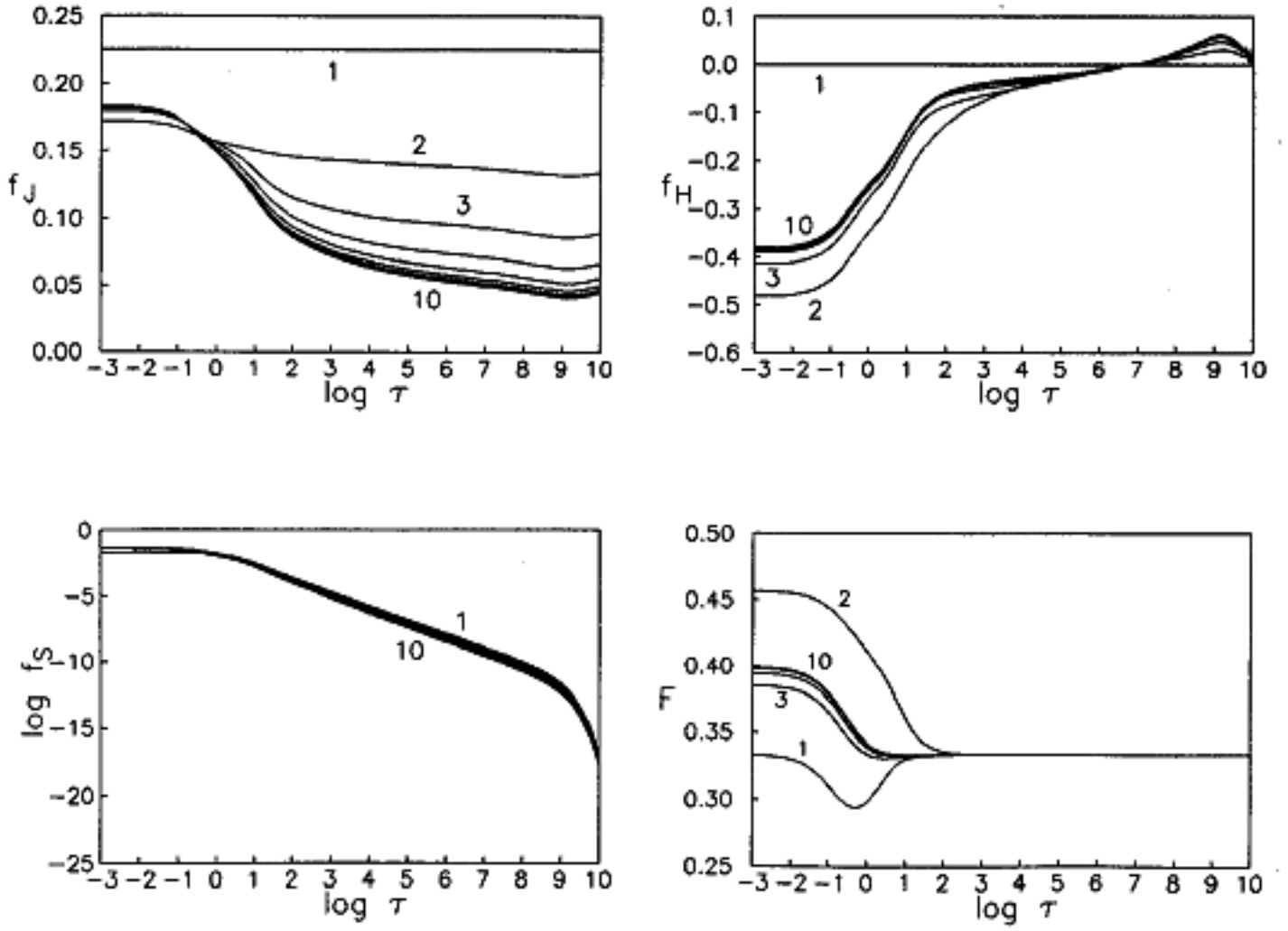

Fig. 7. The variation of the coefficients of the closure relations $f_J(\tau)$, $f_H(\tau)$, $f_S(\tau)$ and $F(\tau)$ for the case $\epsilon = 10^{-8}$ and $B = 1$ in the labelled number of iterations.

solution because the basic physics of the line formation problem is properly taken into account. We shall try not to simplify the treatment of the problem by reducing the number of iteration factors.

