

## DISCRETE SPACE THEORY OF RADIATIVE TRANSFER

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Introduction. The study of transfer of radiation is an essential part in the stellar atmospheric research. The complex physical processes that occur in stellar atmospheres do not permit us to obtain the solution of radiative transfer equation easily. Various people working with the problems of stellar atmospheres have developed different techniques depending on their needs and tastes. Among the most notable methods of solving the equation of radiative transfer is the one based on the principles of invariant imbedding due to Ambartsumian (1943) and Chandrasekhar (1950). These principles are a special case of the interaction principle and the star product (Redheffer 1962 and Preisendorfer 1965) which we shall describe later. The interaction principle and the star product algorithm are general and applicable to any inhomogeneous media in curved geometries. In general the following steps are taken in obtaining the solution.

1 We divide the medium into a number of 'cells' whose thickness is defined by  $\tau$  which is less than a critical thickness ( $\tau_{crit}$ ). The critical thickness is determined on the basis of the physical characteristics of the medium.

2 The integration of the transfer equation is performed on the 'cell' which is a two-dimensional grid bounded by  $[r_n, r_{n+1}] \times [\mu_{j-\frac{1}{2}}, \mu_{j+\frac{1}{2}}]$

3 We compare these discrete equations with the canonical equations of the interaction principle and obtain the transmission and reflection operators of the cell.

4 Lastly, we combine all the cells by star algorithm and obtain the radiation field.

Note. We can divide the medium into shells whose thickness are larger than  $\tau_{crit}$  but integration is done only on 'cell' and star algorithm is used to obtain the transmission and reflection of the composite 'cell' or shell.

In this article, we describe the basic theory and give two examples where it has been applied. We also give necessary details of the formulae and procedures so that users need not refer to the articles cited here for details.

We shall divide the article into following sections:

A Discrete Space Theory

- I. Interaction principle
- II. Star product
- III. Calculation of radiation field at internal points.

B Application

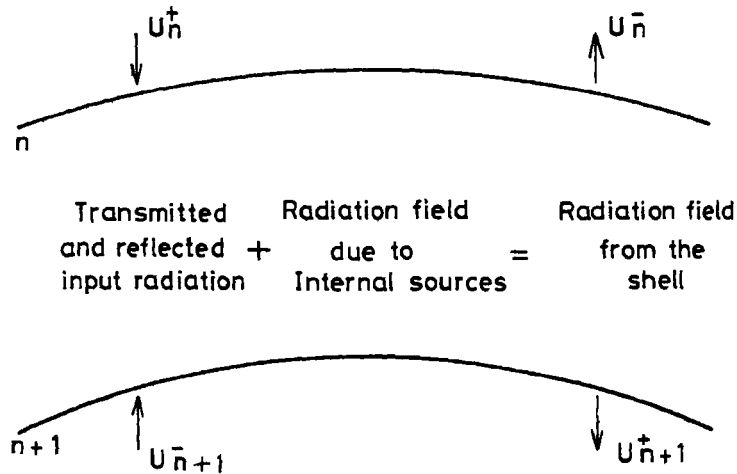
- I. Integration of monochromatic radiative transfer equation and derivation of r & t operators for the 'cell'.
- II. Flux conservation and temperature correction in the polychromatic case.
- III. Line formation in expanding media.

A Discrete Space Theory.

A.I Interaction Principle.

The interaction principle relates the incident and emergent radiation field from a medium of given optical thickness. In figure 1, we have shown a shell of optical thickness  $\tau$  with incident and emergent intensities. We assume that specific intensities  $U_n^+$  and  $U_{n+1}^-$  are incident at the boundaries  $n$  and  $n+1$  respectively of the shell with optical thickness  $\tau$ . The symbols with signs + and - represent specific intensities of the rays travelling in opposite directions.

Figure 1. Schematic diagram showing the interaction principle.



If  $\mu$  represents the cosine of the angle made by a ray relative to the common normal to the stratification in the direction in which  $n$  increases. That is

$$U_n^+ \{U_n(\mu) : 0 < \mu \leq 1\}$$

and  $U_n^- \{U_n(-\mu) : 0 < \mu \leq 1\}$

$U_n^+$  represents the specific intensity of the ray travelling in the direction  $\mu$  and  $U_n^-$  represents the specific intensity of the ray travelling in the opposite direction. We select a finite set of values of  $\mu$  ( $\mu_j : 1 \leq j \leq m; 0 < \mu_1 < \mu_2 < \mu_3 \dots \mu_m \leq 1$ ). Or

$$U_n^+ = \begin{bmatrix} U_n(\mu_1) \\ U_n(\mu_2) \\ \vdots \\ U_n(\mu_m) \end{bmatrix} \quad \text{and} \quad U_n^- = \begin{bmatrix} U_n(-\mu_1) \\ U_n(-\mu_2) \\ \vdots \\ U_n(-\mu_m) \end{bmatrix}$$

are  $m$  - dimensional vectors on Euclidean space.

The incident intensity vectors are

$$U_n^+ \quad \text{and} \quad U_{n+1}^-$$

The emergent intensity vectors are

$$U_n^- \quad \text{and} \quad U_{n+1}^+$$

The emergent radiation field will have the contributions from the internal sources say,  $\Sigma^+(n+1, n)$  and  $\Sigma^-(n, n+1)$  corresponding to the output intensity vectors  $U_{n+1}^+$  and  $U_n^-$  respectively.

We assume certain linear operators which reflect and transmit the incident radiation namely,  $t(n+1, n)$ ,  $r(n, n+1)$ ,  $t(n, n+1)$  and  $r(n+1, n)$ . Then we can write the output intensities in terms of the transmitted and reflected input intensities together with the internal sources as

$$\begin{aligned} U_{n+1}^+ &= t(n+1, n) u_n^+ + r(n, n+1) u_{n+1}^- + \Sigma^+(n+1, n) \\ U_n^- &= r(n+1, n) u_n^+ + t(n, n+1) u_{n+1}^- + \Sigma^-(n, n+1) \end{aligned} \quad (1)$$

The introduction of the internal source terms namely,  $\Sigma^+(n+1, n)$  and  $\Sigma^-(n, n+1)$  was due to Grant and Hunt (1969a). The relationship given by equation (1) is called the Interaction Principle. Equation (1) can also be written concisely as

$$\begin{bmatrix} U_{n+1}^+ \\ U_n^- \end{bmatrix} = S(n,n+1) \begin{bmatrix} U_n^+ \\ U_{n+1}^- \end{bmatrix} + \Sigma(n,n+1) \quad (2)$$

where

$$S(n,n+1) = \begin{bmatrix} \bar{t}(n+1,n)r(n,n+1) \\ r(n+1,n)t(n,n+1) \end{bmatrix} \quad (3)$$

A.II Star Products

If there is another shell with boundaries (n+1,n+2) adjacent to (n,n+1), interaction principle for this shell can be written as

$$\begin{bmatrix} U_{n+2}^+ \\ U_{n+1}^- \end{bmatrix} = S(n+1,n+2) \begin{bmatrix} U_{n+1}^+ \\ U_{n+2}^- \end{bmatrix} + \Sigma(n+1,n+2) \quad (4)$$

where S(n+1,n+2) is similarly defined as in equation (3). If we combine the two shells (n,n+1) and (n+1,n+2) then the interaction principle for the combined shell is written as, (for the thickness is arbitrarily defined)

$$\begin{bmatrix} U_{n+2}^+ \\ U_n^- \end{bmatrix} = S(n,n+2) \begin{bmatrix} U_n^+ \\ U_{n+2}^- \end{bmatrix} + \Sigma(n,n+2) \quad (5)$$

