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An accelerated lambda iteration method for multilevel radiative transfer

II. Overlapping transitions with full continuum

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Abstract. The ALI method of Paper I has been generalized to include treatment of overlapping, active continuum transfer and overlapping lines. The linearity of the iterative equations is maintained in this method by consistent use of the psi operator rather than the lambda operator. The method has been applied to a sample problem of pure helium, which includes 23 levels, 31 lines, 22 continua, three stages of ionization, and electron scattering. Velocity fields of order of a few Doppler widths were also included by means of an observer's frame formulation. The convergence of the solutions was found to be comparable to that achieved in the previous pure line method.

Key words: radiative transfer – non-LTE – stellar atmospheres

1. Introduction

In Paper I (Rybicki & Hummer 1991) we presented a method of solving multilevel transfer equations with their associated equations of statistical equilibrium by a form of the approximate lambda iteration (ALI) method in which the latter always retain their linearity. This feature, which eliminates the need for an internal linearization cycle to obtain the updated level populations, is achieved by "preconditioning" the equations of statistical equilibrium at each step, in order to eliminate the slow convergence of the classical iteration caused by photons trapped in strong lines. Although many versions of the ALI procedure have been developed (references are given in Paper I), ours is the only one in which the treatment of multilevel transfer is an integral part of the formulation. For this reason we refer to our procedure as a multilevel approximate lambda (MALI) method.

In Paper I, we developed the MALI method for isolated transitions, and applied it to problems which involve only line transfer. In the present paper we generalize the method to include any number of overlapping lines and continua. The guiding principle is that the equations of statistical equilibrium must remain linear in the population numbers at every stage of the calculation. This is facilitated by use of the Ψ operator introduced in Paper I, rather than the more familiar Λ operator. The analysis has been incorporated into a computer code, with the temporary restriction that overlapping *lines* cannot yet be treated. In addition to the bound–free continua of the element in question, we can include self-consistently electron scattering and free–free continua, as well as any prespecified "background" continuum. As before, macroscopic velocity fields can be treated in the observers frame.

The analysis leading to various preconditioning strategies for overlapping transitions is developed in the next section. Methods of treating the electron scattering emissivity are also considered. Section 3 then describes the implementation of the generalized preconditioning in our code; other newly added facilities are briefly mentioned. In the final section the application of the code to a pure helium atmosphere containing three stages of ionization is discussed.

Because this paper is of interest only as an extention of the method described in Paper I, we assume that the reader is thoroughly familiar with that paper in order not to have to repeat material developed there.

2. The iterative method

The treatment of the statistical equilibrium equations is central to the present method. We show how to incorporate an iterative transfer scheme directly into these equations, extending the preconditioning method given in Paper I, which should be consulted for notation and background. The development given here applies to quite arbitrarily overlapping continua and lines with velocity fields, but it has been restricted to plane geometry and to the assumption of complete redistribution in the lines. Generalizations to more complex geometries is straightforward. The treatment of partial redistribution within this formalism will be considered in a future paper.

2.1. *The ordinary statistical equilibrium equations*

Before introducing our generalized method of preconditioning, we shall review the ordinary equations of statistical equilibrium, introducing notation that will be convenient for the further developments. As in Paper I, we label the levels by indices $l, l', \ldots$. We denote the population of level l by n_l its energy by E_l, and its satistical weight by g_l. Here the energies E_l are measured relative to the ground level of the neutral species, so that, for example, the energy of the ground level of the first stage of ionization is equal to the first ionization potential. We use the

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notations $l \succ l'$ and $l \prec l'$ to imply $E_l > E_{l'}$ and $E_l < E_{l'}$, respectively.

The ordinary equations of statistical equilibrium can be written

$$\sum_{l'} n_{l'}(C_{l'l}+R_{l'l})=\sum_{l'} n_l(C_{ll'}+R_{ll'}), \tag{2.1}$$

where $C_{ll'}$ are the collisional rate coefficients, $R_{ll'}$ are the radiative rate coefficients. Included in the definitions of the rate coefficients may be factors of the electron density n_e, which is considered known, either because it is prescribed as part of the specified model, or because it may be calculated adequately from the results of a previous iteration Similar remarks hold for the temperature field in the medium. Thus, the collisional rate coefficients $C_{ll'}$ are to be considered as known quantities at each stage of the calculation. We note that these equations are linear and homogeneous in the populations n_l of the treated species. An additional relation is therefore required, usually that the sum of populations over all levels must equal the given total population of the species.

It will be convenient for our further development to be able to write expressions for the radiative rate coefficients $R_{ll'}$ that apply to both lines and continua, apply to both orderings of the indices, $l \succ l'$ and $l \prec l'$, and explicitly display the dependence of these rates on the radiation field $I_{\mu\nu}$. Thus, for the transition connecting l and l' we define the quantities $U_{ll'}(\nu)$ and $V_{ll'}(\nu)$, which for line transitions are given by

$$U_{ll'}(\mu,\nu)\equiv\begin{cases}\dfrac{h\nu}{4\pi}A_{ll'}\varphi_{ll'}(\mu,\nu), & l\succ l',\\ 0, & l\prec l',\end{cases}$$

$$V_{ll'}(\mu,\nu)\equiv\frac{h\nu}{4\pi}B_{ll'}\varphi_{ll'}(\mu,\nu), \tag{2.2}$$

in terms of the Einstein coefficients $A_{ll'}$, $B_{ll'}$, and $B_{l'l}$ and the line profile function $\varphi_{ll'}=\varphi_{l'l}$. The result for $V_{ll'}$ has the same form for either $l \succ l'$ or $l \prec l'$, although the Einstein coefficients then refer to downward or upward transitions, respectively. A dependence of the profile function on the angle μ is included to take into account macroscopic velocity fields.

