

RAPIDLY-CONVERGING METHODS FOR SOLVING MULTILEVEL TRANSFER PROBLEMS

Eugene H. Avrett
Harvard-Smithsonian Center for Astrophysics
60 Garden Street
Cambridge, MA 02138, USA
avrett@cfa.harvard.edu

ABSTRACT

It is well known that lambda iterations can be used to solve multilevel non-LTE transfer equations in a reasonable number of iterations when the lambda operator is preconditioned, e.g., when the diagonal part of the operator is combined with other terms analytically. This approach is currently used successfully for the solution of model atoms with many line transitions, but sometimes a very large number of iterations is needed.

Lambda iteration consists of alternate solutions of the separate transfer and rate equations. For any given line transition the transfer and rate equations can be combined so that a solution can be obtained directly for that transition with no iterations needed between the transfer and rate equations. However, iterations are needed to determine the coupling between transitions. This can be time-consuming for model atoms with a large number of transitions that are treated in this way.

Here we show that 1) a hybrid approach involving such a direct solution for a few of the strongest transitions, and lambda iterations for the rest, gives rapid convergence, often with oscillations that need to be damped, and 2) this approach should include preconditioning of the lambda operator that occurs in the radiative coupling terms.

We illustrate these results with a simple three-level hydrogen atom and a finite, plane-parallel, symmetric atmosphere resembling a solar prominence, with a temperature of 8,000 K at the center, rising to very large values at each boundary (so that hydrogen is only partly ionized at the center and fully ionized at each boundary). Lambda iterations essentially fail to give a solution for this problem, while the hybrid solution converges in 5 to 10 iterations.

I. INTRODUCTION

The fundamental problem to be solved for low-density optically thick atmospheres where local thermodynamic equilibrium cannot be assumed is the simultaneous solution of the rate and transfer equations. The rate equations are used to determine the number densities of various energy levels at any location in the atmosphere given the angle-averaged radiation intensities at that location. The transfer equation is used to determine the radiation intensity at any location and direction given the number densities along a line extending from that location in the opposite direction. For simple problems the rate and transfer equations can be combined and solved directly, but this approach becomes impractical when the number of energy levels and radiative transitions is very large, because the coupling between transitions depends on the solution and must be treated iteratively.

Rather than solving the combined rate and transfer equations, one can iterate between the two. The transfer equation can be solved for the angle- and frequency-integrated mean intensity \bar{J} at each depth given starting values of the number densities throughout the atmosphere. This \bar{J} then can be

used in the rate equations to obtain new number densities everywhere, replacing the starting values. These updated number densities can be used to obtain a new \bar{J} , etc. This is called the lambda iteration method. (The lambda operator is the function used to determine the mean intensity at one depth in terms of source-function values throughout the atmosphere.) Such a direct lambda-iteration method converges too slowly to be practical, but various techniques have been developed to achieve convergence in a reasonable number of iterations.

A comprehensive review of this topic has been provided by Hubeny (2003). The term ‘‘Accelerated Lambda Iteration’’ (ALI) ordinarily refers to removing the diagonal elements (and sometimes principal off-diagonal elements) from the lambda operator and combining these elements analytically with other terms. ‘‘Acceleration’’ thus refers to the faster convergence that results. Typically the convergence is still rather slow, and monotonic, so that purely numerical acceleration techniques can be applied as well.

Here we formulate the ALI method in an equivalent way but with slightly different terminology than used in Hubeny (2003) and in earlier papers. Instead of using the term ‘‘acceleration’’ we refer to the special treatment of diagonal elements as ‘‘preconditioning’’.

We use the simple case of a two-level atom to illustrate the much faster convergence that results from preconditioning, and compare with a direct solution that requires no iteration.

For a three-level case we show how to obtain a direct solution for each transition, and how to derive the coupling terms that relate each transition to the others. We use preconditioning in these coupling terms. Only the strongest transitions need to be solved directly in this way. Preconditioned lambda iterations can be used for weaker transitions. We call this a hybrid approach.

Finally, we show an example for which the ALI method essentially fails, while such a hybrid method converges in 5 to 10 iterations.

II. THE RADIATIVE TRANSFER AND RATE EQUATIONS

The rate equation for level m of an \mathcal{N} -level atom with a continuum is

$$\frac{\partial n_m}{\partial t} + \nabla \cdot (n_m V_m) = \sum_{\substack{\ell=1 \\ \neq m}}^{\mathcal{N}} n_\ell P_{\ell m} + n_\kappa P_{\kappa m} - n_m \left(\sum_{\substack{\ell=1 \\ \neq m}}^{\mathcal{N}} P_{m\ell} + P_{m\kappa} \right) \quad (1)$$

where n_a is the number density of level a , P_{ab} is the transition rate from a to b per atom in level a , κ refers to the next higher ionization stage, and V_m is the mean flow velocity of atoms in level m .