Redheffer (1962) calls S(n,n+2) the star product of the two S-matrices S(n,n+1) and S(n+1,n+2) written as

$$S(n,n+2) = S(n,n+1) * S(n+1,n+2) \quad (6)$$

Equation (5) is obtained by eliminating  $U_{n+1}^+$  and  $U_{n+1}^-$  from equations (2) and (4). We can write r & t operators for the composite shell as

$$\begin{aligned} t(n+2,n) &= t(n+2,n+1) [\bar{I} - r(n,n+1)r(n+2,n+1)]^{-1} t(n+1,n) \\ t(n,n+2) &= t(n,n+1) [\bar{I} - r(n+2,n+1)r(n,n+1)]^{-1} t(n+1,n+2) \\ r(n+2,n) &= r(n+1,n) + t(n,n+1)r(n+2,n+1) [\bar{I} - r(n,n+1)r(n+2,n+1)]^{-1} x \\ &\quad t(n+1,n) \\ r(n,n+2) &= r(n+1,n+2) + t(n+2,n+1)r(n,n+1) [\bar{I} - r(n+2,n+1)r(n,n+1)]^{-1} t(n+1,n+2) \end{aligned}$$

and

$$\Sigma(n,n+2) = \Lambda(n,n+1;n+2)\Sigma(n,n+1) + \Lambda'(n;n+1,n+2)\Sigma(n+1,n+2)$$

where I is the identity matrix and

$$\Lambda(n, n+1; n+2) = \begin{bmatrix} t(n+2, n+1) [\bar{I} - r(n, n+1)r(n+2, n+1)]^{-1} & 0 \\ t(n, n+1)r(n+2, n+1) [\bar{I} - r(n, n+1)r(n+2, n+1)]^{-1} & \bar{I} \end{bmatrix}$$

$$\Lambda'(n; n+1, n+2) = \begin{bmatrix} \bar{I} t(n+2, n+1)r(n, n+1) [\bar{I} - r(n+2, n+1)r(n, n+1)]^{-1} \\ 0 t(n, n+1) [\bar{I} - r(n+2, n+1)r(n, n+1)]^{-1} \end{bmatrix} \quad (9)$$

and  $\Sigma(n, n+1) = \begin{bmatrix} \Sigma^+(n+1, n+2) \\ \Sigma^-(n, n+1) \end{bmatrix}$  (10)

Similarly  $\Sigma(n+1, n+2)$  is defined.

If we write  $S(\alpha)$  to designate the shell  $\alpha$  then

$$S(\alpha*\beta) = S(\alpha)*S(\beta) \quad (11)$$

where  $\alpha*\beta$  denotes the region obtained by putting the two shells  $\alpha$  and  $\beta$  together. If the shells are homogeneous and plane parallel then

$$\alpha*\beta = \beta*\alpha \quad (12)$$

In general star multiplication is non-commutative. However, star multiplication is associative. If we have to add several layers  $\alpha, \beta, \gamma \dots$

then  $S[\alpha*(\beta*\gamma)*\dots] = S[(\alpha*\beta)*\gamma*\dots]$  etc. (13)

If the medium is homogenous and very thick then we can use what is known as 'doubling method' (see van de Hulst 1965). For example,

$$S(2^p d) = S(2^{p-1} d) * S(2^{p-1} d), (p=1, 2, 3, \dots) \quad (14)$$

which means that we can generate the S-matrix for a layer of thickness  $2^p d$  in  $p$  cycles starting with  $S(d)$  rather than in  $2^p$  cycles of adding the  $S(d)$ 's one by one. If  $p=10$ , then only a fraction  $10/2^{10} \approx 10^{-2}$  of the computational work is needed to add  $2^{10}$  layers of thickness  $d$ .

A.III Calculation of Radiation Field at Internal Points.

We expect the reflection and transmission operators to be non-negative. This condition will be satisfied only when the optical thickness of the shell is less than certain value called the 'critical size' or  $\tau_{crit}$  (this will be discussed in section B). If the optical thickness  $T$  of the shell in question is larger than the  $\tau_{crit}$  then we can divide the shell into several subshells whose  $\tau$  is less than the  $\tau_{crit}$  and then use star algorithm to calculate combined response from the subshells whose total thickness is  $T$ . If, for example we need the radiation field at some internal points in the atmosphere, we shall have to divide the entire medium into as many shells as we need and calculate the radiation field at these points. Let us divide the medium into  $N$  shells. One can write down the interaction principle for each shell and solve the whole system of equations (see Grant and Hunt 1968).

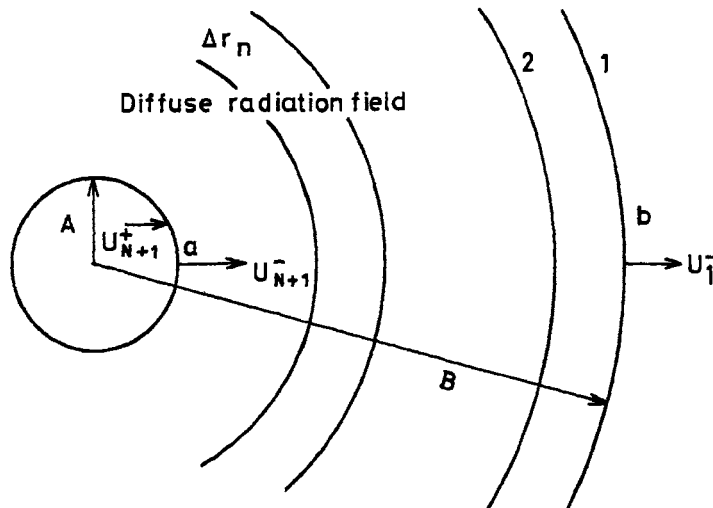
In figure 2, we show the atmosphere in which we calculate the internal radiation field. The atmosphere is divided into N shells with a and b as the inner and outer radii. The solution  $U_{n+1}^+$  and  $U_n^-$  (for any shell between shell 1 and shell N) are obtained from the relations

$$U_{n+1}^+ = r(1,n+1)U_{n+1}^- + v_{n+1/2}^+ \tag{15}$$

$$U_n^- = \hat{t}(n,n+1)U_{n+1}^- + v_{n+1/2}^-$$

with the boundary condition  $U_{N+1}^- = U^-(a)$ .

Figure 2. Schematic diagram showing the diffuse radiation.



The quantities  $r(1,n+1)$ ,  $v_{n+1/2}^+$  and  $v_{n+1/2}^-$  are calculated (with the initial conditions  $r(1,1)=0$  and  $v_{1/2}^+ = U^+(b)$ ) by computing recursively

$$r(1,n+1) = r(n,n+1) + t(n+1,n)r(1,n) [1 - r(n+1,n)r(1,n)]^{-1} t(n,n+1)$$

$$v_{n+1/2}^+ = \hat{t}(n+1,n)v_{n-1/2}^+ + \Sigma^+(n+1,n) + R_{n+1/2}^- \Sigma^-(n,n+1)$$

$$v_{n+1/2}^- = \hat{r}(n+1,n)v_{n-1/2}^+ + T_{n+1/2}^- \Sigma^-(n,n+1)$$

where

$$\left. \begin{aligned} \hat{t}(n+1,n) &= t(n+1,n) [\bar{I} - r(1,n)r(n+1,n)]^{-1} \\ \hat{r}(n+1,n) &= r(n+1,n) [\bar{I} - r(1,n)r(n+1,n)]^{-1} \\ R_{n+\frac{1}{2}} &= \hat{t}(n+1,n)r(1,n) \\ T_{n+\frac{1}{2}} &= [\bar{I} - r(n+1,n)r(1,n)]^{-1} \end{aligned} \right\} \quad (17)$$

and

$$\hat{t}(n,n+1) = T_{n+\frac{1}{2}} t(n,n+1) \quad (18)$$

To calculate the radiation field at the internal points we proceed as follows.