Similarly, if the transition between l and l' is a continuum transition, then we define

$$U_{ll'}(\nu)\equiv\begin{cases}n_e\Phi_{ll'}(T)\dfrac{2h\nu^3}{c^2}e^{-h\nu/kT}a_{ll'}(\nu), & l\succ l',\\ 0, & l\prec l',\end{cases}$$

$$V_{ll'}(\nu)\equiv\begin{cases}n_e\Phi_{ll'}(T)e^{-h\nu/kT}a_{ll'}(\nu), & l\succ l',\\ a_{ll'}(\nu), & l\prec l',\end{cases} \tag{2.3}$$

where $a_{ll'}(\nu)$ is the photoionization cross section, and $\Phi_{ll'}(T)$ is the Saha–Boltzmann function,

$$\Phi_{ll'}(T)=\frac{g_{l'}}{2g_l}\left(\frac{h^2}{2\pi mkT}\right)^{3/2}\exp[(E_l-E_{l'})/kT], \tag{2.4}$$

(see, e.g. Mihalas 1978).

The opacity $\chi_{ll'}$ and emissivity $\eta_{ll'}$ in the transition connecting l and l' can be conveniently expressed in terms of the quantities $U_{ll'}$ and $V_{ll'}$. For $l \succ l'$ these are

$$\chi_{ll'}(\mu,\nu)=n_{l'}V_{l'l}-n_lV_{ll'},\quad \eta_{ll'}(\mu,\nu)=n_lU_{ll'}. \tag{2.5}$$

The total opacity and emissivity can be written as

$$\chi_{\mu\nu}=\sum_{l\succ l'}\chi_{ll'}+\chi_c=\sum_{l\succ l'}(n_{l'}V_{l'l}-n_lV_{ll'})+\chi_c, \tag{2.6}$$

$$\eta_{\mu\nu}=\sum_{ll'}\eta_{ll'}+\eta_c=\sum_{ll'}n_lU_{ll'}+\eta_c. \tag{2.7}$$

It is permissible to write the total emissivity using unrestricted summations over l and l', since the terms for $l \prec l'$ in fact vanish by Eq. (2.2) or (2.3). The quantities χ_c and η_c in these equations are the *background* opacity and emissivity. These background quantities may be one or a combination of two types: quantities given as part of the original specification of the problem; or quantities for which it has been determined that it is adequate to use a *lagged* evaluation, i.e. an evaluation with results of the previous iteration. Either way, these quantities are to be considered known at each stage of the iterations. The special case of electron scattering emissivity is discussed below.

In terms of these quantities the radiative rate coefficient from level l and level l' is given by

$$R_{ll'}=\int d\Omega\int\frac{d\nu}{h\nu}[U_{ll'}(\mu,\nu)+V_{ll'}(\mu,\nu)I_{\mu\nu}], \tag{2.8}$$

which applies to both lines and continua, and for both $l \succ l'$ and $l \prec l'$. The equations of statistical equilibrium (2.1) can now be written in the form

$$\sum_{l'}n_{l'}C_{l'l}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}(n_{l'}U_{l'l}+n_{l'}V_{l'l}I_{\mu\nu})$$
$$=\sum_{l'}n_lC_{ll'}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}(n_lU_{ll'}+n_lV_{ll'}I_{\mu\nu}). \tag{2.9}$$

It is a property of this formulation that the radiation field appears simply through the single quantity $I_{\mu\nu}$ at angle μ and at physical frequency ν, and there is no explicit separation of the integration into "line" or "continuum" frequencies. As a consequence, this formulation automatically takes into account overlapping of continua and lines in any combination, including the overlapping of lines.

2.2. *Preconditioned statistical equilibrium equations*

We now consider the problem of preconditioning the equations of statistical equilibrium by appropriate treatment of the radiative rates terms. A detailed discussion of preconditioning was given in Paper I for the case of a pure line problem with a background continuum and with velocity fields. As shown in Paper I it is possible to retain the linearity and homogeneity of the satistical equilibrium equations in their preconditioned form, which vastly simplifies the iteration process, since *no further linearizations of the equations are required.* In Paper I this was done by judicious evaluation of some quantities using the previous iteration. By straightforward generalizations of the techniques of Paper I, we shall show that linear and homogeneous preconditioned equations can also be obtained in the present case, which includes non-LTE continuum transition and overlapping lines.

For the purposes of the present application, we have found it very convenient to express the formal solution of the transfer equation not by means of the lambda operator acting on the source function, but rather by means of an operator acting on the

emissivity:

$$I_{\mu\nu}=\Psi_{\mu\nu}[\eta_{\mu\nu}], \tag{2.10}$$

where $\Psi_{\mu\nu}$ is the *monochromatic psi operator* and $\eta_{\mu\nu}$ is the total emissivity, given by Eq. (2.7). The psi operator differs from the lambda operator by a factor of the total opacity $\chi_{\mu\nu}$.