The anisotropy of the radiation field is already taken into account through the generalized Eddington factors [cf. Eq. (16)]. Therefore, instead of the "form factors" $\alpha^{\pm}$ and $\theta^{\pm}$ of Eq. (34), we could try to retain the single coefficient

$$f_J \equiv \frac{J_{\varphi^3} - S(\varphi^3 - M_{03}/2)}{J_\varphi - S(1 - M_{01}/2)}, \tag{39}$$

which accounts for the redistribution of the photons over the core and the wings. Such a factor leads to the closure relation:

$$J_{\varphi^3} - \varphi^3 S = f_J(J_\varphi - S) + f_S S. \tag{40}$$

Now the coefficient f_S takes the form

$$f_S = \tfrac{1}{2}(f_J M_{01} - M_{03}). \tag{41}$$

The closure relation given by Eq. (40) contains the same physical information as that of the more general relation given by Eq. (35). However formal difficulties might be introduced by a null denominator, possible in academic cases. When the denominator becomes zero, it holds $J_\varphi = S(1 - M_{01}/2)$, so that the second-order equation is no longer necessary. To make use of the latter relation just implies a slight change in the algorithm. Therefore it is much better to circumvent this possibility by using the closure relation given by Eq. (35).

The denominators of the iteration factors defined by Eqs. (34) have the same form. But there the differences (of opposite sign for the outward and inward radiation field) are of the order of the first derivative of the source function, that becomes zero only at the thermalization depth (for this academic case), where it is possible to predict the correct behaviour of the iteration factors.

Thus, from practical considerations, it is more convenient to separate the outgoing and incoming intensities, that it is to describe the radiation field in terms of a two-stream model. Under such conditions a new direct approach becomes possible to define the moment system and the relevant iteration factors.

From the direct application of such a model to the specific RT equations, we have

$$\pm\mu \frac{\mathrm{d}I^{\pm}_{x\mu}}{\mathrm{d}\tau} = \varphi_x (I^{\pm}_{x\mu} - S). \tag{42}$$

By performing the μ-integration over the interval [0, 1], and the frequency-profile integration, we eventually obtain the system:

$$+\frac{\mathrm{d}H^{+}_{\varphi}}{\mathrm{d}\tau} = (J^{+}_{\varphi^2} - \varphi^2 S)$$

$$-\frac{\mathrm{d}H^{-}_{\varphi}}{\mathrm{d}\tau} = (J^{-}_{\varphi^2} - \varphi^2 S), \tag{43}$$

coupled by the source term:

$$S = \epsilon B + (1-\epsilon)\left(\frac{J^{+}_{\varphi} + J^{-}_{\varphi}}{2}\right). \tag{44}$$

Note that we have used the same notation for the φ_x-integrated moments as before. To close the system we need additional relationships, namely the corresponding iteration factors. Keeping in mind the previous discussion, such factors can be defined in the following way:

$$\alpha^{\pm} = \frac{\tilde{J}^{\pm}_{\varphi^2}}{\tilde{J}^{\pm}_{\varphi}}$$

as the "form" factors, and

$$\theta^{\pm} = \frac{\tilde{H}^{\pm}_{\varphi}}{\tilde{J}^{\pm}_{\varphi}}$$

as the "anisotropy" factors. They can be rewritten as

$$\alpha^{+} \equiv \frac{J^{+}_{\varphi^2} - S\varphi^2}{J^{+}_{\varphi} - S} \qquad \alpha^{-} \equiv \frac{J^{-}_{\varphi^2} - S(\varphi^2 - M_{02})}{J^{-}_{\varphi} - S(1 - M_{01})}$$

$$\theta^{+} \equiv \frac{H^{+}_{\varphi} - S/2}{J^{+}_{\varphi} - S} \qquad \theta^{-} \equiv \frac{H^{-}_{\varphi} - S(1/2 - M_{11})}{J^{-}_{\varphi} - S(1 - M_{01})}.$$

Numerically, this approach is the same as the previous one. We might expect that the treatment of the wing photons is now better because the "form" factors $\alpha^{\pm}$ are here obtained by integration of the radiation field intensities over the wider profile function φ^2_x. However, the convergence properties of the solution obtained by using this new approach are the same. One or the other is just the matter of personal choice.