- 1 Divide the medium into a number of shells (say N) with N+1 boundaries.
- 2 Start calculating the two pairs of reflection and transmission operators  $r(n+1,n), r(n,n+1), t(n+1,n)$  and  $t(n,n+1)$  in each shell (if the optical thickness in each shell is larger than  $\tau_{crit}$ , then apply star algorithm or use doubling procedure if the medium is homogeneous).
- 3 With the boundary condition that  $r(1,1)=0$  and  $v_{\frac{1}{2}}^+ = u^+(a)$  and the  $r$  &  $t$  operators mentioned in 2 compute recursively  $r(1,n+1), v_{\frac{1}{2}}^+$  and  $\hat{t}(n,n+1)$  given in equations (16) to (18) from shell 1 to shell N (i.e. from b to a in fig 2 ).
- 4 Next we shall sweep back from a to b (see fig 2) calculating the radiation field given in equation (15) with the boundary condition  $U_{n+1}^- = U^-(a)$ .

Note. We have to retain the operators  $r(1,n+1), \hat{t}(n,n+1), v_{n+\frac{1}{2}}^+$  and  $v_{n+\frac{1}{2}}^-$  for each shell that are calculated in the steps 2 and 3 above until we start calculating the radiation field from a. (The storage of these operators will not increase the virtual memory of the machine required for computations. The operators can be stored on a magnetic disc and can be recalled whenever necessary).

If the surface at a is reflecting, we can write

$$U_{N+1}^- = r_G U_{N+1}^+ \quad (19)$$

where  $r_G$  is the reflection operator. For a totally reflecting surface  $r_G = I$ . Therefore, we have

$$U_{N+1}^+ = [\bar{I} - r(1,N+1)r_G]^{-1} v_{N+\frac{1}{2}}^+ \quad (20)$$

from which one can calculate  $U_{N+1}^-$  from equation (19). Rest of the calculations follow equation (15).

B Applications

B.I Integration of Radiative Transfer Equation over 'cell'

As the solution of the radiative transfer equation in plane parallel approximation can be obtained as a special case of the solution in spherically symmetric transfer equation we shall try to obtain the solution in the latter case. The equation of radiative transfer in spherical symmetry is written (see Peraiah and Grant, 1973)

$$\frac{\mu}{r^2} \frac{\partial}{\partial r} \{r^2 I(r, \mu)\} + \frac{1}{r} \frac{\partial}{\partial \mu} \{(1-\mu^2) I(r, \mu)\} + \sigma(r) I(r, \mu) = \sigma(r) \left\{ [1-\omega(r)] b(r) + \frac{1}{2} \omega(r) \int_{-1}^{+1} p(r, \mu, \mu') I(r, \mu') I(r, \mu) d\mu' \right\} \quad (21)$$

where  $\omega(r)$  is the albedo for single scattering,  $b(r)$  represents the sources inside the medium,  $r$  is the radius,  $\mu$  is the cosine of the angle made by the ray with the radius vector  $\sigma(r)$  is the absorption coefficient,  $I(r, \mu)$  is the specific intensity of the ray and  $p(r, \mu, \mu')$  is the phase function. The phase function is normalised such that

$$\frac{1}{2} \int_{-1}^{+1} p(r, \mu, \mu') d\mu' = 1 \quad (22)$$

and  $p(r, \mu, \mu') \geq 0$  and  $-1 \leq \mu, \mu' \leq 1$

if we write

$$U(r, \mu) = 4\pi r^2 I(r, \mu)$$

$$B(r) = 4\pi r^2 b(r)$$

Equation (21) can be rewritten as

$$\mu \frac{\partial u(r, \mu)}{\partial r} + \frac{1}{r} \frac{\partial}{\partial \mu} [(1-\mu^2) u(r, \mu)] + \sigma(r) u(r, \mu) = \sigma(r) \left\{ [1-\omega(r)] B(r) + \frac{1}{2} \omega(r) \int_{-1}^{+1} p(r, \mu, \mu') u(r, \mu') d\mu' \right\} \quad (23)$$

for outward going rays and

$$-\mu \frac{\partial u(r, -\mu)}{\partial r} - \frac{1}{r} \frac{\partial}{\partial \mu} [(1-\mu^2) u(r, -\mu)] + \sigma(r) u(r, -\mu) = \sigma(r) \left\{ [1-\omega(r)] B(r) + \frac{1}{2} \omega(r) \int_{-1}^{+1} p(r, -\mu, \mu') u(r, \mu') d\mu' \right\} \quad (24)$$

for inward going rays and we choose the discrete points of  $\mu$  to lie between 0 and 1.

We integrate the equations (23) and (24) on the 'cell' whose boundaries are defined by

$$[r_n, r_{n+1}] \times [\mu_n - \frac{1}{2}, \mu_n + \frac{1}{2}]$$



a two dimensional grid (Carlson 1963, Lathrop and Carlson 1967).

First consider the angle integration. The choice of the set of  $\{\mu_{j+\frac{1}{2}}\}$  is dictated by convenience. We have utilised the roots  $\mu_j$  and their corresponding weights  $c_j$  of the Gauss - Legendre quadrature formula of order J in the interval  $\mu \in [0, 1]$ .

putting  $\mu_{\frac{1}{2}} = 0$  we define

$$\mu_{j+\frac{1}{2}} = \sum_{k=1}^j c_k, \quad j=1, 2, \dots, J \tag{25}$$

Integrating equations (23) on the interval  $[\mu_{j-\frac{1}{2}}, \mu_{j+\frac{1}{2}}]$  we obtain

$$\begin{aligned} c_j \mu_j \frac{\partial u_j^+(x)}{\partial x} + \frac{1}{r} [(1-\mu_{j+\frac{1}{2}}^2) u_{j+\frac{1}{2}}^+(x) \\ - (1-\mu_{j-\frac{1}{2}}^2) u_{j-\frac{1}{2}}^+(x)] + c_j \sigma(x) u_j^+(x) = \sigma(x) c_j [(1-\omega(x)) B(x) + \frac{1}{2} \omega(x) \\ \Sigma(p^{++}(x)_{jj}, c_j u_j^+(x) + p^{+-}(x)_{jj}, c_j u_j^-(x))] \end{aligned} \tag{26}$$

where  $u_j^+(x) = u(x, \mu_j), u_j^-(x) = u(x, -\mu_j),$

$p^{++}(x)_{jj} = p(x, \mu_j, \mu_j), p^{+-}(x)_{jj} = p(x, -\mu_j, \mu_j),$  etc.

The quantities  $u_{j+\frac{1}{2}}^\pm$  are defined as

$$u_{j+\frac{1}{2}}^\pm = \frac{(\mu_{j+1} - \mu_{j+\frac{1}{2}}) u_{j+\frac{1}{2}}^\pm + (\mu_{j+\frac{1}{2}} - \mu_j) u_{j+1}^\pm}{\mu_{j+1} - \mu_j}, \quad j=1, 2, \dots, J-1 \tag{27}$$

and put

$$u_{\frac{1}{2}}^+ = u_{\frac{1}{2}}^- \text{ by interpolation}$$

$$u_{\frac{1}{2}}^+ = u_{\frac{1}{2}}^- = \frac{1}{2} (u_1^+ + u_1^-) \tag{28}$$

By writing

$$u^\pm(x) = \begin{bmatrix} u_1^\pm(x) \\ u_2^\pm(x) \\ \vdots \\ u_J^\pm(x) \end{bmatrix} \tag{29}$$

and making use of equations (27), (28) and (29), the equation (26) can be rewritten for all the angles in matrix form. This is given by

$$\begin{aligned} M \frac{\partial u^+(x)}{\partial x} + \frac{1}{r} [A^+ u^+(x) + A^- u^-(x)] + \sigma(x) u^+(x) \\ = \sigma(x) [(1-\omega(x)) B^+(x) + \frac{1}{2} \omega(x) [P^{++}(x) C^+ u^+(x) + P^{+-}(x) C^- u^-(x)]] \end{aligned} \tag{30}$$