The approximate iterative scheme to be introduced here results from replacing Eq. (2.10) by

$$I_{\mu\nu}=\Psi^*_{\mu\nu}[\eta_{\mu\nu}]+(\Psi_{\mu\nu}-\Psi^*_{\mu\nu})[\eta^\dagger_{\mu\nu}] \tag{2.11}$$

where $\Psi^*_{\mu\nu}$ is an appropriately chosen *approximate psi operator*, and where $\eta^\dagger_{\mu\nu}$ is the total emissivity from the previous iteration,

$$\eta^\dagger_{\mu\nu}=\sum_{ll'} n_l^\dagger U_{ll'}+\eta_c. \tag{2.12}$$

As in Paper I, a dagger denotes quantities evaluated using "old" populations $n_l^\dagger$, from the previous iteration. The theory presented here applies to quite general approximate opertors, but in our practical applications we use approximate operators of the type proposed by Olson et al. (1986), as discussed in Paper I.

The iteration method described by Eq. (2.11) is a variant of the method of approximate lambda operators (ALI), sometimes known as Cannon's method. They are not exactly equivalent, however. In each of the two iterative methods, the basic operator, either lambda or psi, is implicitly constructed from old variables, so that the two methods differ as to whether the total opacity factor connecting them is to be evaluated with old or new variables. We find that for the present problem the implicit choice made with the psi operator is the most useful one. For example, the intensity given by Eq. (2.11) is *linear* in the new populations, through the dependence on the emissivity [Eq. (2.7)].

In the following development, the operators $\Psi_{\mu\nu}$ and $\Psi^*_{\mu\nu}$, and also $\Lambda_{\mu\nu}$ and $\Lambda^*_{\mu\nu}$, are always to be interpreted as numerical operators constructed out of old variables. The relationship betweeen these operators is then simply

$$\Psi_{\mu\nu}[\ldots]=\Lambda_{\mu\nu}[(\chi^\dagger_{\mu\nu})^{-1}\ldots], \quad \Psi^*_{\mu\nu}[\ldots]=\Lambda^*_{\mu\nu}[(\chi^\dagger_{\mu\nu})^{-1}\ldots], \tag{2.13}$$

where $\chi^\dagger_{\mu\nu}$ is the total opacity evaluated with the old populations. We shall use the psi operators exclusively in this paper. However, if desired, lambda operators can easily be substituted in the final formulas, using Eq. (2.13). If this is done, the resulting iteration scheme will then be an approximate *lambda* operator method, but with a particularly advantageous choice for the total opacity factors having been made automatically.

Another form for Eq. (2.11) results from substituting for $\eta_{\mu\nu}$ and $\eta^\dagger_{\mu\nu}$ using Eqs. (2.7) and (2.12),

$$I_{\mu\nu}=\Psi_{\mu\nu}[\eta^\dagger_{\mu\nu}]-\sum_{mm'}\Psi^*_{\mu\nu}[n_m^\dagger U_{mm'}]+\sum_{mm'}\Psi^*_{\mu\nu}[n_m U_{mm'}], \tag{2.14}$$

where we have used the fact that the background opacity η_c is assumed to be the same quantity in evaluating both the old and new emissivities. Using this expression for $I_{\mu\nu}$ in the equations of statistical equilibrium, we obtain the iterative equations,

$$\sum_{l'} n_{l'} C_{l'l}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}\Big(n_{l'}U_{l'l}+n_{l'}V_{l'l}\Psi_{\mu\nu}[\eta^\dagger_{\mu\nu}]$$
$$-\sum_{mm'} n_{l'}V_{l'l}\Psi^*_{\mu\nu}[n_m^\dagger U_{mm'}]+\sum_{mm'} n_{l'}V_{l'l}\Psi^*_{\mu\nu}[n_m U_{mm'}]\Big)$$
$$=\sum_{l'} n_l C_{ll'}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}\Big(n_l U_{ll'}+n_l V_{ll'}\Psi_{\mu\nu}[\eta^\dagger_{\mu\nu}]$$
$$-\sum_{mm'} n_l V_{ll'}\Psi^*_{\mu\nu}[n_m^\dagger U_{mm'}]+\sum_{mm'} n_l V_{ll'}\Psi^*_{\mu\nu}[n_m U_{mm'}]\Big), \tag{2.15}$$

As it stands, Eq. (2.15) is not linear in the new populations, because of the last summations on each side (the *critical summations*), which involve the product of $n_{l'}$ and n_m on the left, and the product of n_l and n_m on the right. We may obtain linear equations by appropriately modifying these terms by replacing some quantities by corresponding ones evaluated from the previous iteration. It is easily seen that, in order to maintain both the linearity and homogeneity of the equations, for each term of critical summation on the left, one should choose *either* $n_{l'}$ or n_m to be replaced by its old value, *but not both.* An analogous replacement is made on the right side in each term of the critical summation involving n_l and n_m.

Which population should be chosen to be the old one? Considerable insight into this question is gained by supposing, for the moment, that we choose to evaluate all the n_m in the critical summations in Eq. (2.15) using the old populations (and thus evaluate the corresponding factors of n_l and $n_{l'}$ using the new populations). The the last term on each side of that equation would be identical with preceding term except for sign, which would then cancel, leaving an equation that is precisely equivalent to classical lambda iteration.