The bound-bound rates are

$$P_{u\ell} = A_{u\ell} + B_{u\ell} \bar{J}_{u\ell} + C_{u\ell}, \quad u > \ell \quad (2)$$

$$P_{\ell u} = B_{\ell u} \bar{J}_{u\ell} + C_{\ell u}, \quad u > \ell \quad (3)$$

where A and B are the Einstein coefficients, $C_{\ell u}$ and $C_{u\ell}$ are the collisional excitation and de-excitation rates, and \bar{J} is the integrated mean intensity for the $u\ell$ transition, which must be calculated from the transfer equation.

The transfer equation for the $u\ell$ line transition is

$$\frac{dI_\nu}{ds} = -\frac{h\nu_{u\ell}}{4\pi} \varphi_\nu [(n_\ell B_{\ell u} - n_u B_{u\ell}) I_\nu - n_u A_{u\ell}] - \kappa_\nu^C I_\nu + \epsilon_\nu^C \quad (4)$$

where s is geometrical depth in the direction of the intensity I_ν . Here, for simplicity, we assume complete frequency redistribution (CRD, i.e., absorption and emission have the same uncorrelated dependence on frequency ν , and have the common profile function φ_ν). Using the well-known relationships between the Einstein coefficients, we can write

$$\frac{dI_\nu}{ds} = -\kappa_\nu^L(I_\nu - S^L) - \kappa_\nu^C(I_\nu - S_\nu^C) \quad (5)$$

where the line absorption coefficient is

$$\kappa_\nu^L = \frac{h\nu_{u\ell}}{4\pi} \varphi_\nu (n_\ell B_{\ell u} - n_u B_{u\ell}) \quad (6)$$

and the line source function is

$$S_{u\ell}^L = \frac{2h\nu_{u\ell}^3/c^2}{(g_u n_\ell / g_\ell n_u) - 1}. \quad (7)$$

For simple illustrative purposes we consider the plane-parallel semi-infinite case for which $\kappa_\nu^C \ll \kappa_\nu^L$. Then the transfer equation reduces to

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S^L \quad (8)$$

where $d\tau_\nu = \kappa_\nu^L dz$, $dz = -\mu^{-1} ds$, and where μ is the cosine of the angle between the direction of I_ν (along ds) and the inward normal direction.

Solving for I_ν in terms of S^L , the mean intensity $J_\nu = \frac{1}{2} \int_{-1}^{+1} I_\nu(\mu) d\mu$ is given by

$$J_\nu(\tau_\nu) = \frac{1}{2} \int_0^\infty E_1(|t - \tau_\nu|) S^L(t) dt, \quad (9)$$

where E_1 is the first exponential integral. The mean intensity can be expressed in the discrete form

$$J_{ik} = \sum_j W_{ijk}^\Lambda S_j^L \quad (10)$$

where i and j are depth indices and k is the frequency index. Various quadrature representations can be used to determine the lambda-operator weighting coefficients W_{ijk}^Λ which depend on the monochromatic optical depths τ_{ik} .

The integrated mean intensity is

$$\bar{J} = \int \varphi_\nu J_\nu d\nu, \quad \int \varphi_\nu d\nu = 1, \quad (11)$$

so that

$$\bar{J} = \sum_j W_{ij}^\Lambda S_j^L, \quad W_{ij}^\Lambda = \int \varphi_\nu W_{ijk}^\Lambda d\nu. \quad (12)$$

The net rate coefficient $\rho_{u\ell}$ is defined by

$$n_u A_{u\ell} \rho_{u\ell} = n_u (A_{u\ell} + B_{u\ell} \bar{J}_{u\ell}) - n_\ell B_{\ell u} \bar{J}_{u\ell}, \quad (13)$$

so that

$$\rho_{u\ell} = 1 - \frac{\bar{J}_{u\ell}}{S_{u\ell}^L}. \quad (14)$$

We can write \bar{J}_i (i.e., \bar{J} at depth i for the $u\ell$ transition) either as

$$\bar{J}_i = \sum_j W_{ij}^\Lambda S_j^L, \quad \text{or as} \quad \bar{J}_i = S_i + \sum_j W_{ij}^{\Lambda-1} S_j^L, \quad (15)$$

where $W_{ij}^{\Lambda-1} = W_{ij}^\Lambda - U_{ij}$ and U_{ij} is the unit matrix. Then we obtain

$$\rho_i = -\frac{1}{S_i^L} \sum_j W_{ij}^{\Lambda-1} S_j^L, \quad (16)$$

to be used in the rate equations in place of $\bar{J}_{u\ell}$.