Similarly equation (24) can be written as

$$\begin{aligned}
 & -M \frac{\partial \underline{u}^-(r)}{\partial r} - \frac{1}{r} \left[ \underline{\Lambda}^+ \underline{u}^-(r) + \underline{\Lambda}^- \underline{u}^+(r) \right] + \sigma(r) \underline{u}^-(r) \\
 & = \sigma(r) \left\{ (1-\omega(r)) \underline{B}^-(r) + \frac{1}{2} \omega(r) (p^+(r) c \underline{u}^+(r) + p^-(r) c \underline{u}^-(r)) \right\} \quad (3)
 \end{aligned}$$

where  $\underline{c}$  and  $\underline{M}$  are diagonal matrices with elements  $[c_j \delta_{jj}]$  and  $[M_j \delta_{jj}]$  respectively.  $\underline{B}^+$  and  $\underline{B}^-$  are source vectors and  $\underline{\Lambda}^+$  and  $\underline{\Lambda}^-$  are matrices of dimension  $J \times J$  called curvature scattering matrices. They are described in Appendix I. These matrices should satisfy the identity

$$\sum_{j=1}^J c_j (\underline{\Lambda}_{jk}^+ - \underline{\Lambda}_{jk}^-) = 0 \quad (32)$$

Now we integrate over the radial coordinate from  $r_n$  to  $r_{n+1}$ .

Integration of equations (30) and (31) from  $r_n$  to  $r_{n+1}$  gives us

$$\begin{aligned}
 M \left[ \underline{U}_{n+1}^+ - \underline{U}_n^+ \right] + \tau_{n+\frac{1}{2}} \underline{U}_{n+\frac{1}{2}}^+ = \tau_{n+\frac{1}{2}} \left[ (1-\omega_{n+\frac{1}{2}}) \underline{B}_{n+\frac{1}{2}}^+ + \left( \frac{1}{2} \omega_{n+\frac{1}{2}} p_{n+\frac{1}{2}}^{++} c_{n+\frac{1}{2}} - \frac{\rho \Delta^+}{\tau_{n+\frac{1}{2}}} \right) \underline{U}_{n+\frac{1}{2}}^+ \right. \\
 \left. + \left( \frac{1}{2} \omega_{n+\frac{1}{2}} p_{n+\frac{1}{2}}^{+-} c_{n+\frac{1}{2}} - \frac{\rho \Delta^-}{\tau_{n+\frac{1}{2}}} \right) \underline{U}_{n+\frac{1}{2}}^- \right] \quad (33)
 \end{aligned}$$

$$\begin{aligned}
 M \left[ \underline{U}_n^- - \underline{U}_{n+1}^- \right] + \tau_{n+\frac{1}{2}} \underline{U}_{n+\frac{1}{2}}^- = \tau_{n+\frac{1}{2}} \left[ (1-\omega_{n+\frac{1}{2}}) \underline{B}_{n+\frac{1}{2}}^- + \left( \frac{1}{2} \omega_{n+\frac{1}{2}} p_{n+\frac{1}{2}}^{-+} c_{n+\frac{1}{2}} + \frac{\rho \Delta^-}{\tau_{n+\frac{1}{2}}} \right) \underline{U}_{n+\frac{1}{2}}^- \right. \\
 \left. + \left( \frac{1}{2} \omega_{n+\frac{1}{2}} p_{n+\frac{1}{2}}^{--} c_{n+\frac{1}{2}} + \frac{\rho \Delta^+}{\tau_{n+\frac{1}{2}}} \right) \underline{U}_{n+\frac{1}{2}}^+ \right] \quad (34)
 \end{aligned}$$

where

$$\underline{U}_n^+ = \underline{U}^+(\underline{r}_n)$$

and variables subscripted with  $n+\frac{1}{2}$  such as  $\underline{U}_{n+\frac{1}{2}}^+$ ,  $\tau_{n+\frac{1}{2}}$ ,  $\omega_{n+\frac{1}{2}}$  are averages over the cell whose radial boundaries are  $r_n$  and  $r_{n+\frac{1}{2}}$ . We define  $\Delta r_{n+\frac{1}{2}} = r_{n+1} - r_n$ ,  $\tau_{n+\frac{1}{2}} = \sigma_{n+\frac{1}{2}} \Delta r_{n+\frac{1}{2}}$  and  $\rho = \bar{\rho} r_{n+\frac{1}{2}} / r_{n+\frac{1}{2}}$  where  $r_{n+\frac{1}{2}}$  is a suitable mean radius such as  $(r_n + r_{n+1})/2$

The quantities  $\underline{U}_{n+\frac{1}{2}}^+$  and  $\underline{U}_{n+\frac{1}{2}}^-$  are replaced by

$$\underline{U}_{n+\frac{1}{2}}^+ = \frac{1}{2} (\underline{U}_{n+1}^+ + \underline{U}_n^+) \quad \text{and} \quad \underline{U}_{n+\frac{1}{2}}^- = \frac{1}{2} (\underline{U}_n^- + \underline{U}_{n+1}^-) \quad (35)$$

which is nothing but the 'diamond' difference scheme. We substitute equations (35) into equations (33) and (34) and rearrange the input and output intensities in the form of the interaction principle. Comparing these equations with those given in (1), we obtain the transmission and reflection operators. These are given in Appendix II.

These operators should be non negative and for this condition to be satisfied, we must have

$$\Delta^+, \Delta^-, S^{++}, S^{--} \geq 0. \text{ See Appendix II.}$$

This can be achieved only if

$$\tau_{n+\frac{1}{2}} \leq \tau_{\text{crit}} = \min_j \left| \frac{\mu_j \pm \frac{1}{2} \rho \Lambda_{jj}^+}{\frac{1}{2}(1-\omega_{n+\frac{1}{2}} p_{jj}^{++} c_j)} \right| \quad (36)$$

Generally, we take the critical step size to be approximately equal to

$$\tau_{\text{crit}} \approx 2\mu_1 \quad (37)$$

For a 4 angle quadrature  $\tau_{\text{crit}} \approx .14$ . Once we calculate the  $r$  &  $t$  operators corresponding to this optical depth, we can use star algorithm for obtaining the radiation field for a shell of larger optical thickness.

B.II Flux Conservation and Temperature correction.

Flux Conservation.

We must have the solution checked for flux conservation. The system should neither create nor destroy energy and we must show that the solution obtained in the frame work of discrete space theory does conserve flux. (see Grant and Hunt 1969b and Peraiah and Grant 1973). The simplest case is that when we have purely scattering media. In this case we have  $\omega=1$ . We solve the transfer equation as described in the previous section and obtain the operators

$$r(n, n+1), r(n+1, n); t(n, n+1) \text{ and } t(n+1, n)$$

Then we should show that

$$\|t(n+1, n) + r(n+1, n)\| = 1 + O(\Delta\tau) \quad (38)$$

where  $\| \cdot \|$  means that we take the norm defined by

$$\|A\| = \sum_{j=1}^m \left| (DAD^{-1})_{jk} \right|, k=1, 2, \dots, J \quad (39)$$

and

$$D = 2\pi M C$$

As a consequence of condition (38)

$$(1) \frac{1}{2} \sum_{j=1}^J c_j \left[ p_{jk}^{++}(n) + p_{jk}^{--}(n) \right] = 1, k=1, 2, \dots, J \quad (40)$$

This is due to scattering. And

$$(2) \sum_{j=1}^J c_j (\Lambda_{jk}^+ - \Lambda_{jk}^-) = 0, k=1, 2, \dots, J \quad (41)$$

This is due to the nature of the curvature terms (see Appendix AI).