The preceding discussion strongly suggests that to maximize the degree of preconditioning (as opposed to approaching the lambda iteration limit), in the critical summations in Eq. (2.15) one should use the old populations for n_l and $n_{l'}$, and the new populations for all the n_m. Such a choice leads to *full preconditioning* of the equations. However, such a full preconditioning can put large demands on the numerical work; for example, it can create couplings betweeen levels that may have been uncoupled in the original statistical equilibrium equations. As we shall see, the preconditioning of some terms may have little effect on the convergence rate. Therefore, it may not always be desirable to make the maximum preconditioning choice in all terms, and there exist many types of *partial preconditioning* strategies. We shall treat full preconditioning first, and then treat one partial preconditioning strategy, namely, preconditioning within the same transition. These two cases should make clear the general ideas and procedures. Finally, we discuss briefly some other possible strategies that may be useful in particular cases.

2.3. *Full preconditioning strategy*

As discussed above, this strategy leads to the iterative scheme

$$\sum_{l'} n_{l'} C_{l'l}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}\Big(n_{l'}U_{l'l}+n_{l'}V_{l'l}\Psi_{\mu\nu}[\eta^\dagger_{\mu\nu}]$$
$$-\sum_{mm'} n_{l'}V_{l'l}\Psi^*_{\mu\nu}[n_m^\dagger U_{mm'}]+\sum_{mm'} n_l^\dagger V_{l'l}\Psi^*_{\mu\nu}[n_m U_{mm'}]\Big)$$
$$=\sum_{l'} n_l C_{ll'}+\sum_{l'}\int d\Omega\int\frac{d\nu}{h\nu}\Big(n_l U_{ll'}+n_l V_{ll'}\Psi_{\mu\nu}[\eta^\dagger_{\mu\nu}]$$
$$-\sum_{mm'} n_l V_{ll'}\Psi^*_{\mu\nu}[n_m^\dagger U_{mm'}]+\sum_{mm'} n_l^\dagger V_{ll'}\Psi^*_{\mu\nu}[n_m U_{mm'}]\Big). \tag{2.16}$$

This system of equations determines the set of new populations

n_l. Because of their homogeneity, one of them must be replaced by the equation expressing the total population of the species, summed over all levels.

For practical calculations it is convenient to rewrite these equations to emphasize their linear dependence on the n_l. It is straightforward to show that they may be put into the form

$$\sum_{l'} \Gamma_{ll'} n_{l'} = \sum_{l'} (\Gamma^C_{ll'} + \Gamma^R_{ll'}) n_{l'} = 0, \tag{2.17}$$

where

$$\Gamma^C_{ll'} = C_{l'l} - \delta_{ll'} \sum_{l''} C_{l'l''}, \tag{2.18}$$

$$\Gamma^R_{ll'} = \int d\Omega \int \frac{d\nu}{h\nu} \left[U_{l'l} + V_{l'l} I^{\text{eff}}_{\mu\nu} - \left(\sum_{l''} \chi^{\dagger}_{l''l} \right) \Psi^*_{\mu\nu} \left(\sum_{l'''} U_{l'l'''} \right) - \delta_{l'l} \left(\sum_{l''} U_{l'l''} \right) - \delta_{l'l} \left(\sum_{l''} V_{l'l''} \right) I^{\text{eff}}_{\mu\nu} \right], \tag{2.19}$$

and

$$I^{\text{eff}}_{\mu\nu} = \Psi_{\mu\nu}[\eta^{\dagger}_{\mu\nu}] - \Psi^*_{\mu\nu}[\eta^{\dagger}_{\mu\nu}] + \Psi^*_{\mu\nu}[\eta_c]. \tag{2.20}$$

In Eq. (2.19) the old opacity is defined by the same equation

$$\chi^{\dagger}_{l''l'} = n^{\dagger}_{l'} V_{l'l''} - n^{\dagger}_{l''} V_{l''l'}, \tag{2.21}$$

for either orderings of the indices (i.e. it is antisymmetric in the two indices).

We now briefly discuss some of the considerations that go into the numerical implementation of the method. First of all, one notes that, because of the conservation property

$$\sum_{l} \Gamma^R_{ll'} = 0, \tag{2.22}$$

one only needs to compute the nondiagonal elements of $\Gamma^R_{ll'}$, the diagonal elements being expressed as a row sum over the nondiagonal elements. Thus, the terms involving $\delta_{l'l}$ in Eq. (2.19) can be ignored for the numerical computations.

Upon the introduction of an appropriate frequency and angular quadrature formula, the numerical evaluation of the elements of Γ^R_{ll} proceeds by accumulating the contributions from each frequency and angle, using the formal solution of the transfer equation to compute the old radiation field $\Psi_{\mu\nu}[\eta^{\dagger}_{\mu\nu}]$ and the elements of the approximate psi operator $\Psi^*_{\mu\nu}$. Since the number of active radiative transitions is ordinarily substantially smaller than the number of level pairs, considerable savings can be effected by maintaining a list of transitions active at the current frequency. This is used first to compute the two relevant summations in Eq. (2.19), and then to find the contributions to $\Gamma^R_{ll'}$ only for the relevant pairs of indices ll'. This list can be quickly updated as one proceeds through the frequency grid, knowing where each process begins and ends.

