

## SOLUTIONS TO RADIATIVE TRANSFER PROBLEMS USING APPROXIMATE LAMBDA OPERATORS

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### ABSTRACT

Two new techniques for obtaining solutions to non-LTE problems are developed. The essence of the first technique is that the core-saturation approximation, the Eddington-Barbier relation, and the upper boundary condition are used to derive a simple first-order differential equation for  $S_l$ . This approximate equation is solved analytically for a two-level atom in an atmosphere with constant properties and zero continuum opacity. The correct surface source function,  $S_l(0) = (\epsilon)^{1/2}B$ , and the correct thermalization depth are obtained.

Second, we develop a new efficient perturbation technique for numerical solutions to non-LTE problems. Using a linear test function, a one-point quadrature relation between  $I_\nu$  and  $S_\nu$  is derived. From this relation it is possible to obtain an approximate solution of the transfer equation with a small amount of computing time. Higher order correction terms are then obtained from a perturbation series or by iteration using LTE techniques. A 1% accuracy in  $S_l$  is usually obtained after approximately four iterations. The computing time required to solve a one-dimensional non-LTE problem with velocity fields for a two-level atom is of the order of 5 times the computing time required to solve the corresponding LTE problem.

*Subject headings:* line formation — numerical methods — radiative transfer

### I. INTRODUCTION

The present paper deals with the solution of the non-LTE radiative transfer equation in situations where the source function,  $S_\nu$ , may be expressed as

$$S_\nu = \frac{\phi_\nu}{\phi_\nu + r} S_l + \frac{r}{\phi_\nu + r} B. \quad (1)$$

Here,  $\phi_\nu$  is the line absorption profile normalized to unit area, and  $r$  is the ratio between the continuum and the integrated line opacities. The frequency  $\nu$  is measured in units of the Doppler width.  $B$  is the Planck function, and  $S_l$  is the line source function, which can be written as (cf. Athay 1972a)

$$S_l = \frac{\langle J \rangle + \epsilon^* B}{1 + \epsilon^\dagger}. \quad (2)$$

In this expression,  $\epsilon^*$  and  $\epsilon^\dagger$  are related to the various creation and destruction mechanisms of photons. The mean intensity  $\langle J \rangle$  is defined as

$$\langle J \rangle = \frac{1}{2} \int_{-1}^1 \int_{-\infty}^{\infty} \phi_\nu I_\nu d\mu d\nu, \quad (3)$$

where  $I_\nu$  is the specific intensity. Using this general expression for  $\langle J \rangle$ , we may account for the effect of velocity fields on the specific intensity.

The difficulty of solving the transfer equation is a result of the homogeneous term  $\langle J \rangle$ . Mathematically, this term produces a coupling between different frequencies and angles at each depth. Physically, this coupling is caused by scattering events during which photons, absorbed at a certain frequency and angle, are reemitted at other frequencies and in all directions. A small number of photons are emitted far out in the wings, where the opacity is low. These photons travel large distances before they are reabsorbed. This leakage of photons in the wings leads to interactions over very large distances. The nonlocal behavior of the radiation field is the main cause of the numerical difficulties of solving the transfer equation when  $\epsilon^*$  and  $\epsilon^\dagger$  are much smaller than unity.

In the past, a number of methods have been developed to solve the transfer equation. Here we shall mention only those which are related to the present work. The first method, developed by Rybicki (1971), is called the core-saturation method. The essence of this method is that inactive photons are removed from the transfer problem by the approximation

$$I_\nu = S_\nu, \quad (4)$$

in the core of the line. This approximation is based on the fact, mentioned earlier, that wing photons are very efficient in transferring radiation, whereas core photons

play an essentially passive role (Osterbrock 1962; Rybicki and Hummer 1969). Using this approximation, Rybicki derived an expression for  $S_l$  which involves only the radiation field in the wings of the line. Here and in the following, the wings of a line are defined as those frequencies and angles for which

$$\tau_\nu < \gamma, \quad (5)$$

where  $\tau_\nu$  is the monochromatic optical depth, and  $\gamma$  is a free parameter, the value of which should be on the order of unity. The equation for  $S_l$  is solved by direct iteration. Thus, the use of machine core storage is minimal and there is no need for matrix inversions. The drawback of the method is that, in order to make the approximation  $I_\nu = S_\nu$  sufficiently good for a high accuracy in the final solution, it is necessary to choose a relatively large  $\gamma$ . This, of course, decreases the rate of convergence of the lambda iteration, so that typically 40–50 iterations are needed for a 1% accuracy in  $S_l$ . The core-saturation method has been successfully applied to two-dimensional problems by Stenholm (1977).

An entirely different approach to radiative transfer problems is developed by Athay (1972*b*, 1976) and Delache (1974). Using probabilistic arguments, these authors derive a simple first-order differential equation for the quantity  $\langle J \rangle$ . This equation can be solved analytically in certain situations. However, the solutions are accurate only to within a factor of 2. Also, it is somewhat unsatisfactory that probabilistic arguments are used to derive this equation, since the transfer equation contains *all* relevant physics. Thus, it must be possible to derive an equation for  $\langle J \rangle$  directly from the transfer equation, provided some suitable approximations are made. This was done by Frisch and Frisch (1975) in a beautiful paper. These authors derive an equation for  $S_l$  which gives very good agreement with numerical solutions of the transfer equation.

Finally, we mention the perturbation technique of Cannon (1973*a*, *b*). This method consists of replacing the integral over frequency and angle by a quadrature sum of a much lower order than is normally required for a given accuracy. This is equivalent to replacing the ordinary lambda operator  $\Lambda$  by a more approximate operator  $\Lambda^*$ , such that

$$S_l = \Lambda S_l + \epsilon B = \Lambda^* S_l + \epsilon B + (\Lambda - \Lambda^*) S_l. \quad (6)$$

The last term is considered to be a small error term, which is calculated iteratively or by using a perturbation technique. Note that in contrast to the core-saturation method, the accuracy of the final solution is independent of the choice of  $\Lambda^*$  if the solution converges. The advantage of Cannon's method is that the required matrices and their inverses corresponding to  $\Lambda^*$  can be calculated much more rapidly than those corresponding to  $\Lambda$ . The extra time required to solve for the correction terms is insignificant.

In the present work, we will first derive a simple equation for  $S_l$  using three approximations, one of which is the core-saturation approximation. We then use a technique similar to that of Cannon (1973*a*, *b*) to obtain more accurate solutions. Finally, some refinements and generalizations are made, resulting in a simple and very efficient method for solving non-LTE problems.