A more practical way of testing the system for flux conservation is as follows.

We introduce some flux at the point a and calculate the fluxes that emerge out at a and b. (see fig.2) Thus if F denotes flux, we must have

$$F^-(a) = F^-(b) + F^+(a) \tag{42}$$

(Notice that we did not give any flux at b (i.e)  $u_1^+ = 0$ ), where  $F^-(b)$  is the flux emerging at  $r=b$  and  $F^+(a)$  is the flux back scattered into the inner region. We give  $F^-(a) = \pi$ . We present the quantities  $F^-(b)$  and  $F^+(a)$  in the table and we can see that the equation(42) can be satisfied to within the machine accuracy (1 part in  $10^9$ ).

Table 1 Global conservation for a conservative isotropically scattering shell illuminated isotropically on the inner boundary  $r=a$ . The columns give the total flux emerging from the shell at radii a and b and verify the equation  $F^+(a) + F^-(b) = F^-(a) = \pi$ . Calculations are based on 8 point Gauss-Legendre quadrature. A and B are the inner and outer radii of the shell. Notice that when  $B/A=1$ , the approximation becomes plane parallel. The results are taken from Peraiah and Grant (1973).

$\tau$	2		5		10	
	$F^-(b)/2\pi$	$F^+(a)/2\pi$	$F^-(b)/2\pi$	$F^+(a)/2\pi$	$F^-(b)/2\pi$	$F^+(a)/2\pi$
1.00	0.19503	0.30497	.10383	.39617	0.05387	0.44163
1.30	0.24617	0.25383	.13354	.36646	0.07550	.42450
1.50	0.27325	0.22675	.15177	.34823	.08650	.41350
1.7	0.29611	0.20389	.16881	.33119	.09716	.40284
2.0	0.32439	0.17561	.19227	.30773	.11254	.38746

Figure 3. Angular distribution of the specific intensity from inside ( $n=100$ ) to the outside ( $n=1$ ) of a spherical atmosphere. Here  $\tau=10$ ,  $B/A=1.5$ ,  $N=100$ ,  $w=1.0$ , isotropic scattering. Taken from Peraiah and Grant (1973).

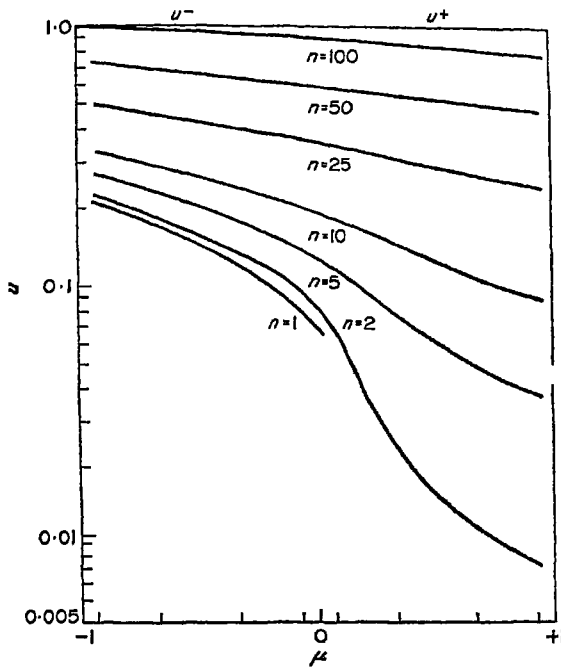
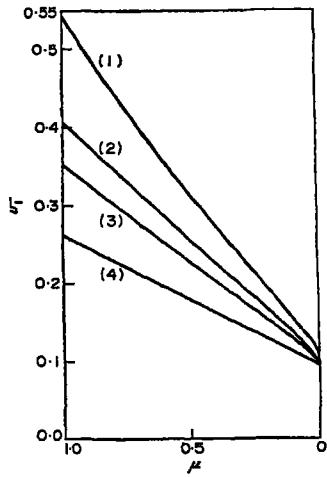


Figure 4. Angular distribution of emergent intensity for  $\tau=5$ ,  $w=1.0$ , isotropic scattering (1)  $B/A=2$ ; (2)  $B/A=1.5$ ; (3)  $B/A=1.3$ ; (4)  $B/A=1.0$ . Taken from Peraiah and Grant (1973).



In figure 3, we have presented the solution of the transfer equation and the emergent solution is given in figure 4, for the specified parameters.

Temperature Correction

The temperature correction for the discrete space theory had been worked out by Wehrse (1981). We shall outline his procedure here and those who are interested further may look into the above reference. We begin from the interaction principle given in equation (1), written for all the shells. Let us write

$$\underline{A} \underline{U} = \underline{\Sigma} \tag{43}$$

where  $\underline{A}$  is a tridiagonal block matrix and  $\underline{U}$  and  $\underline{\Sigma}$  condition all the specific intensities and source vectors respectively from shell 1 to N. From equation (43), we have

$$\underline{U} = \underline{A}^{-1} \underline{\Sigma} \tag{44}$$

To calculate flux vector we multiply  $\underline{U}$  by a matrix  $\underline{G}$  which contains the weight factors for interaction

$$\int_{-1}^{+1} \dots \mu d\mu \tag{45}$$

The total flux in a shell  $F'_{tot}$  over all frequency points is

$$F'_{tot} = \sum_{i=1}^{n_f} g_i (G U_i) = \sum_{i=1}^{n_f} g_i (G A^{-1} \Sigma_i) \tag{46}$$

where  $g_i$  are the integration weights and  $n_f$  is the total number of frequency points. Let the temperature stratification vector be  $T = [T_1, T_2, \dots, T_N]^t$  for which the total flux is conserved. We write,

$$F_{tot}^k = \sum_{i=1}^{n_f} g_i (T^k + \Delta T) = \sum_{i=1}^{n_f} g_i \left\{ G A^{-1} \left( \Sigma_i^k + \frac{\partial \Sigma_i^k}{\partial T} T \right) \right\} \tag{47}$$

where  $k$  is the iteration number. The temperature correction vector is given by

$$\Delta T^k = \left\{ \sum_{i=1}^{n_f} g_i (G A^{-1} \frac{\partial \Sigma_i^k}{\partial T}) \right\}^{-1} \Delta F \tag{48}$$

$$\Delta F = F - \sum_{i=1}^{n_f} g_i (G A^{-1} \Sigma_i^k) \tag{49}$$

This procedure has been successfully used by Wehrse (1981) for computing the models of M-super giant stars.

B.III Line Formation in Expanding Stellar Atmospheres.

The problem of calculating the spectral lines in an expanding stellar atmosphere is considerably complicated because the physical properties of the medium are affected by the local conditions of the moving matter. If the velocity of expansion is small (say one or two mean thermal units) one can use the rest frame and simulate the spectral lines. In this frame we have to deal with a large angle-frequency mesh and the size of this mesh increases with the velocity of expansion because of Doppler effect. On the other hand in a comoving frame, one need not worry about the Doppler effect and can employ very high velocities, with a much smaller angle-frequency mesh. Therefore, we shall formulate the algorithm in a comoving frame and indicate how the same procedure can be utilised in a rest frame.