In this derivation we have assumed that the line source function is frequency-independent, but the general case with partial frequency redistribution (PRD), with the continuum included (and using either plane-parallel or spherical geometry), can be treated by methods very similar to those discussed here. (See Avrett & Loeser 1984.)

III. PRECONDITIONING

Let $W_{ij}^{\Lambda-1} = d_i + W_{ij}^r$ where $d_i = W_{ii}^{\Lambda-1}$ and where W_{ij}^r is the same as $W_{ij}^{\Lambda-1}$ but with zero diagonal elements. Then

$$\rho_i = -d_i - \frac{1}{S_i^L} \sum_j W_{ij}^r S_j^L. \quad (17)$$

From equation (7), the S_i^L term in the denominator (for the $u\ell$ transition) can be written as

$$S_{u\ell}^L = \left(\frac{n_u}{n_\ell}\right) q_{u\ell}, \quad (18)$$

where

$$q_{u\ell} = \left(\frac{g_\ell}{g_u}\right) \frac{2h\nu_{u\ell}^3/c^2}{1 - (g_\ell n_u)/(g_u n_\ell)}. \quad (19)$$

Note that $q_{u\ell}$ has only a secondary dependence on n_u/n_ℓ except when stimulated emission is important. Equation (17) for $\rho_{u\ell}$ at depth i may then be written as

$$n_u \rho_{u\ell} = -n_u d_{u\ell} - n_\ell \chi_{u\ell}, \quad (20)$$

where, at depth i ,

$$\chi_i = \frac{1}{q_i} \sum_j W_{ij}^r S_j^L. \quad (21)$$

Expressing $n_u \rho_{ul}$ in terms of d_{ul} and χ_{ul} in the rate equation gives much better results than using ρ_{ul} obtained directly from S_{ul}^L .

IV. THE SIMPLE TWO-LEVEL ATOM

The time-independent rate equation for a two-level atom without a continuum, and without mass flow, is

$$n_2(A_{21} + B_{21}\bar{J}_{21} + C_{21}) = n_1(B_{12}\bar{J}_{21} + C_{12}), \quad (22)$$

or

$$n_2(A_{21}\rho_{21} + C_{21}) = n_1C_{12}. \quad (23)$$

Using $n_2\rho_{21} = -n_2d_{21} - n_1\chi_{21}$ gives

$$n_2(-A_{21}d_{21} + C_{21}) = n_1(A_{21}\chi_{21} + C_{12}) \quad (24)$$

or

$$\frac{n_2}{n_1} = \frac{A_{21}\chi_{21} + C_{12}}{C_{21} - A_{21}d_{21}}. \quad (25)$$

Let $R = n_2/n_1$ and ignore stimulated emission. Then at depth i ,

$$R_i = \frac{\sum_j W_{ij}^r R_j + \epsilon_i R_i^*}{\epsilon_i - d_i}, \quad (26)$$

where $\epsilon = C_{21}/A_{21}$ and

$$R_i^* = C_{12}/C_{21} = \left(\frac{g_2}{g_1}\right) \exp^{-h\nu_{21}/kT} = n_2^*/n_1^*. \quad (27)$$

This shows that n_2/n_1 approaches the LTE ratio n_2^*/n_1^* at large optical depths, as d_i and W_{ij}^r approach zero.

Thus we can have three forms of the equation for R_i , as a result of:

- 1) preconditioning, using $W_{ij}^r = W_{ij}^{\Lambda-1} - d_i$:

$$R_i = \frac{\sum_j W_{ij}^r R_j + \epsilon_i R_i^*}{\epsilon_i - d_i} \quad (28)$$

- 2) using $W_{ij}^{\Lambda-1}$:

$$R_i = \frac{\sum_j W_{ij}^{\Lambda-1} R_j + \epsilon_i R_i^*}{\epsilon_i} \quad (29)$$

- 3) using the usual lambda operator, W_{ij}^Λ :

$$R_i = \frac{\sum_j W_{ij}^\Lambda R_j + \epsilon_i R_i^*}{1 + \epsilon_i} \quad (30)$$

Example 1:

Let $R_i^* = 1$ and $\epsilon_i = 0.01$ at all depths i :

With preconditioning:

Without preconditioning:

$$R_i = \frac{\sum_j W_{ij}^r R_j + 0.01}{0.01 - d_i}$$

$$R_i = \frac{\sum_j W_{ij}^\Lambda R_j + 0.01}{1 + 0.01}$$

Numerical solution:

τ	0	0.1	1	3	10	30	100
R	0.1	0.123	0.260	0.476	0.842	0.999	1.000

Number of iterations required to reach $R = 0.1 \pm 0.001$ at $\tau = 0$

	<u>With</u> preconditioning	<u>Without</u> preconditioning
initial $R = 1$	76	189
initial $R = 0$	79	334

Alternatively, as shown below, we can solve the set of linear equations for R_i directly without any iterations, and in much less time than required by the preconditioned lambda iterations.