## II. AN APPROXIMATE EQUATION FOR $S_l$

In this section we shall derive a simple first-order differential equation for  $S_l$  directly from the transfer equation. It is a well-known fact that virtually all solutions of the transfer equation display the same three characteristic properties for semi-infinite atmospheres with no incident radiation:

$$I_\nu \approx S_\nu, \quad \tau_\nu \gg 1; \quad (7)$$

$$\frac{F}{R} : \text{constant}; I_\nu \approx S_\nu(\tau_\nu = 1), \quad \tau_\nu \ll 1, \mu > 0; \quad (8)$$

$$I_\nu \approx 0, \quad -\tau_\nu \ll 1, \mu < 0. \quad (9)$$

Note that the monochromatic optical depth,  $\tau_\nu$ , is calculated along a ray, i.e.,

$$d\tau_\nu = (\phi_\nu / r + 1) d\tau / \mu, \quad (10)$$

where  $\tau$  is the *continuum* optical depth. The first of the above relations is the core-saturation approximation discussed in § I. The second relation is the Eddington-Barbier relation, which is valid for the emergent radiation at  $\tau_\nu = 0$ . However, this relation is approximately valid also for the interior radiation field if  $\tau_\nu$  is less than unity. The third relation is the upper boundary condition, which of course has an important influence on  $S_l$ .

We now assume that  $\phi_\nu$  and  $r$  are independent of  $\tau$  and  $\mu$ . Then we can write

$$\langle J \rangle = \int_{-\infty}^{\infty} J_\nu \phi_\nu d\nu, \quad (11)$$

and

$$\tau_\nu = \tau(\phi_\nu / r + 1) / \mu. \quad (12)$$

Integrating equation (7) over  $\mu$ , we obtain an approximate relation between  $J_\nu$  and  $S_\nu$ , valid in the core of the line (Rybicki 1971):

$$J_\nu \approx S_\nu, \quad \tau_\nu > 1. \quad (13)$$

To calculate a similar relation between  $J_\nu$  and  $S_\nu$  valid in the wings of the line, we employ the *test function*

$$S_\nu = a + b\tau. \quad (14)$$

Using equations (8), (12), and (14), we obtain

$$I_\nu = a + b\mu / (\phi_\nu / r + 1), \quad (15)$$

for  $\mu > 0$ . Integrating equations (15) and (9) over  $\mu$ , we find

$$J_\nu = \frac{1}{2} \left[ a + \frac{1}{2} b / (\phi_\nu / r + 1) \right] \quad (16)$$

Comparing this expression to equation (14), we obtain

$$J_\nu(\tau) \approx \frac{1}{2} S_\nu(\tau') \quad (17)$$

which can be considered a *one-point quadrature formula*, valid in the wings of the line. The depth  $\tau'(\nu)$  is given by

$$\tau'(\nu) = [2(\phi_\nu / r + 1)]^{-1}. \quad (18)$$

Note that  $\tau'$  is independent of  $\tau$ .

We can now relate  $\langle J \rangle$  to  $S_\nu$  by writing

$$\langle J \rangle = \langle J_c \rangle + \langle J_w \rangle \equiv \int_{\text{core}} J_\nu \phi_\nu d\nu + \int_{\text{wings}} J_\nu \phi_\nu d\nu. \quad (19)$$

The transition between the core and the wings is defined by the frequency,  $\nu_c$ , for which  $\tau'(\nu) = \tau$ . Comparing equation (18), we find that

$$\phi_{\nu_c} = r(1/2\tau - 1) = \nu_c'(\tau') \quad (20)$$

Inserting equations (13) and (17) into (19), we can write

$$\langle J \rangle \approx \int_{\text{core}} S_\nu \phi_\nu d\nu + \frac{1}{2} \int_{\text{wings}} S_\nu(\tau') \phi_\nu d\nu. \quad (21)$$

Using equations (1) and (2), we finally obtain an approximate equation for  $S_\nu$ :

$$\begin{aligned} (1 + \epsilon^\dagger) S_\nu - \epsilon^* B = & 2 \int_0^{\nu_c} \left[ \frac{\phi_\nu}{\phi_\nu + r} S_\nu + \frac{r}{\phi_\nu + r} B \right] \phi_\nu d\nu \\ & + \int_{\nu_c}^\infty \left[ \frac{\phi_\nu}{\phi_\nu + r} S_\nu(\tau') + \frac{r}{\phi_\nu + r} B(\tau') \right] \\ & \times \phi_\nu d\nu, \end{aligned} \quad (22)$$

where  $\nu_c = \nu_c(\tau)$ , and  $\tau' = \tau'(\nu)$ . The wing integral in this equation contains the long-range interactions resulting from the efficient transfer of radiation by the wing photons. Note also that the upper boundary condition is included in the wing integral. Thus, the above approximate equation indeed contains the *basic* mechanisms of radiation transport in spectral lines.

### III. THE PSEUDO-LINE TRANSFER EQUATION

Equation (22) is a simple integral equation for the line source function  $S_\nu$ . It can very easily be converted into a general differential equation. However, here we shall only study the two-level atom with no continuum. In this case, we have  $r=0$  and

$$\epsilon^* = \epsilon^\dagger = \epsilon', \quad (23)$$

where  $\epsilon'$  is the photon destruction probability. Equation (22) simplifies to

$$(1 + \epsilon') S_\nu - \epsilon' B = 2 S_\nu \int_0^{\nu_c} \phi_\nu d\nu + \int_{\nu_c}^\infty S_\nu(\tau') \phi_\nu d\nu. \quad (24)$$

Noting the normalization of  $\phi_\nu$ , we find that

$$\epsilon' (S_\nu - B) = -2 S_\nu \int_{\nu_c}^\infty \phi_\nu d\nu + \int_{\nu_c}^\infty S_\nu(\tau') \phi_\nu d\nu. \quad (25)$$

It is particularly convenient to use the probability of photon escape,  $P_e$  (Osterbrock 1962),

$$P_e(\tau) = \int_{\nu_c(\tau)}^\infty \phi_\nu d\nu \quad (26)$$

as depth variable.  $P_e$  is equal to the probability that a photon is emitted outward ( $\mu > 0$ ) in the optically thin wings of the line. We obtain

$$\epsilon' (S_\nu - B) = -2 S_\nu P_e + \int_0^{P_e} S_\nu dP_e', \quad (27)$$

which has a simple interpretation: The number of photons created or destroyed at a depth,  $\tau$ , is balanced by a leakage of photons in the wings of the line minus a similar inflow of radiation coming from all other depths. Since the leakage is isotropic while the inflow comes only from below, the former flux tends to be twice as large as the latter, which is the reason why  $S_\nu$  usually is smaller than  $B$ . Note that this interpretation is in conflict with the derivation of Delache (1974). He derives an approximate equation for  $\langle J \rangle$ , using the  $(N)^{1/2}$  law for random walks or diffusion processes. However, this argument is incorrect (cf. Frisch and Frisch 1975). In our derivation the only probability of importance is the probability  $P_e$  that a photon is emitted in the wings. Such an emission is the *only* mechanism in our equation by which a photon may be transferred from one depth to another.