If $\Psi^*_{\mu\nu}$ is a local operator, then all the terms in Eq. (2.19) are ordinary numbers, and it can be solved independently at each point in the medium. However, if it is a nonlocal operator, then the terms involving $\Psi^*_{\mu\nu}$ are to be regarded as spatial operators acting on all quantities to the right, that is, on the $n_{l'}$ and also on the sum over the $U_{l'l'''}$. This requires that the equations be solved as a coupled set between different spatial points. A tridiagonal operator (or wider band approximation) can be treated efficiently by well-known block band methods, but the computational time and storage requirements are increased over those of the local operator.

2.4. *Preconditioning within the same transition only*

The preceding full preconditioning strategy can easily be seen to be unnecessarily complete for many types of problems. For example, in the critical summations in Eq. (2.15), the product $V_{ll'} U_{mm'} \equiv 0$ for all frequencies when ll' and mm' refer to nonoverlapping radiative transitions. Even when some frequency overlap occurs, the mathematical overlap of the functions $V_{ll'}$ and $U_{mm'}$ is clearly much greater for one transition with itself than between two differing transitions. This suggests that a useful strategy is to precondition within the same transition only. This is accomplished by using the new populations n_m in each critical summations only for those two terms for which mm' is the same as ll' or $l'l$. In the other terms the use of $n^{\dagger}$ will cancel an identical term in the preceding summation. Therefore, all summations in Eq. (2.19) will reduce to just two terms corresponding to the transition ll' and $l'l$, yielding the iterative scheme

$$\begin{aligned} &\sum_{l'} n_{l'} C_{l'l} + \sum_{l'} \int d\Omega \int \frac{d\nu}{h\nu} (n_{l'} U_{l'l} + n_{l'} V_{l'l} \Psi_{\mu\nu}[\eta^{\dagger}_{\mu\nu}] \\ &\quad - n_{l'} V_{l'l} \Psi^*_{\mu\nu}[n^{\dagger}_{l} U_{ll'}] - n_{l'} V_{l'l} \Psi^*_{\mu\nu}[n^{\dagger}_{l'} U_{l'l}] + n^{\dagger}_{l'} V_{l'l} \Psi^*_{\mu\nu}[n_l U_{ll'}] \\ &\quad + n^{\dagger}_{l'} V_{l'l} \Psi^*_{\mu\nu}[n_{l'} U_{l'l}]) \\ &\quad = \sum_{l'} n_l C_{ll'} + \sum_{l'} \int d\Omega \int \frac{d\nu}{h\nu} (n_l U_{ll'} + n_l V_{ll'} \Psi_{\mu\nu}[\eta^{\dagger}_{\mu\nu}] \\ &\quad - n_l V_{ll'} \Psi^*_{\mu\nu}[n^{\dagger}_{l} U_{ll'}] - n_l V_{ll'} \Psi^*_{\mu\nu}[n^{\dagger}_{l'} U_{l'l}] \\ &\quad + n^{\dagger}_{l} V_{ll'} \Psi^*_{\mu\nu}[n_l U_{ll'}] + n^{\dagger}_{l} V_{ll'} \Psi^*_{\mu\nu}[n_{l'} U_{l'l}]), \end{aligned} \tag{2.23}$$

A similar reduction to the form (2.17) can be done here, where now

$$\Gamma^R_{ll'} = \int d\Omega \int \frac{d\nu}{h\nu} \left\{ (1 - \chi^{\dagger}_{l'l} \Psi^*_{\mu\nu}) U_{l'l} + V_{l'l} I^{\text{eff}}_{\mu\nu;ll'} - \delta_{l'l} \sum_{l''} [(1 - \chi^{\dagger}_{l'l''} \Psi^*_{\mu\nu}) U_{l'l''} + V_{l'l''} I^{\text{eff}}_{\mu\nu;l'l''}] \right\}, \tag{2.24}$$

and

$$I^{\text{eff}}_{\mu\nu;ll'} = \Psi_{\mu\nu}[\eta^{\dagger}_{\mu\nu}] - \Psi^*_{\mu\nu}[n^{\dagger}_{l} U_{ll'}] - \Psi^*_{\mu\nu}[n^{\dagger}_{l'} U_{l'l}]. \tag{2.25}$$

Although two terms involving $\Psi^*_{\mu\nu}$ appear in Eq. (2.25), for any particular values of l and l' only one survives, because of the vanishing of either $U_{ll'}$ or $U_{l'l}$ by Eq. (2.2) or (2.3). These equations are very similar to the ones presented in Paper I, and indeed they reduce to those under the same restrictive assumptions of nonoverlapping lines with background continuum.

Many of the remarks made at the end of the preceding section concerning the numerical solution of these equations also applies here. The numerical effort is smaller here, since only one transition contributes to each element of $\Gamma_{ll'}$.

2.5. *Other strategies*

One can easily imagine other partial preconditioning strategies that may be advantageous for particular problems. For example, one might augment the partial strategy of Sect. 2.4 in order to include special cases of unusual overlap. In case of strong line overlap, this could be done by including not only the same transition in the preconditioning, but also include any line or lines that overlap it. The general guiding principle is that additional preconditioning should be done in those terms for which

there is a significant frequency overlap, but probably only experience will show what a "significant" overlap really means.