The equation of radiative transfer for a Non LTE two level atom in the comoving frame in spherical symmetry is written as (see Peraiah 1980)

$$\begin{aligned} \mu \frac{\partial I(x, \mu, r)}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial I(x, \mu, r)}{\partial \mu} &= K(x, r) S_L(r) + K_c(r) S_c(r) \\ &- [K(x, r) + K_c(r)] I(x, \mu, r) + \left[ (1-\mu^2) \frac{V(r)}{r} + \mu^2 \frac{dV(r)}{dr} \right] \frac{\partial I(x, \mu, r)}{\partial x} \\ \text{and} \quad -\mu \frac{\partial I(x, -\mu, r)}{\partial r} - \frac{1-\mu^2}{r} \frac{\partial I(x, -\mu, r)}{\partial \mu} &= K(x, r) S_L(r) + K_c(r) S_c(r) - [K(x, r) + \\ &K_c(r)] I(x, -\mu, r) + \left\{ (1-\mu^2) \frac{V(r)}{r} + \mu^2 \frac{dV(r)}{dr} \right\} \frac{\partial I(x, -\mu, r)}{\partial x} \end{aligned} \quad (51)$$

Where  $I(x, \mu, r)$  is the specific intensity of the ray making angle  $\cos^{-1} \mu$  with the radius vector  $r$  at the radial point  $r$  corresponding to frequency point  $x(=(v-v_0)/\Delta s)$ ,  $\Delta s$  being some standard frequency interval in the line).  $V(r)$  is the velocity of the gases at  $r$  and  $K(x, r)$  and  $K_c(r)$  are the absorption coefficients per unit frequency interval in the line and continuum respectively. The quantities  $S_L(r)$  and  $S_c$  are the line and continuum source functions respectively and are given by

$$S_L(r) = \frac{(1-\epsilon)}{2} \int_{-\infty}^{+\infty} J(x, r) \phi(x) dx + \epsilon B(r) \quad (52)$$

$$S_c = \rho(r) B(r) \quad (53)$$

$$K(x, r) = K_L(r) \phi(x) \quad (54)$$

where  $K_L(r)$  is the line-centre absorption coefficient and  $\phi(x)$  is the normalised line profile.  $B(r)$  is the Planck function and  $\rho(r)$  is an unspecified parameter.  $\epsilon$  is the probability per scattering that a photon

is lost from the line by collisional de-excitation of the excited states.  $J(x,r)$  is the mean intensity.

We integrate equations (50) and (51) in the same manner as described section BI. The corresponding discrete equations are written as

$$M \left[ \begin{matrix} U_{n+1}^+ \\ U_n^+ \end{matrix} \right] + \rho_c \left[ \begin{matrix} \Lambda^+ U_{n+1/2}^+ + \Lambda^- U_{n+1/2}^- \\ \Lambda^+ U_{n+1/2}^+ + \Lambda^- U_{n+1/2}^- \end{matrix} \right] + \tau_{n+1/2} \phi_{n+1/2} U_{n+1/2}^+ = \tau_{n+1/2} S_{n+1/2} + \frac{1}{2} (1-\epsilon) \tau_{n+1/2} \left[ \begin{matrix} \phi \phi^t \omega \\ \phi \phi^t \omega \end{matrix} \right] \left[ \begin{matrix} U^+ \\ U^- \end{matrix} \right]_{n+1/2} + M_{-1} dU_{n+1/2}^+ \tag{55}$$

similarly

$$M \left[ \begin{matrix} U_n^- \\ U_{n+1}^- \end{matrix} \right] - \rho_c \left[ \begin{matrix} \Lambda^+ U_{n+1/2}^- + \Lambda^- U_{n+1/2}^+ \\ \Lambda^+ U_{n+1/2}^- + \Lambda^- U_{n+1/2}^+ \end{matrix} \right] + \tau_{n+1/2} \phi_{n+1/2} U_{n+1/2}^- = \tau_{n+1/2} S_{n+1/2} + \frac{1}{2} (1-\epsilon) \tau_{n+1/2} \left[ \begin{matrix} \phi \phi^t \omega \\ \phi \phi^t \omega \end{matrix} \right] \left[ \begin{matrix} U^+ \\ U^- \end{matrix} \right]_{n+1/2} + M_{-1} dU_{n+1/2}^- \tag{56}$$

where

$$U_n^+ = \left[ \begin{matrix} U_{1,n}^+ \\ U_{2,n}^+ \\ U_{3,n}^+ \\ \dots \\ U_{i,n}^+ \\ \dots \\ U_{I,n}^+ \end{matrix} \right]^t \tag{57}$$

$t$  indicates the transpose of the vector.

$$U_{-1,n}^+ = 4\pi r_n^2 \begin{bmatrix} \bar{I}(\tau_n, \mu_1, x_1) \\ I(\tau_n, \mu_2, x_1) \\ \dots \\ I(\tau_n, \mu_J, x_1) \end{bmatrix} \tag{58}$$

Here  $I$  and  $J$  are the total number of frequency points and angle points respectively.

$$\phi_{n+1/2} = \left[ \begin{matrix} \phi_{kk'} \end{matrix} \right]_{n+1/2} = (\beta + \phi_k)_{n+1/2} \delta_{kk'} \tag{59}$$

where

$$\beta = \frac{Kc}{KL}$$

and

$$k = j + (i-1)J, 1 \leq k \leq K = IJ$$

$j$  and  $i$  being the running indices of angle and frequency quadrature. The subscript  $n+1/2$  represents the average of the parameter over the shell bounded by radii  $r_n$  and  $r_{n+1}$ . Moreover,

$$\begin{aligned} \phi_k &= \phi(x_j, \mu_j) \\ S_{n+1/2} &= (\rho\beta + \epsilon\phi_k) B'_{n+1/2} \delta_{kk'} \\ B'_{n+1/2} &= 4\pi r_{n+1/2}^2 B(r_{n+1/2}) \\ \phi_{-1}^+ V_k &= a_{1c} c_j \end{aligned} \tag{60}$$

with



$$a_i = \frac{A_i \phi_i}{\sum_{i=1}^I A_i \phi(x_i)} \tag{61}$$

$A_i^{\pm}$  being the quadrature weights for the frequency points. The matrices  $\underline{M}$  and  $\underline{\Lambda}^{\pm}$

$$\underline{M} = \begin{bmatrix} M_m & & & \\ & M_m & & \\ & & \ddots & \\ & & & M_m \end{bmatrix}, \underline{\Lambda}^+ = \begin{bmatrix} \Lambda_m^+ & & & \\ & \Lambda^+ & & \\ & & \ddots & \\ & & & \Lambda^+ \end{bmatrix} \tag{62}$$

with

$$M_m = [\mu_j \delta_{jk}] \text{ and similarly } \underline{\Lambda}^- \text{ is defined.}$$

and  $\underline{\Lambda}^{\pm}$  are the curvature matrices given Appendix AI. The quantity  $M_{n+1/2}$  in equations (55) and (56) are the equivalents of the comoving terms in equations (50) and (51). We have

$$M_{n+1/2} = [\underline{M}^1 \Delta V_{n+1/2} + M^2 \rho_c V_{n+1/2}] \tag{63}$$

$$M_m^1 = \begin{bmatrix} M_m^1 & & & \\ & M_m^1 & & \\ & & \ddots & \\ & & & M_m^1 \end{bmatrix}, M_m^1 = [(\mu_j^2 \delta_{j1})] \tag{64}$$

$$M_m^2 = \begin{bmatrix} M_m^2 & & & \\ & M_m^2 & & \\ & & \ddots & \\ & & & M_m^2 \end{bmatrix}, M_m^2 = [(1-\mu_j^2) \delta_{j1}] \tag{65}$$

$$j, 1=1, 2, \dots, J, \Delta V_{n+1/2} = V_{n+1} - V_n$$

The matrix  $d$  is determined from the condition of flux conservation and is given by

$$d = \begin{bmatrix} -d_1 & d_1 & \dots & & \\ -d_2 & 0 & d_2 & \dots & \\ & -d_3 & 0 & & \\ & & -d_4 & & d_{I-1} \\ & & & -d_I & d_I \end{bmatrix} \tag{66}$$

where  $d_i = (x_{i+1} - x_{i-1})^{-1}$  for  $i=2, 3, \dots, I-1$

We set  $d_1 = d_I = 0$  as boundary condition on the frequency integration.