Equation (27) can be written as a differential equation:

$$(\epsilon' + 2P_e) \frac{dS_\nu}{dP_e} = -S_\nu + \epsilon' \frac{dB}{dP_e} - (S_\nu - B) \frac{d\epsilon'}{dP_e}. \quad (28)$$

Assuming that  $\epsilon'$  and  $B$  are independent of  $P_e$ , the solution of this simple equation is

$$S_l = B[\epsilon' / (\epsilon' + 2P_e)]^{1/2}. \quad (29)$$

This solution is remarkable, since it gives the correct thermalization depth,  $S_l \rightarrow B$  at  $P_e \approx 1/2\epsilon'$ , and the exact value for the source function at the surface:

$$S_l(\tau_o = 0) = S_l(P_e = \frac{1}{2}) = B[\epsilon' / (\epsilon' + 1)]^{1/2} = B\epsilon^{1/2}, \quad (30)$$

where  $\tau_o$  is the integrated line opacity. Solutions similar to equation (29) have been obtained by Ivanov (1973) and Frisch and Frisch (1975), who used other methods of derivation.

The simplicity of equation (28) suggests that  $P_e$  is the most natural depth variable. The solutions expressed in terms of this variable are independent of the type of line profile considered. However, it is customary to express  $S_l$  in terms of  $\tau_o = \tau/r$ . The transformation between  $P_e$  and  $\tau_o$  is given by equation (26), where  $\nu_c$  now is defined by

$$\tau_{\nu_c} = \tau_o \phi_{\nu_c} = \frac{1}{2}. \quad (31)$$

For a pure Doppler profile  $P_e \propto \tau_o^{-1}$ , whereas for a Voigt profile  $P_e \propto \tau_o^{-1/2}$  (cf. Rybicki 1971). Thus, our approximate equation for  $S_l$  gives

$$S_l \propto \tau_o^{1/2} \text{ (Doppler);} \quad (32)$$

$$S_l \propto \tau_o^{1/4} \text{ (Voigt),} \quad (33)$$

when  $2P_e \gg \epsilon'$ . This result is in excellent agreement with numerical calculations.

In spite of the crudeness of our approximations, we have been able to derive an equation for  $S_l$  which is simple to solve and yet gives surprisingly accurate results regarding the depth variation of  $S_l$ . This shows that the basic physics of radiation transport in spectral lines has been retained in spite of the rather crude treatment. In particular we have been able to show explicitly that the source function is controlled by the exchange of photons between distant parts of the atmosphere, and that this exchange occurs in the transparent wings of the line. The solution obtained here is valid for the simple case when  $r=0$  and when  $\epsilon'$  and  $B$  are depth-independent. However, there is no reason why equation (22) should be inappropriate in more complicated situations, since our *basic* assumptions are not in any way less valid if  $r \neq 0$  or if  $\epsilon'$  and  $B$  vary with depth.

As far as we know, the method for solving non-LTE problems presented here is new, even though the approximations on which the method is based are all

well-known. Our simple approach to the derivation of an equation for  $S_l$  is more straightforward than the heuristic derivations of Athay (1972*b*, 1976) and Delache (1974). These authors derive an equation for  $S_l$  using widely different arguments. The results obtained from their equation are less accurate than those presented here. The derivations of Ivanov (1973) and Frisch and Frisch (1975) are elegant and more rigorous but also more complicated than ours. Their solutions contain a more accurate definition of the escape probability, but basically the equation obtained by these authors is identical to the one derived here, even though the methods of derivation are entirely different.

#### IV. THE VALUE OF $\gamma$

We have derived an equation for  $S_l$  by employing a linear test function,  $S_l = a + b\tau$ . Using this function, we found a value of 0.5 for  $\gamma$ . As we have seen, this somewhat arbitrary test function gives accurate results. However, we point out that there can be no unique choice of the value of  $\gamma$ , since this parameter does in fact depend on the source function itself. Therefore, we have calculated  $S_l(\tau_o)$  obtained from equations (26) and (29), using the wing approximation

$$J_\nu = \frac{1}{2} S_\nu(\tau_\nu = \gamma) \quad (34)$$

for different values of  $\gamma$ . The frequency  $\nu_c$  was determined from the equation

$$\tau_{\nu_c} = \tau_o \phi_{\nu_c} = \gamma. \quad (35)$$

In Figure 1, we show  $S_l(\tau_o)$  obtained from our equations together with the exact solutions obtained by Avrett and Hummer (1965). We have made calculations for  $B=1$ ,  $r=0$ , and  $\epsilon=10^{-4}$ , using  $\gamma=0.5$  and 1.0 for a pure Doppler profile and for a Lorentz profile with  $\gamma=0.25$  and 0.5. It can be seen from the figure that the best overall agreement occurs for  $\gamma \approx 0.45-0.8$ , which is in good agreement with our earlier estimate. We can also see that the approximate solution does not depend too strongly on the value of  $\gamma$ . In particular, we note that the surface value of  $S_l$  is independent of  $\gamma$ .

The core-saturation approximation works very well in the optically thick parts of the line, and the wing approximation is rather accurate in the far wings, where  $\tau_\nu \ll 1$ . Both of these approximations are poor near the transition between the core and the wing, where  $\tau_\nu \approx 1$ . Therefore, the errors in the approximate solution for  $S_l$  always tend to be largest for  $\tau_o \approx \gamma$ . Also, we see from Figure 1 that  $S_l$  is constant above  $\tau_o \approx \gamma$ . The reason for this is that the wing approximation is equivalent to ignoring all emissions and absorptions above the depth where  $\tau_\nu = \gamma$ . Thus, effectively the atmosphere ends at  $\tau_o \approx \gamma$ . Later we shall see how this inconvenience may be removed.