From

$$R_i = \frac{\sum_j W_{ij}^{\Lambda-1} R_j + \epsilon_i R_i^*}{\epsilon_i} \quad (31)$$

we write

$$R_i - \frac{1}{\epsilon_i} \sum_j W_{ij}^{\Lambda-1} R_j = R_i^*. \quad (32)$$

Then, if M_{ij}^{-1} is the inverse of

$$M_{ij} = U_{ij} - \frac{1}{\epsilon_i} W_{ij}^{\Lambda-1}, \quad (33)$$

the solution is

$$R_i = \sum_j M_{ij}^{-1} R_j^*. \quad (34)$$

V. A THREE-LEVEL ATOM

We illustrate the basic properties of the general multilevel case by considering a three-level atom. The rate equations for levels 2 and 3 (again ignoring other stages of ionization for simplicity) are

$$n_2(A_{21}\rho_{21} + C_{21} + C_{23}) = n_1C_{12} + n_3(A_{32}\rho_{32} + C_{32}) \quad (35)$$

and

$$n_3(A_{31}\rho_{31} + C_{31} + A_{32}\rho_{32} + C_{32}) = n_1C_{13} + n_2C_{23}. \quad (36)$$

These two equations can be solved for the two unknowns (n_2/n_1) and (n_3/n_1) if, from the transfer equations, we know the values of ρ_{21} , ρ_{31} , and ρ_{32} . Ordinary lambda iteration consists of successively solving these two rate equations and the three transfer equations.

Alternatively, we can write

$$n_u\rho_{u\ell} = -n_u d_{u\ell} - n_\ell \chi_{u\ell} \quad (37)$$

to get a better-conditioned set of equations. This is the basic preconditioning step, as in the two-level case. The preconditioned rate equations for levels 2 and 3 are

$$n_2(C_{21} - A_{21}d_{21} + C_{23} + A_{32}\chi_{32}) = n_1(C_{12} + A_{21}\chi_{21}) + n_3(C_{32} - A_{32}d_{32}) \quad (38)$$

and

$$n_3(C_{31} - A_{31}d_{31} + C_{32} - A_{32}d_{32}) = n_1(C_{13} + A_{31}\chi_{31}) + n_2(C_{23} + A_{32}\chi_{32}). \quad (39)$$

We can iterate between the χ values and the rate equations, just as in the two-level case, with slow convergence using W_{ij}^A , but with much faster convergence using W_{ij}^T .

Direct numerical solutions for each transition can be used in the multilevel case, just as in the two-level case. The above equations can be written as

$$\left(\frac{n_2}{n_1}\right)(x_{21} + y_{32}) - \left(\frac{n_3}{n_1}\right)x_{32} = y_{21}, \quad (40)$$

and

$$-\left(\frac{n_2}{n_1}\right)y_{32} + \left(\frac{n_3}{n_1}\right)(x_{31} + x_{32}) = y_{31}, \quad (41)$$

where

$$y_{u\ell} = C_{\ell u} + A_{u\ell}\chi_{u\ell}, \quad (42)$$

and

$$x_{u\ell} = C_{u\ell} - A_{u\ell}d_{u\ell}. \quad (43)$$

Then we can eliminate n_3/n_1 to obtain

$$\left(\frac{n_2}{n_1}\right)(x_{21} + \bar{x}_{21}) = y_{21} + \bar{y}_{21}. \quad (44)$$

Finally, the coefficients ϵ_{21} and B_{21}^S in the expression

$$S_{21}^L = \frac{\bar{J}_{21} + \epsilon_{21}B_{21}^S}{1 + \epsilon_{21}} \quad (45)$$

can be expressed in terms of the x and y coefficients. The results are

$$\epsilon_{21} = \epsilon_{21}^a - \beta_{21}\epsilon_{21}^b, \quad \beta_{21} = e^{-h\nu/kT}, \quad (46)$$

and

$$B_{21}^S = \alpha_{21}\beta_{21}(\epsilon_{21}^b/\epsilon_{21}), \quad \alpha_{21} = 2h\nu_{21}^3/c^2, \quad (47)$$

where

$$\epsilon_{21}^a = \frac{1}{A_{21}}(C_{21} + \bar{x}_{21}), \quad \epsilon_{21}^b = \frac{g_1}{g_2\beta_{21}A_{21}}(C_{12} + \bar{y}_{21}). \quad (48)$$