The average intensities  $\underline{U}_{n+1/2}^+, \underline{U}_{n+1/2}^-$  are approximated

by the diamond scheme given by

$$\frac{1}{2}(U_{-n}^+ + U_{-n+1}^+) = U_{-n+\frac{1}{2}}^+ \quad (67)$$

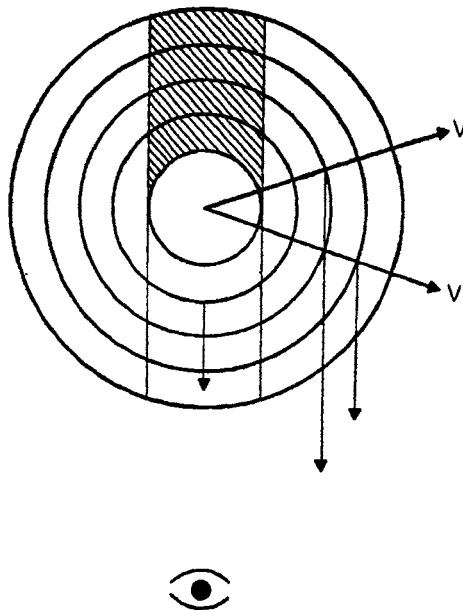
and

$$\frac{1}{2}(U_{-n}^- + U_{-n+1}^-) = U_{-n+\frac{1}{2}}^-$$

Substituting equation (63) into equations (55) and (56) and arranging the resulting equations in the form of the equations of interaction principle, we obtain the  $r$  &  $t$  operators for the cell. These are given in the Appendix III. The critical optical thickness can be estimated from the condition that the  $r$  and  $t$  operators be non negative.

Using the source functions that are obtained in the comoving frame, one can obtain the radiation field transformed to a point at infinity (see figure 5), or on to a rest frame whichever is necessary. We shall present calculations of spectral lines obtained in the static and moving media (rest-frame and comoving frame).

Figure 5. Schematic diagram showing how fluxes are calculated at infinity



In a static medium we have no velocity fields and all the comoving frame terms in equations (50) and (51) vanish (assuming that the velocity gradients are also absent). We have performed some calculations in this situation and these results are presented in figure 6 and 7.

Figure 6. Symmetric line profiles for LTE and non LTE and plane parallel (pp) and spherically symmetric media. Calculations have been done in static media with  $(B/A)^2=1$  for pp and  $(B/A)^2=2$  for SS. The total optical depth is taken to be 200 and the Planck function is set  $B(r)=\exp(-T/n^2)$  where  $n$  is the number of the shell ( $n=1$  at  $r=b$  and  $n=N$  at  $r=a$  and  $N=150$ ). This Planck function represents an atmosphere with decreasing temperature outwards. Taken from Peraiah (1973).

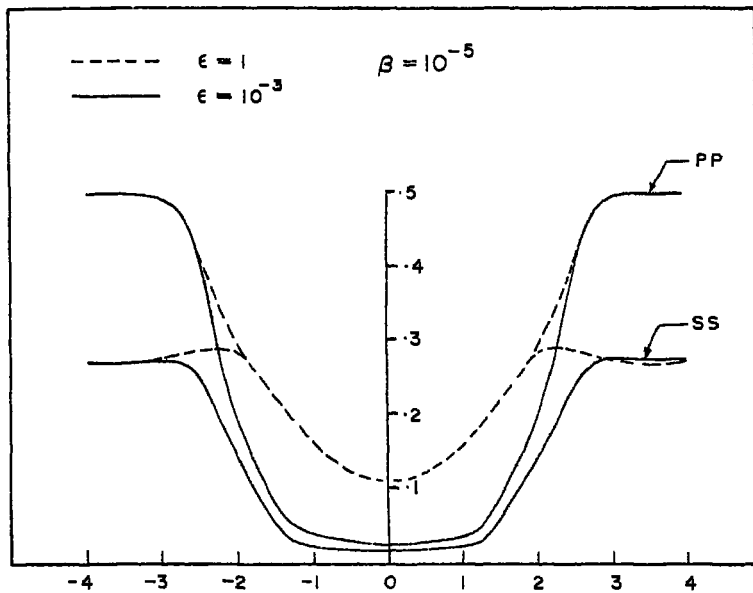
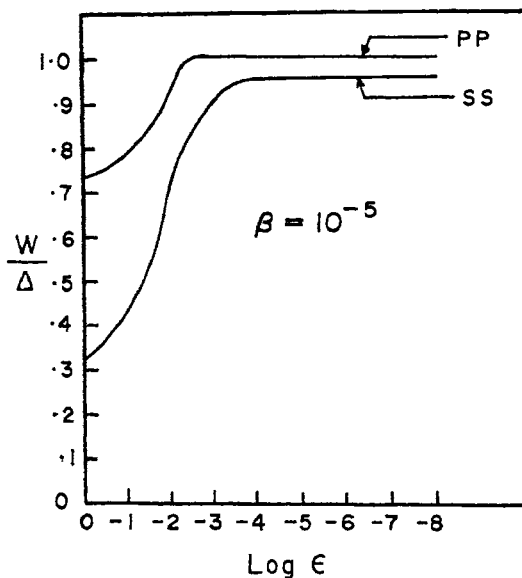


Figure 7. Equivalent widths are plotted against  $\log \epsilon$  for PP and SS with the same parameters given in figure 6. Taken from Peraiah (1973).



We need not employ the full angle-frequency mesh for differencing as we are calculating the line in a static medium and it is enough if we solve half the number of equations necessary to obtain the line profile. We employed 14 frequency points in  $X\epsilon(-4,+4)$  and 2 angle points  $(\mu_1, \mu_2)$  over  $\mu\epsilon(0,1)$ . These points are taken from Gauss-Legendre quadrature. (see Grant and Peraiah 1972). In figure 6, we have plotted frequency dependant fluxes in the line for  $\beta=10^{-5}$  and  $\epsilon=1$  for LTE and  $\epsilon=10^{-3}$  for Non LTE situation, with a two level atom approximation. We performed calculations in plane parallel (PP) stratification with  $(B/A)^2=1$  and in spherically symmetric shells with  $(B/A)^2=2$  where B and A are the outer and inner radii in the spherical medium. Effects due to non LTE physics and sphericity are conspicuous. In figure 7, we have shown how the equivalent widths change due to changes in  $\epsilon$  and B/A.

In figure 8, we have given the line profiles of the emergent hydrogen Lyman alpha line for a nebula expanding uniformly with twice the thermal velocity, (see Peraiah and Wehrse 1978). These calculations are done in the restframe, and for details the reader may refer to the

above paper.

**Figure 8.** Profiles of the emergent hydrogen Ly $\alpha$  line for a nebula expanding uniformly with twice the thermal velocity. These profiles are calculated in the rest frame.  $\tau_d$  is the dust optical depth. Taken from Peraiah and Wehrse (1978).