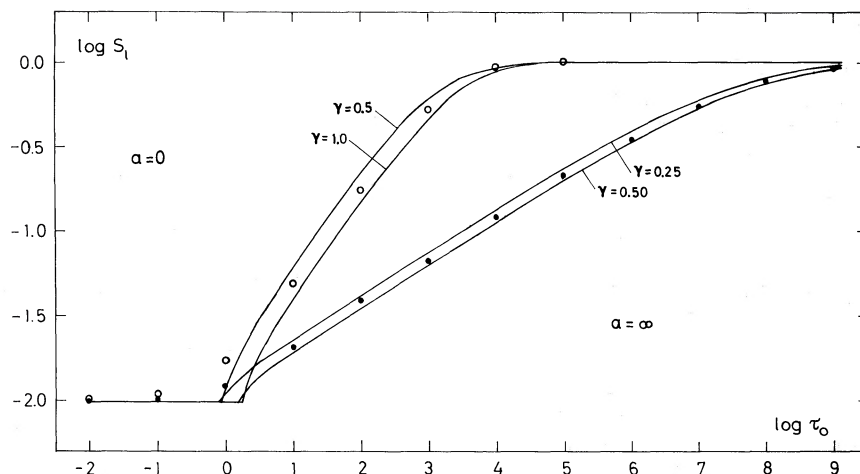


FIG. 1.— $S_l(\tau_0)$  obtained from eqs. (29), (34), and (35) for different values of  $\gamma$ . The calculations were made with  $\epsilon = 10^{-4}$  for a pure Doppler profile ( $a=0$ ) and for a Lorentz profile ( $a=\infty$ ). Shown are also the more exact calculations of Avrett and Hummer (1965) (dots and circles).

#### V. AN ITERATIVE SOLUTION OF THE TRANSFER EQUATION

To find the correct variation of the source function with depth, we must use the *exact* relation

$$J_\nu = \Lambda_\nu S_\nu, \quad (36)$$

where  $\Lambda_\nu$  is the monochromatic lambda operator. Our approximate equation for  $\langle J \rangle$  results from replacing  $\Lambda_\nu$  by the more approximate operator  $\Lambda_\nu^*$ :

$$\Lambda_\nu^* = \begin{cases} 1, & \tau_\nu > \gamma; \\ \frac{1}{2} \int d\tau_\nu \delta(\tau_\nu - \gamma), & \tau_\nu < \gamma. \end{cases} \quad (37)$$

As we have seen, this approximation gives a rather good accuracy. The advantage of the operator  $\Lambda_\nu^*$  is that it results in an equation for  $S_l$  which is very rapidly solved numerically. We therefore propose a method for solving the transfer equation which is similar to the technique of Cannon (1973*a, b*). We rewrite equation (36) in the form

$$J_\nu = \Lambda_\nu^* S_\nu + (\Lambda_\nu - \Lambda_\nu^*) S_\nu. \quad (38)$$

Calculating  $\langle J \rangle$ , we find

$$\langle J \rangle = \int_{-\infty}^{\infty} \phi_\nu \Lambda_\nu^* [S_\nu] d\nu + \int_{-\infty}^{\infty} \phi_\nu (\Lambda_\nu - \Lambda_\nu^*) [S_\nu] d\nu. \quad (39)$$

Inserting equations (1) and (2), we obtain

$$\begin{aligned} (1 + \epsilon^\dagger) S_l &= \int_{-\infty}^{\infty} \phi_\nu \Lambda_\nu^* \left[ \frac{\phi_\nu}{\phi_\nu + r} S_l \right] d\nu \\ &= \epsilon^* B + \int_{-\infty}^{\infty} \phi_\nu \Lambda_\nu \left[ \frac{r}{\phi_\nu + r} B \right] d\nu \\ &\quad + \int_{-\infty}^{\infty} \phi_\nu (\Lambda_\nu - \Lambda_\nu^*) \left[ \frac{\phi_\nu}{\phi_\nu + r} S_l \right] d\nu. \end{aligned} \quad (40)$$

This equation is solved by iteration: The “error” term involving the operator  $(\Lambda_\nu - \Lambda_\nu^*)$  is first put equal to zero, which gives an initial solution  $S_l^{(0)}$ . Then this solution is used to recalculate the error term. The process is iterated until convergence. It should be pointed out that the operator  $\Lambda_\nu$  is never calculated *explicitly*. The terms involving  $\Lambda_\nu$  are instead obtained simply by calculating  $\langle J \rangle$  from the *known* source functions:

$$S_{\nu_1} = \frac{r}{\phi_\nu + r} B, \quad \text{or} \quad S_{\nu_2} = \frac{\phi_\nu}{\phi_\nu + r} S_l, \quad (41)$$

using the Feautrier LTE technique. Thus, the only matrix which is calculated and inverted explicitly is that corresponding to  $\Lambda_\nu^*$ .

To calculate numerically the operator  $\Lambda_\nu^*$ , we must know the frequencies,  $\nu_j$ , which separate the core from the wings at each depth point,  $\tau_j$ . Thus, the frequencies  $\nu_j$  are determined from the equations

$$\tau_j(\tau_j) = \gamma, \quad j \geq j_0, \quad (42)$$



where  $\tau_o$  is the first depth point for which the line is optically thick at the frequency  $\nu=0$ .

The integrals over frequency are replaced by quadrature formulae. To avoid interpolations, the set of frequencies defined by equation (42) were used as quadrature points. This makes the numerical representation of the  $\Lambda_\nu^*$  operator particularly simple:

$$\Lambda_\nu^*[f(\nu, \tau)] \rightarrow \begin{cases} f_{jk}, & k \geq j, \\ f_{jj}, & k \leq j, \end{cases} \quad (43)$$

where the index  $k$  corresponds to the depth variable  $\tau$ , and the index  $j$  to the frequency  $\nu$ . The frequency quadrature weights are calculated from the trapezoidal rule. However, it must be noted that the operator  $\Lambda_\nu^*$  is discontinuous at the transition between the core and the wing.

Equation (40) can be written as a matrix equation in the standard form:

$$\Lambda^*s = e, \quad (44)$$

where the vector  $s$  corresponds to the line source function, and  $e$  to the right-hand side of equation (40). The matrix  $\Lambda^*$  is an upper triangular matrix, i.e., there are no terms below the diagonal. The reason for this desirable property is that  $\tau' > \tau$ , which implies that  $S_l(\tau)$  is controlled solely by sources below  $\tau$ . Equation (44) therefore can be solved by back substitution, which requires very little computing time.