3.3. Iteration factors for a frequency dependent source function

It is easy to generalize the previous method to the case of a spectral line superposed to a background continuum. From the numerical point of view, this problem should be easier and its solution more stable, due to the fact that the additional opacity decreases the thermalization length making the line closer to the condition of LTE.

When the continuum opacity is taken into account, the radiative transfer equation takes the form:

$$\mu \frac{\mathrm{d}I_{x\mu}}{\mathrm{d}\tau} = (\varphi_x + \beta)[I_{x\mu}(\tau) - S_x(\tau)]. \tag{45}$$

Here β denotes the ratio of continuum to the line opacity ($\beta = k^c/k^l$) and $S_x(\tau)$ is the total source function

$$S_x(\tau) = \frac{\varphi_x}{\varphi_x + \beta} S^l(\tau) + \frac{\beta}{\varphi_x + \beta} S^c(\tau), \tag{46}$$

where S^l [given by Eq. (7)] and S^c are the relevant line and continuum contributions. We will assume that the continuum source function S^c is equal to the Plack function B. Both B and the ratio β will be supposed constant and known "*a priori*".

Equations (45) and (46) can be solved by a direct use of the procedure described in Sec. 3.2. By performing the integration of Eq. (45) over angles by using the operators $\int [\cdot]\,d\mu$ and $\int \mu[\cdot]\,d\mu$ and over frequencies by using $\int \varphi_x(\varphi_x + \beta)[\cdot]\,dx$ and $\int \varphi_x[\cdot]\,dx$, we obtain the two moment equations:

$$\frac{dH_{\varphi^2}(\beta)}{d\tau} = J_{\varphi^3}(\beta) - S_{\varphi^3}(\beta) \tag{47a}$$

$$\frac{dK_\varphi}{d\tau} = H_{\varphi^2}(\beta) \tag{47b}$$

where the frequency integrated moments are given by

$$Q_{\varphi^n}(\beta) \equiv \int Q_x \varphi_x (\varphi_x + \beta)^{n-1}\,dx. \tag{48}$$

The system (47a,b) must be closed by means of two additional relations. Like in Sec. 3.2. one can take the generalized Eddington factor $F(\tau) \equiv K_\varphi / J_\varphi$ as the first closure relation and, similarly to Eq. (35)

$$J_{\varphi^3}(\beta) - S_{\varphi^3}(\beta) = f_J(J_\varphi - S_\varphi) + f_H H_{\varphi^2}(\beta) + f_S, \tag{49}$$

as the second one. Here, S_φ—the frequency integrated total source function S_x has the form:

$$S_\varphi \equiv \int S_x \varphi_x\,dx = (1-\epsilon)\psi_1 J_\varphi + (\epsilon\psi_1 + \psi_2)B, \tag{50}$$

where

$$\psi_1 = \int \frac{\varphi_x^2\,dx}{\varphi_x + \beta}, \quad \psi_2 = \beta \int \frac{\varphi_x\,dx}{\varphi_x + \beta}. \tag{51}$$