Then, from equation (45), we can obtain n_2/n_1 at each depth i from the solution of the set of equations

$$S_i^L - \frac{1}{\epsilon_i} \sum_j W_{ij}^{\Lambda-1} S_j^L = B_i^S. \quad (49)$$

Here ϵ and B^S depend on χ_{31} and χ_{32} , but not on χ_{21} .

We can derive similar equations for S_{31}^L that depend on χ_{21} and χ_{32} , and for S_{32}^L that depend on χ_{21} and χ_{31} .

The direct approach applied to each of the transitions would consist of assuming initial values of χ_{21} , χ_{31} , and χ_{32} , and solving each set of simultaneous equations to get S_{21}^L , S_{31}^L , and S_{32}^L , thus giving new iterative values of χ_{21} , χ_{31} , and χ_{32} from equation (21). (Equation 21 represents the solution of the transfer equation.)

Preconditioned lambda iteration in this case would consist of substituting the initial χ values into equations (40) and (41) to obtain n_2/n_1 and n_3/n_1 at each depth, and then using equation (21) to obtain new χ values. Each lambda iteration needs fewer computations than the direct approach, but many more iterations are required, and sometimes the lambda iterations do not converge.

It is not necessary to apply the direct approach to all transitions, only to the strongest ones that control the large-scale behavior of the solution. Thus in Example 2 below we use such a hybrid method, solving the simultaneous equations for S_{21}^L and S_{31}^L but using preconditioned lambda iteration for the 32 transition, i.e., the χ_{32} used in equations (40) and (41) is determined directly from n_3/n_2 rather than by solving the set of simultaneous equations for S_{32}^L .

The derivation given above for a three-level atom with no continuum can be extended without difficulty to cases with an arbitrary number of bound levels together with other stages of ionization.

Example 2:

Consider a 3-level hydrogen atom with a continuum (i.e., with the bound-free rates in equation 1 included), and a finite, symmetric atmosphere extending over the geometrical depth range $-700 \leq s(\text{km}) \leq +700$, with the total hydrogen density $n_H = 10^{11} \text{cm}^{-3}$, constant with depth, and the temperature varying as $T = 8000 \exp(s^2/10^5)$, so that $T = 8000$ K at $s = 0$, and $T = 10^6$ K at $s = \pm 700$. In this case $n_H \approx n_e \approx n_p$. Let n_1 represent the number density of hydrogen atoms in level 1 calculated from 1) the rate equations that include the bound-free transitions, and 2) the transfer equations for continuum radiation as well as line radiation.

Numerical solution: $n_1 = 2.4 \times 10^4$ at each surface

$$n_1 = 5.6 \times 10^6 \text{ at the center}$$

Total line-center optical thickness: $\tau_{21} = 19$, $\tau_{31} = 3.0$, $\tau_{32} = 0.0027$

Note that in this example there are large temperature variations, but not large optical depths.

Parameters of the (21)-line solution:

	<u>surface</u>	<u>center</u>
ϵ	1.4×10^{-4}	1.4×10^{-5}
B	1.9	8.3×10^{-8}
S	4.9×10^{-7}	1.3×10^{-6}

Results for two methods of solution:

Case I

Direct solutions for (21) and (31)
Preconditioned lambda iterations for (32).

< 0.1% convergence
after 8 iterations;
solution oscillating
with diminishing changes

computer time 10 min.

Case II

Preconditioned lambda iterations
for (21), (31), and (32)

far from convergence
after 50 iterations;
 $n_2(\text{center}) = 19100$ and slowly
decreasing toward the
correct value of 129

computer time > 50 min.

VI. CONCLUSIONS

1. We illustrate the well-known improvement in lambda-iteration solutions that results from preconditioning.
2. The strongest line transitions of a multilevel atom should be treated by solving the simultaneous equations corresponding to the combined rate and transfer equations, and not by lambda iteration.
3. Preconditioning should be used to determine the coupling between transitions that are needed in the simultaneous-equation solutions.

The methods described here are used in the Pandora atmosphere program (Avrett & Loeser 2003). I am very grateful to Rudolf Loeser for his continued collaboration in this work.

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