Another partial strategy might start from the full strategy of Sect. 2.3, but would avoid preconditioning some terms in order to maintain some desirable structure of the rate matrix $\Gamma_{ll'}$, for example, its overall block tridiagonal form in cases where only transitions between neighboring stages of ionization are treated.

The above represent only a few suggestions for partial preconditioning strategies. No special equations will be given to implement them, since it is probably best to do this in the numerical code itself.

2.6. *Electron scattering*

In the energy ranges of interest here, the scattering coefficient for electron scattering has the classical Thomson value and, as such, can be easily incorporated into the absorption (extinction) coefficient $\chi_{\mu\nu}$. However, the inclusion of electron scattering in the emissivity $\eta_{\mu\nu}$ is not straightforward. Electron scattering is often treated as coherent in the context of steller atmospheres, and this is usually a very good approximation for transfer in the continuum. However, coherence is manifestly incorrect for spectral lines, since scattered photons are redistributed over the electron Doppler width (see e.g. Chandrasekhar 1960, §86; Hummer & Mihalas 1967), which is broader than the line Doppler width by the large factor $(m_{\rm ion}/m_{\rm e})^{1/2}$.

While the treatment of noncoherence is probably necessary to determine the effects on lines, there are more efficient methods that apply to the continuum, where electron scattering may be well-approximated as coherent and isotropic. For simplicity in this preliminary investigation, we have used this approximation for both lines and continua.

The simplest conceptual treatment of coherent and isotropic electron scattering is to include it in the terms $\chi_{\rm c}$ and $\eta_{\rm c}$ in Eqs. (2.6) and (2.7), with contributions to these terms being updated using the results of the previous iteration. In this way, the non-LTE parts of the transfer are treated by ALI, while the electron scattering part is treated by classical lambda iteration. One advantage of this kind of lambda iteration method is that it would be easy to generalize to include the effects of noncoherence by evaluating the emissivity using the full redistribution function.

Another approach to the monochromatic transfer problem is to write the transfer equation in the form introduced by Feautrier (1964),

$$\mu^2 \frac{\partial^2 u_{\mu\nu}}{\partial \tau_\nu^2} = u_{\mu\nu} - \frac{\chi^{\rm a}_{\mu\nu}}{\chi^{\rm a}_{\mu\nu}+\chi^{\rm s}_\nu} S^{\rm a}_{\mu\nu} - \frac{\chi^{\rm s}_\nu}{\chi^{\rm a}_{\mu\nu}+\chi^{\rm s}_\nu} J_\nu, \tag{2.26}$$

where $\chi^{\rm a}_{\mu\nu}$ and $\chi^{\rm s}_\nu = n_{\rm e}\sigma_{\rm T}$ are, respectively, the "absorption" and electron scattering opacities, and $S^{\rm a}_{\mu\nu}$ is the "absorption" source function. The term "absorption" here refers to all proceses for which the absorption and emission coefficients can be expressed in terms of populations; this includes all non-LTE lines and continua, and background LTE processes such as free–free.

For the two-stream approximation, $u_{\mu\nu}=u_\nu\equiv J_\nu$, so that Eq. (2.1) can be written,

$$\mu^2 \frac{\partial^2 u_\nu}{\partial \tau_\nu^2} = \varepsilon_\nu (u_\nu - S^{\rm a}_\nu), \tag{2.27}$$

where

$$\varepsilon_\nu \equiv \frac{\chi^{\rm a}_\nu}{\chi^{\rm a}_\nu+\chi^{\rm s}_\nu}. \tag{2.28}$$

Equation (2.27) can be solved using a trivial modification of the usual Feautrier method, which takes into account the extra factor ε_ν. This method worked very well on our test problem, giving convergence rates very much like those without scattering. Although we have not actually done so, it is possible to generalize this method to include explicitly the coupling of a number of radiation streams at various angles. This would give rise to multicomponent transfer equations at each frequency in the form of a block tridiagonal system, which could be solved by block Gaussian elimination.

When the number of discrete angles per hemisphere is greater than one, scattering can also be treated by introducing the geometrical factor

$$r_{\mu\nu} \equiv \frac{J_\nu}{u_{\mu\nu}}, \tag{2.29}$$

which is evaluated from the previous iteration, much in the spirit of variable Eddington factors. The major disadvantage of this approach is that it does require a considerable amount of extra storage for all the quantities $r_{\mu\nu}$. We expect that this method could also be generalized to include noncoherence.

3. Implementation

The primary task in implementing numerically the preconditioning strategies above is the evaluation of the coefficient matrices $\Gamma^R_{ll'}$ given by Eq. (2.19) or (2.24). This calculation can be organized conveniently by dividing the frequency interval in which all transitions occur into *zones*, defined by the thresholds of all bound-free transitions and by the red and blue edges of each line, as specified by a band width parameter; the same set of transitions are active for all frequencies in the zone. As only one transition is added (or possibly subtracted in the case of a line) at each zone boundary, it is simple to keep track of the opacities and emissivities entering the solution of the transfer equation at each frequency.

The zone boundary frequencies are first created by running through all transitions in turn, and then are ordered by ascending frequency, along with the identification number of the transition entering or exiting, which is negative in case of a bluc line edge. The algorithms described in Paper I are then employed to generate the frequency mesh in each zone. Photoionization cross sections are generated and stored at all frequencies in the zones where the corresponding bound–free transition is active, and the profile functions are generated and stored for each line.