The coefficients of the second closure relation (49) can be derived from the relevant iteration factors:

$$\alpha^\pm = \frac{\tilde{J}^\pm_{\varphi^3}(\beta)}{\tilde{J}^\pm_\varphi} \quad \theta^\pm = \frac{\tilde{H}^\pm_{\varphi^2}(\beta)}{\tilde{J}^\pm_\varphi}, \tag{52}$$

defined as the ratios of the non-local parts of the corresponding radiation field intensity moments. Using the "two-stream" model and proceeding from the formal solution of (45), the following differences between the radiation field and the "local" source function can be obtained

$$\tilde{I}^+_{x\mu} = I^+_{x\mu} - S_x$$

$$\tilde{I}^-_{x\mu} = I^-_{x\mu} - S_x(1 - e^{-\tau(\varphi_x + \beta)/\mu}).$$

Integrated over angles and frequencies and substituted into (52) they lead to the following iteration factors:

$$\alpha^+ \equiv \frac{J^+_{\varphi^3}(\beta) - S_{\varphi^3}(\beta)}{J^+_\varphi - S_\varphi}$$

$$\alpha^- \equiv \frac{J^-_{\varphi^3}(\beta) - [S_{\varphi^3}(\beta) - M^s_{03}(\beta)]}{J^-_\varphi - (S_\varphi - M^s_{01})}$$

$$\theta^+ \equiv \frac{H^+_{\varphi^2}(\beta) - S_{\varphi^2}(\beta)/2}{J^+_\varphi - S_\varphi}$$

$$\theta^- \equiv \frac{H^-_{\varphi^2}(\beta) - [S_{\varphi^2}(\beta)/2 - M^s_{12}(\beta)]}{J^-_\varphi - (S_\varphi - M^s_{01})}. \tag{53}$$

Here we defined

$$M^s_{mn} = \int \varphi^n_x S_x \, dx \int \mu^m \, d\mu \, e^{-\tau(\varphi_x + \beta)/\mu}$$

$$M^s_{mn}(\beta) = \int \varphi_x (\varphi_x + \beta)^{n-1} S_x \, dx \int \mu^m \, d\mu \, e^{-\tau(\varphi_x + \beta)/\mu}, \tag{54}$$

where the index s denotes that the integrand involves the frequency dependent total source function S_x.

The coefficients f_J and f_H have the same form as in (36), whereas f_S is given in terms of $M^s(\beta)$ and M^s by:

$$f_S = \tfrac{1}{2}[f_J M^s_{01} - M^s_{03}(\beta) - f_H M^s_{12}(\beta)]. \tag{55}$$

We will note that such an approach to the solution of the problem when continuum absorption is taken into account is conceptually the same as the one presented in the previous sections although slightly more complicated from the computational point of view.

The solutions obtained are shown in Fig. 8 where the line source function $S^l(\tau)$ is presented vs τ for a semi-infinite atmosphere with $B = 1$, $\epsilon = 10^{-8}$ and with two values of β (10^{-5} and 10^{-3}). When β grows, ϵ loses its decisive rôle on the behaviour of the line source function $S^l(\tau)$, that approaches its LTE value.

The exact solution of this physically more realistic problem is obtained with 6–7 iterations only. The stability is high and no relaxation technique is needed. Thus the iteration factors method proved to have better convergent properties when applied to physically more complex but numerically more stable problems.