The proposed method was tested for a number of cases with a variable Planck function. In all cases studied,  $S_l$  converged to a 1% accuracy after 6–12 iterations. This compares favorably with the core-saturation method

of Rybicki (1971). To achieve convergence, it was always necessary to choose a  $\gamma$ -value in excess of 0.5. For a Voigt profile with  $a=0.1$ , we obtained a 1% accuracy after only six iterations using a  $\gamma$ -value of 1.0. However, to obtain convergence for a pure Doppler profile, it was necessary to increase  $\gamma$  to about 2.0, which increased the number of iterations to 12. In Figure 2, examples of two such calculations are shown with  $r=0$  and a variable Planck function:  $\log B_\nu = 1.69 - 0.153 \log \tau_o$ . In both cases  $\gamma$  was equal to 2.0. It can be seen that convergence is global and quite rapid. Another notable feature is that the convergence is slowest near  $\tau_o = 1$ , where the initial error is largest. This is because of the poor treatment of the transition between the core and the wings.

The reason for the instability at low  $\gamma$ -values is probably the following: By making  $\Lambda^*$  triangular, we are making the approximation that  $S_l$  is controlled locally and from below. Regarding the numerical value of the source function, this is a rather good approximation, as seen from the high accuracy of the initial solution. However, this approximation ignores the fact that some fraction of the radiation field at  $\tau$  always is from sources above  $\tau$ . Thus, when using  $\Lambda^*$  to correct for the errors of the previous iteration, we may come to a point where most of the true error is caused by an error in  $S_l$  above  $\tau$ , whereas  $\Lambda^*$  interprets the error as being caused by an error in  $S_l$  below  $\tau$ . At this point the instability starts to grow unless the change of  $S_l$  from one iteration to the next is damped. Since  $S_l$  is controlled by transfer of radiation in the wings, increasing  $\gamma$  leads to a damping of the correction terms which stabilizes the solution. However, this also decreases the rate of convergence. To completely get rid of the instability, it is probably necessary to include terms below the diagonal in the matrix  $\Lambda^*$ .

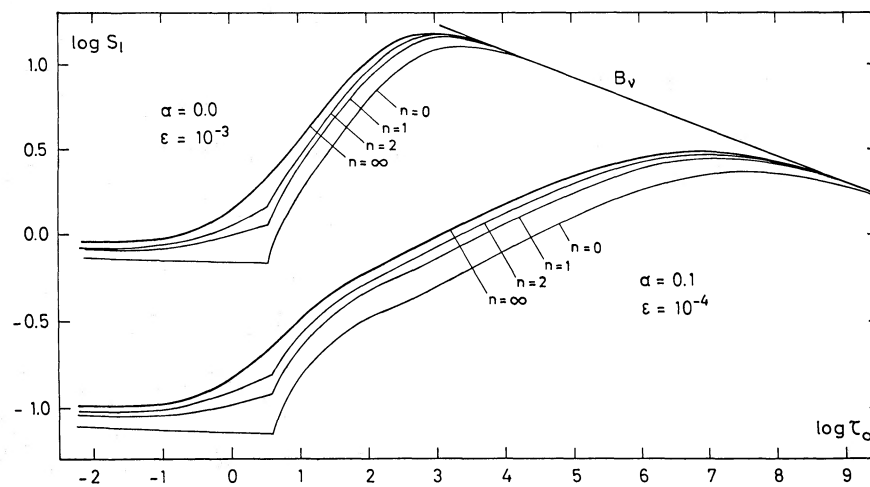


FIG. 2.—The convergence of  $S_l(\tau_o)$  in the case of a variable Planck function for a pure Doppler profile ( $a=0$ ) and a Voigt profile ( $a=0.1$ ). In order to obtain convergence,  $\gamma=2$  was chosen. Using  $\gamma=0.5$  gives a much better initial accuracy, but after one or two iterations the solution becomes unstable.

Nevertheless, the proposed method works very well, provided a sufficiently large  $\gamma$  is chosen. The numerical implementation of the method is very simple. The computing time required to solve a one-dimensional problem scales as

$$c_1 n_\nu n_\tau + n_{it} (c_2 n_\mu n_\nu n_\tau + c_3 n_\tau^2), \quad (45)$$

where  $n_\nu$  is the number of frequencies,  $n_\mu$  the number of angles,  $n_\tau$  the number of depth points, and  $n_{it}$  the number of iterations. The total time is equal to the time required to calculate the matrix  $\Lambda^*$ , the time required to calculate  $\langle J \rangle$  from a known source function, and the time required to solve a triangular system of equations. In actual practice, about 90–95% of the time is used for the calculation of  $\langle J \rangle$ . The total computing time required is therefore a factor of 7–13 greater than the time required to solve the corresponding LTE problem. The storage requirements are modest, since the only matrix stored is  $\Lambda^*$ . If the available core storage is very small, it is possible to recalculate  $\Lambda^*$  during each iteration, since the time required to do so is very short. In this case, only vectors of length  $n_\tau$  need to be stored.

#### VI. AN IMPROVED QUADRATURE FORMULA

The main disadvantages of the operator  $\Lambda_\nu^*$  are the discontinuity at the transition between the core and the wings and the failure to account for the presence of sources located above  $\tau$ . Also, this operator is not well suited for situations where the velocity of the gas is nonzero.

In this section we will derive an improved quadrature formula of the type

$$I_\nu(\tau, \mu, \nu) = W(\tau, \mu, \nu) S_\nu[\tau'(\tau, \mu, \nu), \mu, \nu], \quad (46)$$

which does not have the inconvenient properties of the  $\Lambda_\nu^*$  operator. This allows us to solve the transfer equation in situations where  $\phi$  depends on  $\mu$ , as well as on  $\tau$  and  $\nu$ , and thus where  $\langle J \rangle$  must be written as

$$\langle J \rangle(\tau) = \frac{1}{2} \int_{-1}^1 \int_{-\infty}^{\infty} \phi(\tau, \mu, \nu) I_\nu(\tau, \mu, \nu) d\nu d\mu. \quad (47)$$

To derive a quadrature formula, we write the transfer equation in the form

$$\frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu, \quad (48)$$

where  $\tau_\nu$  is given by equation (10). The formal solution of this equation is written in different ways depending

on the sign of  $\mu$ . For  $\mu > 0$ , we have (cf. Mihalas 1978)

$$I_\nu = e^{\tau_\nu} \int_{\tau_\nu}^{\infty} S_\nu e^{-\tau'_\nu} d\tau'_\nu, \quad (49)$$

and for  $\mu < 0$ , we have

$$I_\nu = -e^{\tau_\nu} \int_0^{\tau_\nu} S_\nu e^{-\tau'_\nu} d\tau'_\nu, \quad (50)$$

if the incident radiation field is zero. Note that  $\tau_\nu < 0$  for  $\mu < 0$  (cf. eq. [10]). Employing the linear test function

$$S_\nu = a + b\tau_\nu, \quad (51)$$

we obtain the standard results

$$I_\nu = a + b + b\tau_\nu, \quad (52)$$

for  $\mu > 0$ , and

$$I_\nu = a + b + b\tau_\nu - (a + b)e^{\tau_\nu} \quad (53)$$

for  $\mu < 0$ .