The monochromatic transfer is the integrated for each frequency and angle, starting with the lowest frequency. The quantities Γ^R are then accumulated frequency by frequency, according to Eqs. (2.19) or (2.24).

In most applications of the present ALI method, the formal solutions of the transfer equations can be done with improved Feautrier method described in Paper I, which is based on the symmetric Feautrier variable $u_\nu=(I_{\mu\nu}+I_{-\mu,\nu})/2$ in the continuum, or $u_\nu=(I_{\mu\nu}+I_{-\mu,\,\nu_0-\nu})/2$ within a single line with a velocity field. However, the Feautrier formulation breaks down when both velocity fields and overlappping lines occur together, because the required symmetries no longer apply. These cases require a method based on the specific intensity $I_{\mu\nu}$ itself, such as the method of short characteristics of Olson & Kunasz (1987). Alternatively, one might use a Feautrier-type method specifically adapted to treat the asymmetry. We have not implemented such

methods in our work, since we have not yet treated problems for which they are necessary.

We implemented several of the methods presented in Sect. 2.6 for treating the electron scattering, in particular the lambda iteration method, the two-stream method of Eq. (2.27), and the iteration factor method of Eq. (2.29).

The code now includes a number of other new facilities. The electron density is expressed as a sum of two contributions, a prespecified "background" component arising from all of the other elements in the atmosphere, and a "self-consistent" part evaluated from the ion populations of the element being treated from the previous iteration. This component is initialized by an input value for the number of free electrons per nucleus of the element in question. Either component can be set to zero as desired. This simple scheme appears to converge much more rapidly than the main ALI calculation. An analogous procedure has been implemented for "background" continuous opacities, augmented by the free–free opacity arising from the ions of element being treated.

In addition to the free or reflecting lower boundary condition described in Paper I, the option of a diffusion-approximation condition is now available. The temperature derivative is replaced by a difference approximation based on the last two depth points for consistency with the treatment of the transfer equations.

Here, as in Paper I, we used the acceleration method of Ng (1974) to improve the convergence of the method. A number of important points about the Ng method and our use of it were not covered in Paper I, and we should like to do so now. Although the original Ng method did not include the possibility of using "weights" for defining the mean square differences, we have found that such weights can be easily included in the method and can lead to substantial improvements. In our work we have chosen to use the set of level populations at the various depths as defining the basic solution. With this choice, weights equal to the inverse squares of the level populations appear to give the best results; these are equivalent to making the method sensitive to the mean square of the *relative* errors rather than *absolute* errors in the populations.

Although the Ng method works on nonlinear equations, it really only works well after the errors in the approximate iterative solution become fairly small, that is, become approximately linear deviations from the true solution. This can be checked by monitoring the maximum relative change in the solution in each iteration (denoted as C_k in Paper I); this should be $\lesssim 0.1$ or 0.01 before starting the Ng steps. Applying the Ng method too soon can produce a subsequent poor convergence rate, or even divergence. The optimum iteration stage to turn on the Ng method depends very much on the type of problem treated, and probably can only be determined with some experimentation. Typically, for the problems we have treated, the optimum starting point occurs about after a number of iterations in the range 15–30.

An important parameter of the Ng method is K_{back}, the number of previous iterations that are used in constructing a single Ng acceleration step. We have found $K_{\text{back}}=5$ to be a good value for our work, but, again, this is probably best determined by experiment with the particular types of problems to be treated.

Conceptually, the simplest way of using the Ng method is to apply it to a set of K_{back} iterations found by the underlying "ordinary" iteration scheme (here ALI). The resulting accelerated iterate is then used to start a new sequence of ordinary iterations; when at least N_{back} of these are determined, the Ng method is again used to give a new accelerated iteration.

However, once started, it is not necessary to wait for K_{back} new ordinary iterates before applying the Ng method, and it can be used for every step. This may seem surprising to those accustomed to acceleration methods that work by extrapolation, such as Aitken's Δ^2-method (see, e.g. Stoer & Bulirsch 1980). Extrapolation methods assume that the iterates follow some simple law in iteration number, such as polynomial or exponential, and it is therefore imporant that the iterates be part of a consistent, analytical progression. The Ng method is quite different in that it works by finding the "best" solution that can be constructed from a linear combination of previous iterates. This best solution depends only on the linear space spanned by these previous iterates and not on their ordering in iteration number. For example, if the iteration numbers of the K_{back} iterations were permuted before applying the Ng method, the results would not change (for extrapolation methods, permuting the iteration numbers would be disastrous!). It is clear that the Ng method does not require a "consistent" set of iterations in the same sense, and, once started, it can be used at every iteration step, even though it initially mixes ordinary and accelerated steps. It is in this form that we have used Ng method here (and in Paper I), and we have found much faster overall convergence that when ordinary iteration steps are interleaved.

It is likely, however, that particularly difficult cases exist where it might be useful to interleave some ordinary iterations between Ng steps, since these will tend to settle the solution down, and possibly prevent a divergence of the iteration scheme. (The same comment may apply to the introduction of some ordinary lambda iteration steps in very difficult cases.)