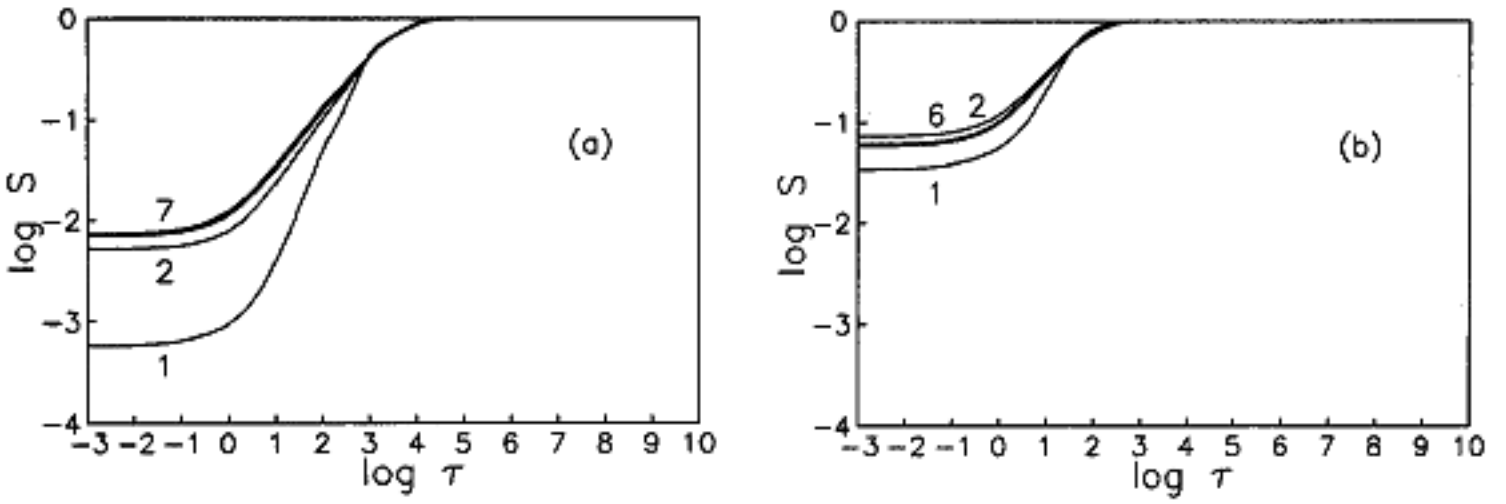

Fig. 8. The line source function $S^l(\tau)$ vs τ for a semi-infinite atmosphere $B = 1$, $\epsilon = 10^{-8}$ and for $\beta = 10^{-5}$ (a) and $\beta = 10^{-3}$ (b).

4. CONCLUSIONS

In this paper we have presented the method of iteration factors for the solution of the NLTE radiative transfer problem in spectral lines. This method represents the generalization of the idea of VEFs to the frequency dependent variables relevant to the line formation problem. Within a mixed iterative procedure, the so-called iteration factors are computed through the RT equation in the first step, to give in the second one the closure relation(s) necessary to solve the frequency-integrated moment equations. Similarly to the Λ-iteration, the procedure does not involve any matrix operation, so that only small memory storage and computational time are required.

In order to achieve a rapid convergence to the exact solution, the iteration factors, defined as the ratios of the relevant intensity moments, have to be good quasi-invariants, that is nearly independent of the initial solution and almost exact since the first iterations. Moreover, they must be simply related to the unknown moments in order to enable their determination in a way as simple as possible.

In this first part of our study, we have applied the method to the solution of the two-level-atom line formation problem, where the explicit form of the source function enables a straightforward definition of the iteration factors. This method provides an accurate and extremely fast convergence to the exact solution at the small additional cost, with respect to the Λ-iteration, of solving just one second-order differential equation.

We have shown that there are several ways to close the moment equations, namely to define the iteration factors. The closure relation, which contains all the relevant variables and is derived from the straightforward mathematical simulation of the physical process, gives the best convergence properties. With the use of this relation, the exact solution is obtained within only a few iterations, even under conditions very far from LTE. The first important conclusions is that a two-stream model, in which the outgoing and incoming directions of the radiation field are treated separately, leads to a much better convergence.

The definition of the appropriate iteration factors, hence the method itself, is of course problem dependent. In this respect the method of the iteration factors and ALI are similar. The choice of the iteration factors is determined by the physics of the problem under study, exactly as is the choice of the approximate operator Λ^*. However, while the optimum choice of Λ^* is always a question of compromise between the two basic requirements that Λ^* has to satisfy, the iteration factors follow almost directly from the structure of the basic equations.

Moreover, the structure of the algorithm easily allows for any further improvement in the definition of the iteration factors, without any extra computational cost. This becomes especially important when the radiative transfer has to be coupled with some physical constraints (e.g., of radiative and hydrostatic equilibrium in the modelling stellar atmospheres) or with some other physical processes (e.g., the presence of hydro-dynamical flows). In such cases it is difficult, and sometimes even impossible, to couple the constraint equations with those of radiative transfer for each frequency and direction. But the solution can be significantly reduced if the system of transfer equations is replaced by a single equation with the iteration factors as coefficients. Moreover, due to such a simple coupling, the occurrence of numerical instabilities is less probable, and the iterative procedure is easily kept under control.

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