Inserting these solutions and equation (51) into equation (46), we obtain

$$W = 1, \quad \tau'_\nu = \tau_\nu + 1 \quad (54)$$

for  $\mu > 0$ , and

$$W = 1 - e^{\tau_\nu}, \quad \tau'_\nu = 1 + \tau_\nu / (1 - e^{\tau_\nu}) \quad (55)$$

for  $\mu < 0$ . These are the required formulae.

The expression for  $\tau'_\nu$  can be used to derive the continuum quadrature point  $\tau'$ . To show how this is accomplished, we assume that  $\phi_\nu$  and  $r$  are depth-independent. Then  $\tau_\nu$  is given by equation (12), and we obtain

$$\tau' = \tau + \mu / (\phi_\nu / r + 1) \quad (56)$$

for  $\mu > 0$ . Note that  $\tau'$  is a function of  $\tau$ ,  $\mu$ , and  $\nu$ .

In the limit of large optical depths, equations (54) and (55) automatically give the core-saturation approximation. In the limit of very small optical depths, we find  $\tau'_\nu \rightarrow 1$ ,  $W \rightarrow 1$  for  $\mu > 0$ , and  $W \rightarrow 0$  for  $\mu < 0$ . When averaged over  $\mu$ , this corresponds to the wing approximation. The improved quadrature formulae derived here do not have a discontinuity at  $\tau_\nu = \gamma$ . By expanding equation (55) to the second order in  $\tau_\nu$ , we find  $\tau'_\nu \rightarrow \frac{1}{2}\tau_\nu$  for  $\mu < 0$  at small optical depths, which implies that equation (55) correctly accounts for the fact that some of the nonlocalness of the radiation field is caused by sources above  $\tau$ .

The quadrature formulae derived in this section correspond to a simple physical model of the radiation field:

The intensity  $I_\nu$  is a result of a point source of strength  $WS_\nu$  located at the depth  $\tau'$ . Numerical calculations show that this simplified model is sufficiently accurate for an understanding of the gross behavior of  $S_\nu$ .

#### VII. THE DEPTH-QUADRATURE PERTURBATION TECHNIQUE

The quadrature formulae derived in § VI correspond to writing

$$I_\nu = \Lambda_{\nu\mu}^\dagger S_\nu + (\Lambda_{\nu\mu} - \Lambda_{\nu\mu}^\dagger) S_\nu, \quad (57)$$

where the approximate operator  $\Lambda_{\nu\mu}^\dagger$  is defined by

$$\Lambda_{\nu\mu}^\dagger = W \int d\tau \delta(\tau_\nu - \tau'_\nu). \quad (58)$$

This operator is obtained by replacing the integral over  $\tau$  in equations (49) and (50) by a one-point quadrature formula. Thus, the method for solving non-LTE problems proposed below is *exactly* analogous to the AQP and FQP techniques of Cannon (1973*a, b*). We therefore refer to our method as the depth-quadrature perturbation technique (DQPT), although we do not formally expand  $I_\nu$  in terms of  $(\Lambda_{\nu\mu} - \Lambda_{\nu\mu}^\dagger)$ . Our technique differs from Cannon's FQPT in one important respect: The quadrature point  $\tau'_\nu$  is chosen in an *optimum* rather than an arbitrary way.

The equation for  $S_\nu$  corresponding to  $\Lambda_{\nu\mu}^\dagger$  is identical to that obtained for  $\Lambda_{\nu\mu}^*$ , except that the integrals over  $\nu$  occurring in equation (40) are replaced by integrals over  $\nu$  and  $\mu$ . In order to decrease the computing time, advantage is taken of the symmetry relations (cf. Mihalas 1978)

$$\phi_\nu(\tau, -\mu, \nu) = \phi_\nu(\tau, \mu, -\nu), \quad (59)$$

and

$$\tau_\nu(\tau, -\mu, \nu) = -\tau_\nu(\tau, \mu, -\nu). \quad (60)$$

By using these relations, we may treat  $\mu$  as a positive variable. Then for each  $\mu$  there are two quadrature points,  $\tau_\nu^+$  and  $\tau_\nu^-$ , and weights,  $W^+$  and  $W^-$ , corresponding to outgoing and ingoing rays. We obtain from equations (54) and (55)

$$W^+ = 1, \quad (61)$$

$$\tau_\nu^+ = \tau_\nu + 1, \quad (62)$$

$$W^- = 1 - e^{-\tau_\nu}, \quad (63)$$

$$\tau_\nu^- = \tau_\nu / W^- - 1. \quad (64)$$

The equation for  $S_\nu$  can be written

$$\Lambda^\dagger s = e. \quad (65)$$

The time required to calculate  $\Lambda^\dagger$  is longer than the time required to calculate  $\Lambda^*$ . Hence, the calculation of  $\Lambda^\dagger$  should be arranged in an efficient way. This can be done conveniently if the vector  $\tau_\nu(k)$ , where  $k=1, \dots, n_\tau$ , is calculated for one frequency and angle at the time. Since  $\phi_\nu$  and  $r$  are positive quantities, we will always find  $\tau_\nu(1) \leq \tau_\nu(2) \leq \dots \leq \tau_\nu(n_\tau)$ . It is easy to show that  $\tau_\nu^+$  and  $\tau_\nu^-$  are increasing functions of  $\tau_\nu$ . This implies that  $\tau_\nu^+(1) \leq \tau_\nu^+(2) \leq \dots \leq \tau_\nu^+(n_\tau)$ , and that  $\tau_\nu^-(1) \leq \tau_\nu^-(2) \leq \dots \leq \tau_\nu^-(n_\tau)$ . Using these inequalities, the depth point  $k^+$ , defined such that  $\tau_\nu(k^+) \leq \tau_\nu^+(k) < \tau_\nu(k^+ + 1)$ , can very rapidly be found for each  $k$ . Then the matrix elements  $\Lambda^\dagger(k, k^+)$  and  $\Lambda^\dagger(k, k^+ + 1)$  are calculated from the linear interpolation formula

$$S_\nu(\tau_\nu^+) = S_\nu(k^+) + \frac{\tau_\nu^+ - \tau_\nu(k^+)}{\tau_\nu(k^+ + 1) - \tau_\nu(k^+)} \times [S_\nu(k^+ + 1) - S_\nu(k^+)]. \quad (66)$$

The same procedure is used to calculate matrix elements corresponding to ingoing rays.