4. Numerical results

A model helium atom including all three stages of ionization was used as the test problem, with 19 levels of He I ($n\leq 4$) and three of He II. All 31 allowed bound–bound transitions were included, as were all 22 bound-free transitions to the ground state of the next ion. The He I radiative data came from the Opacity Project (Fernley et al. 1987) and the collisional rates for He I were those of Berrington & Kingston (1987). Collisional ionization rate coefficients for ground states were obtained from Bell et al. (1983) and those for the excited states were estimated using the formula of Seaton (1962). Up to 1000 frequencies and one or two angle points per hemisphere were used (up to three points per hemisphere for calculating the emergent fluxes).

For simplicity, and to concentrate on the effect of overlapping transitions, the atmospheric model was taken to be isothermal, with a diffusion-approximation boundary condition at a mass column density of 10 g cm^{-2} (simulating a semi-infinite slab) with constant temperature and mass density. For similar reasons of simplicity, electron scattering was treated in the coherent approximation, which ignores frequency redistribution effects in the lines.

For the particular test problem where $T=2\,10^4$ K, $\rho=10^{-10}$ g cm^{-3} and $n_e=10^{14}$ cm^{-3}, we checked our results against a similar model kindly calculated for us by Keith Butler using an implementation of the method of Auer & Heasley (1976) due to Butler & Giddings (1985). We found substantial agree-

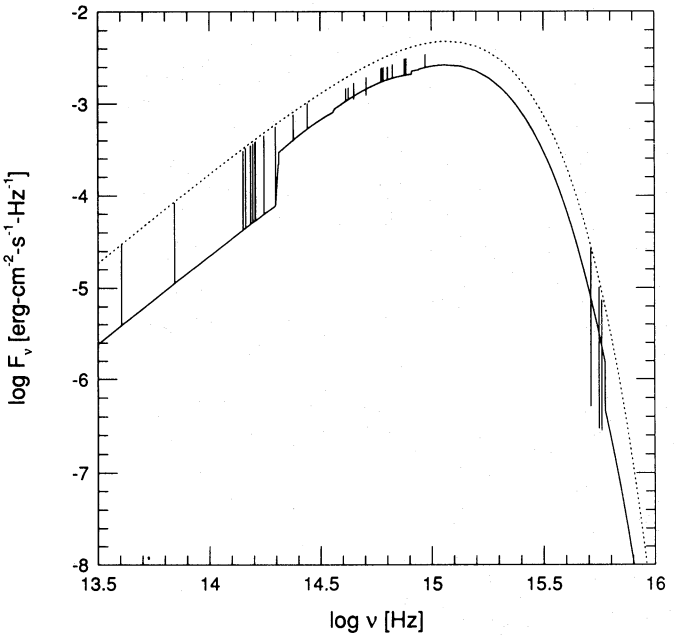

Fig. 1. The emergent flux (solid curve) for pure helium test problem with $T=2\,10^4$ K, $\rho=10^{-10}$ g cm^{-3}, and $n_e=10^{14}$ cm^{-3}. The dotted curve is the emergent flux for a blackbody at $T=2\,10^4$ K. The spectral lines are not resolved, but their positions and range in flux can be clearly seen. The weak emission lines and continua here are mainly due to the Schuster mechanism (see text)

ment between these calculations. The emergent flux calculated by our method for this test problem is given in Fig. 1.

Both the full and the partial preconditioning strategies developed in Sects. 2.3 and 2.4, respectively were coded and tested. For the test problem both strategies required the same number of iterations, although each iteration with full preconditioning required significantly more computer time. Convergence was roughly a factor of two slower than for the 19 Level He I models with similar parameters treated in Paper I.

We also compared the three different methods for treating electron scattering described in Sect. 3. As expected, the lambda iteration method was the slowest in convergence, by about a factor of two. The iteration factor method of Eq. (2.29) converged more quickly but did require quite a bit more storage. The two-stream method of Eq. (2.27) gave the best convergence, but the limitation to two streams produced noticeable deviations from our more accurate calculations with four and six streams. This defect could be presumably be corrected by implementing a multicomponent generalization of Eq. (2.27).

Some models with velocity fields were also computed. Because the code uses the observer's frame, we treated only cases for which the velocities were limited to a few times the thermal ion velocity. The populations for these cases did not differ much from those of the static case, but the emergent fluxes showed substantial effects due to the profile shift in the formal solution. This behavior is consistent with similar results found by other workers.

Although these test models are not meant to apply to any particular physical case, it is interesting in that they exhibit beautifully the Schuster (1905) mechanism. The emergent flux in Fig. 1 shows the strong emission of the weak lines and the weak edges in emission that result when the electron scattering opacity is stronger than the bound–bound or bound–free opacity. One notes that subordinate lines in the region log $\nu \lesssim 14.5$ are formed nearly in LTE, but they still have enough absorptive opacity to dominate the electron scattering opacity. Thus, the emergent fluxes in the cores of these lines are very near to the thermal value (dotted curve). However, the continuum transfer is dominated by scattering opacity, and the continuum emergent flux falls well below the thermal value, giving rise to the emission profiles. A similar discussion applies to the continua that appear in emission.

The helium test problems treated here involve lines and continua that overlap other continua, but not lines that overlap other lines, and they therefore do not yet test the full capabilities of our ALI method. However, since lines and continua are treated in a unified manner in this formalism, there is every reason to expect that the treatment of line–line overlaps will present no difficulties. We are currently planning to apply the method of this paper to molecular line transfer in planetary atmospheres (see e.g. Kutepov et al. 1991), where such line overlaps can be important.

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