A computer program which solves two-level non-LTE problems with macroscopic velocity fields using the DQP technique described in this section has been written. In the calculations,  $\phi_\nu$  was treated as an angle-dependent function. In Table 1 we give the central processing unit (CPU) time used for various parts of the program. The calculations were made with a CDC Cyber 170-720. It can be seen from this table that the time required to calculate  $\Lambda^\dagger$  is approximately a factor of 1.5 longer than the time required to calculate  $\langle J \rangle$  *once* from a known source function. However, these calculations were made using the same number of angles and frequencies in the calculation of  $\Lambda^\dagger$  and the correction terms. This is not necessary, since the depth quadrature formula used in the calculation of  $\Lambda^\dagger$  gives errors in  $S_\nu$  of the order of 30%. Thus, decreasing  $n_\mu n_\nu$  by a factor of 2 or 3 would not affect the accuracy of  $\Lambda^\dagger$  or the rate of convergence. It would cause a reduction of the total computer time by approximately 20%. It is obvious that the DQPT is very conveniently combined with the AQP and the FQPT. However, it is *not* meaningful to use a very small number of angular and frequency points in the calculation of  $\Lambda^\dagger$ , since most of the computer time is used for the calculation of  $\langle J \rangle$ , not  $\Lambda^\dagger$ .

#### VIII. CALCULATIONS USING THE DQPT

We have tested the depth-quadrature perturbation technique on a variety of non-LTE problems. A few representative calculations are described below.



TABLE 1  
CPU TIME FOR COMPUTER PROGRAM SOLVING ONE-DIMENSIONAL NON-LTE PROBLEMS WITH VELOCITY FIELDS

NO. OF ANGLES	NO. OF DEPTH POINTS	CPU TIMES (s)			
		Calculation of Voigt Profiles	Calculation of the Matrix $\Lambda^{\dagger}$	LU factorization of $\Lambda^{\dagger}$	Calculation of $\langle J \rangle$ per Iteration
1.....	40	0.13	0.32	0.30	0.24
3.....	40	0.38	0.94	0.28	0.71
3.....	60	0.57	1.47	0.98	1.02

NOTE.—No. of frequencies: 25. Computer: CDC Cyber 170-720. CPU=central processing unit.

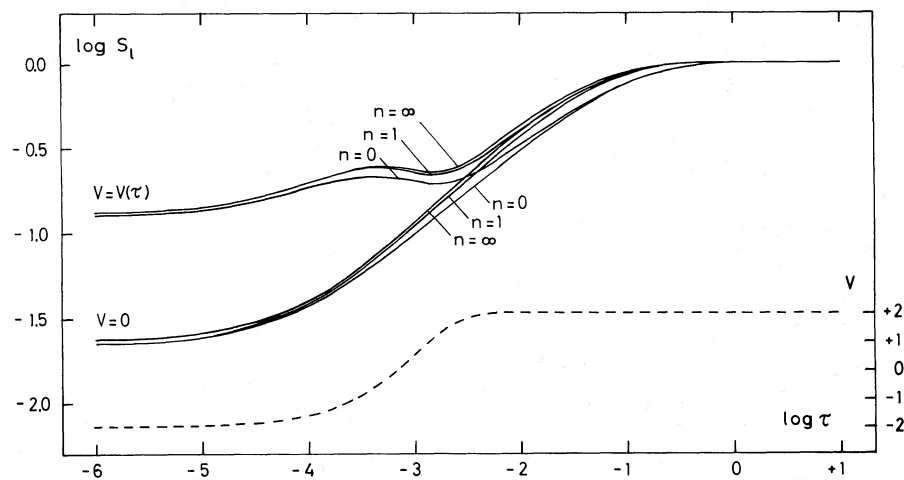


FIG. 3.—The convergence of  $S_l(\tau)$ , using the DQPT for an atmosphere with  $a=0$ ,  $r=10^{-4}$ ,  $\epsilon'=10^{-4}$ , and  $B=1$ . The lower set of curves corresponds to a constant velocity, and the upper set of curves to a variable velocity,  $V$ . The dashed curve shows the variation of  $V$  with  $\tau$ . Note the high accuracy of the initial solution ( $n=0$ ) and the rapid convergence.

Figure 3 shows two examples of calculations for a pure Doppler profile with  $B=1$ ,  $\epsilon'=10^{-4}$ , and a weak continuum,  $r=10^{-4}$ . The macroscopic velocity  $V$  was assumed to have the form

$$V=2-4 \exp(-\tau/\tau_1), \quad (67)$$

which switches from  $-2$  to  $+2$  at approximately  $\tau=\tau_1$ . The calculations were made with  $n_\mu=3$ ,  $n_\nu=35$ , and  $n_\tau=40$  for a stationary atmosphere and for a moving atmosphere with  $\tau_1=10^{-3}$ . In both cases the convergence was very rapid. After four iterations, the maximum error in  $S_l$  was 0.6% for the stationary atmosphere and 1.1% for the nonstationary atmosphere. The presence of large velocity gradients affects the convergence only in a minor way. Contrary to what is often claimed in the literature, we find that the effects of the velocity gradient on  $S_l$  are large. This is because of the reflector effect, i.e., the Doppler displaced profile leads to an illumination by the lower layers which enhances  $S_l$ .

Figure 4 shows examples of calculations for a Voigt profile with  $a=10^{-3}$ ,  $B=1$ ,  $\epsilon'=10^{-4}$ , and  $r_o=r/\phi(v=0)=10^{-6}$ . In these calculations the vertical velocity was

zero, but the Doppler width,  $\Delta$ , changed with depth according to

$$\Delta=\Delta(\infty)[1+2 \exp(-\sqrt{\alpha\tau})]. \quad (68)$$

Calculations were made for  $\alpha=10^6$  and  $\alpha=0$ , the latter corresponding to a constant Doppler width. In these calculations we used  $n_\mu=3$ ,  $n_\nu=30$ , and  $n_\tau=55$  to obtain a high accuracy. Again the convergence was very rapid. After only four iterations the maximum error in  $S_l$  was 0.5% in the case of a constant Doppler width and 0.7% in the case of a variable width. Calculations with the same set of atmospheric parameters were made by Athay (1972a), which gives us the possibility of verifying that the solution converges to the correct values. We note that the variation in  $\Delta$  gives strong effects on  $S_l$  similar to those found for a variable velocity (see Fig. 3).

Calculations using the DQPT have been made for a number of similar cases. The convergence was always very rapid, and no evidence for numerical instabilities was found. The numerical implementation of the technique is very simple; in fact, most of the computer code consists of an assembly of standard LTE routines. The

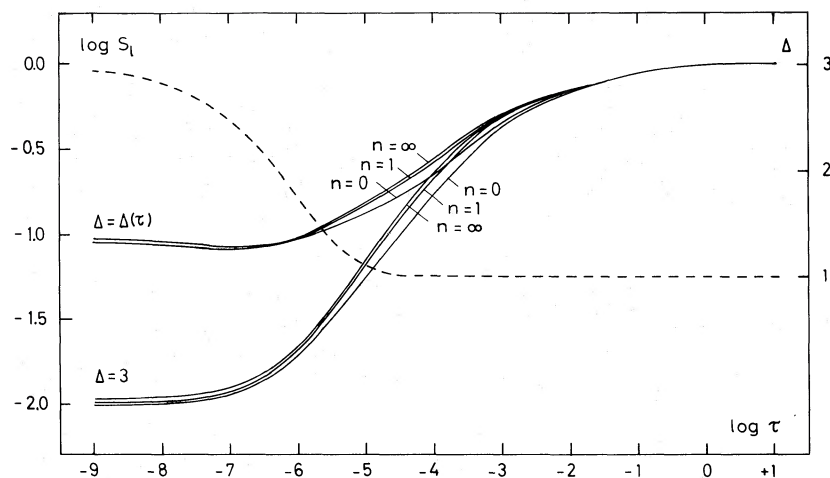


FIG. 4.—The convergence of  $S_l(\tau)$ , using the DQPT for an atmosphere with  $a=10^{-3}$ ,  $r_o=10^{-6}$ ,  $\epsilon'=10^{-4}$ , and  $B=1$ . The lower set of curves corresponds to a constant Doppler width,  $\Delta=3$ , and the upper set of curves to a variable Doppler width. The dashed curve shows the variation of  $\Delta$  with  $\tau$ .

computing time scales as

$$c_4 n_\mu n_\nu n_\tau + n_{it} c_5 n_\mu n_\nu n_\tau + c_6 n_\tau^3, \quad (69)$$

which corresponds to the time required to calculate the matrix  $\Lambda^\dagger$ , the time required to calculate  $\langle J \rangle$  from a known source function, and the time required to perform one *LU* factorization (the time required to solve the resulting triangular system of equations by back substitution is negligible). For very large  $n_\tau$  values it may be rewarding to make use of the fact that in most normal situations  $\Lambda^\dagger$  is almost a triangular matrix having approximately only two subdiagonals. The *LU* factorization of such a matrix requires only  $c_7 n_\tau^2$  operations.

It therefore appears that the computing time requirements of the DPQT are very favorable when compared to any other existing numerical technique for solving non-LTE radiative transfer problems. The reason for this saving is that though we often need a large number of depth points to determine  $S_l$ —because of the large variation of opacity with frequency—for any *single* frequency the number of depth points required is not that large. Thus, inverting full-size tridiagonal matrices means a waste of computing time. By introducing a simple one-point quadrature formula and iterating until a predetermined accuracy in  $S_l$  is reached, we are performing a minimum of arithmetic operations.

In the calculations made so far, we have not tried to minimize the computer time used for the calculation of the correction terms. By ignoring depth points outside the interval  $10^{-2} < \tau_v < 10$ , it should be possible to decrease the computing time by approximately a factor of 2 without any significant loss of accuracy.

The choice of quadrature points in frequency has been rather arbitrary. By combining equations (46) and (47), we may calculate  $\langle J \rangle$  when  $S_l$  is given. Using various expressions for  $S_l$ , it should be possible to discuss thoroughly the *proper* choice of frequency quadrature points and thus to decrease the number of frequencies required.

#### IX. CONCLUSIONS

We have presented one approximate analytical method and one more exact numerical method for solving non-LTE problems. The analytical method relies on simple and well-understood concepts of radiative transfer theory. Using this approach we may understand the basic control mechanisms of non-LTE. This is important also from a pedagogical point of view. It should be possible to use the analytical approach to derive new approximate scaling laws. For example, we have derived expressions for the surface value of  $S_l$  when the incident radiation field is not zero (not published). Finally, the derivation of equation (22) is interesting from a diagnostic point of view because it rests on the assumption of equality between the *observable* intensity  $I_\nu(0)$  and the source function  $S_\nu$  at  $\tau_\nu=1$ . This means that the Eddington-Barbier relation can be used not only to derive the *value* of  $S_\nu$ ; it allows us to probe directly the escape mechanisms which *control* the source function. However, it should be pointed out that the Eddington-Barbier relation may fail badly for differentially moving atmospheres (cf. Athay 1972*a*; Hummer 1976).

We have also presented a new numerical technique, the DQPT, which consists in replacing the integral of  $S_\nu$  over  $\tau$  by a one-point quadrature formula. This method provides an important link between the core-saturation method of Rybicki (1971) and the perturbation tech-

niques of Cannon (1973*a, b*). The efficiency of this method and its easy implementation should make this an attractive method for solving non-LTE problems. Also, the fact that the initial solution is obtained from a quadrature formula which has a simple physical meaning should give good possibilities for interpretations of the calculations. The DQPT can easily be applied to three-dimensional problems.

Finally, we should mention that the original idea of constructing quadrature formulae for evaluating mean intensities seems to be from Bengt Strömgren (cf. Chandrasekhar 1960, p. 69). Such two- and three-point quadrature formulae for evaluating  $J_\nu$  were constructed

by Reiz (1950). The iterative technique developed here to solve non-LTE problems is new.

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