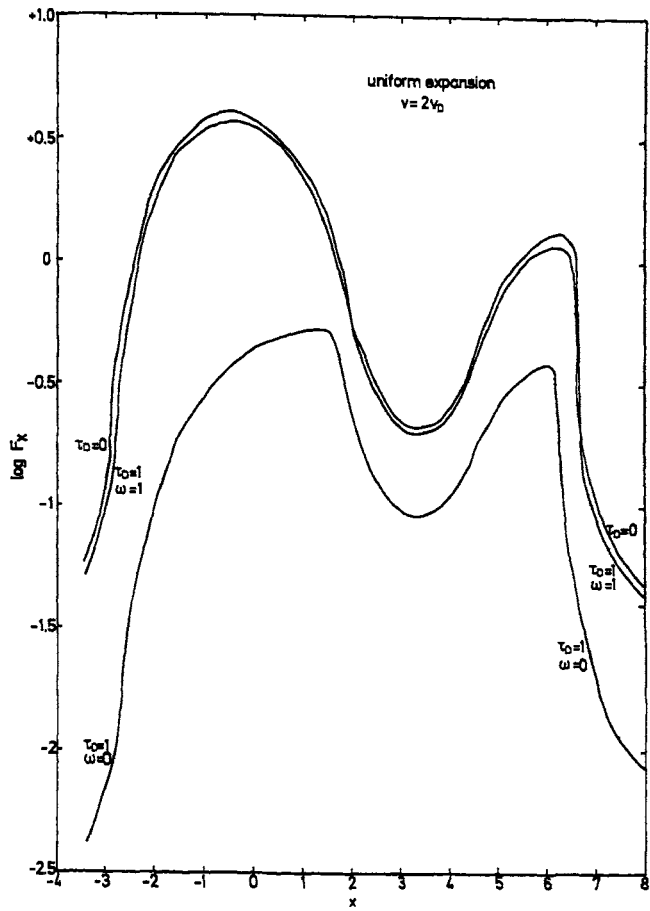
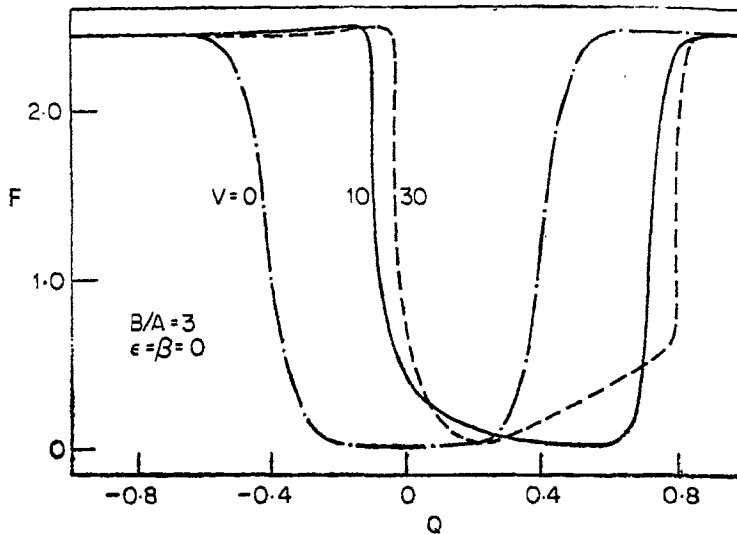


Figure 9. Flux profiles of the lines received at the observer  $F = F(x)/F(X_{max})$  and  $Q = X/X_{max}$ . These profiles are transformed from comoving to a frame at infinity. Taken from Peraiah (1980).



The comoving frame calculations have been done with partial frequency redistribution in an isothermal atmosphere (Peraiah 1980). We calculate the frequency dependent source functions in the comoving frame and it is transformed on to a point at infinity. We have presented in figure 9 such profiles calculated using angle averaged redistribution function  $R_I$  in the comoving frame. Here we have used a velocity law with constant velocity gradients

$$V(r) = V_A + \frac{V_B - V_A}{B - A}(r - A)$$

Where  $V_B$  and  $V_A$  are the velocities (in mean thermal units) at radial points  $a$  and  $b$  respectively. The velocity  $V_A$  is always set equal to 0 and the numbers corresponding to each curve represent the velocities at  $b$  (i.e.)  $V_B$ . When  $V_A = V_B = 0$  (static medium) we obtain a symmetric line profile and when the velocity increases, the line becomes asymmetric.

Appendix I (AI)

The curvature scattering matrices are

$$C_j \Lambda_{jk}^+ = \frac{(1-\mu_{j+\frac{1}{2}}^2)(\mu_{j+\frac{1}{2}}-\mu_j)}{(\mu_{j+1}-\mu_j)}, k=j+1, j=1, 2, \dots, J-1$$

$$= \frac{(1-\mu_{j+\frac{1}{2}}^2)(\mu_{j+1}-\mu_{j+\frac{1}{2}})}{(\mu_{j+1}-\mu_j)} - \frac{(1-\mu_{j-\frac{1}{2}}^2)(\mu_{j-\frac{1}{2}}-\mu_{j-1})}{(\mu_j-\mu_{j-1})}$$

$$k=j, j=1, 2, \dots, J$$

$$= \frac{(1-\mu_{j-\frac{1}{2}}^2)(\mu_j-\mu_{j-\frac{1}{2}})}{(\mu_j-\mu_{j-1})}, k=j-1, j=2, 3, \dots, J$$

and

$$C_j \Lambda_{jk}^- = -\frac{1}{2} \delta_{j,1} \delta_{k,1}$$

The  $\mu$ 's and  $c$ 's are the roots and weights of Gauss - Legendre quadrature on  $\mu \in (0,1)$  (see Abramowitz and Stegun 1970, page 921).

For  $J=2, \mu_1 = .21132, \mu_2 = .78868, c_1 = c_2 = .5$

$$\Lambda^+ = \begin{bmatrix} -.25 & .75 \\ -.75 & -.75 \end{bmatrix} \Lambda^- = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}$$

For  $J=4$

$\mu_1 = .06943 \mu_2 = .33001 \mu_3 = .66999 \mu_4 = .93057$

$c_1 = .17393 c_2 = .32607 c_3 = .32607 c_4 = .17393$

$$\Lambda^+ = \begin{bmatrix} .46494 & 2.23590 & 0 & 0 \\ -1.78139 & -0.04258 & 1.15005 & 0 \\ 0 & -1.15005 & -0.75945 & 0.58343 \\ 0 & 0 & -.73228 & -1.09379 \end{bmatrix}$$

$$\Lambda^- = -2.87476 \delta_{j,1} \delta_{k,1}$$

Appendix AII

The operators of transmission and reflection are given by

$$\underline{t}(n+1, n) = \underline{t}^+ \begin{bmatrix} \underline{\Delta}^+ \underline{S}^{++} + \underline{r}^- & \underline{r}^- \\ \underline{\Delta}^- \underline{S}^{--} + \underline{r}^+ & \underline{r}^+ \end{bmatrix}$$

$$\underline{t}(n, n+1) = \underline{t}^- \begin{bmatrix} \underline{\Delta}^- \underline{S}^{--} + \underline{r}^+ & \underline{r}^+ \\ \underline{\Delta}^+ \underline{S}^{++} + \underline{r}^- & \underline{r}^- \end{bmatrix}$$

$$\underline{r}(n+1, n) = 2 \underline{t}^- \underline{r}^- \underline{\Delta}^+ \underline{M}$$

$$\underline{r}(n, n+1) = \underline{t}^+ \underline{r}^+ \underline{\Delta}^- \underline{M}$$

and the source vectors are

$$\underline{\Sigma}_{n+\frac{1}{2}}^+ = \underline{\tau}_{n+\frac{1}{2}} (1-\omega) \underline{t}^+ \begin{bmatrix} \underline{\Delta}^+ \underline{B}^+ + \underline{r}^- & \underline{r}^- \\ \underline{\Delta}^- \underline{B}^- & \underline{r}^+ \end{bmatrix}$$

$$\underline{\Sigma}_{n+\frac{1}{2}}^- = \underline{\tau}_{n+\frac{1}{2}} (1-\omega) \underline{t}^- \begin{bmatrix} \underline{\Delta}^- \underline{B}^- + \underline{r}^+ & \underline{r}^+ \\ \underline{\Delta}^+ \underline{B}^+ & \underline{r}^- \end{bmatrix}$$

$$\underline{t}^+ = \begin{bmatrix} \underline{I} - \underline{r}^- & \underline{r}^- \\ \underline{r}^- & \underline{r}^- \end{bmatrix}^{-1}, \underline{t}^- = \begin{bmatrix} \underline{I} - \underline{r}^+ & \underline{r}^+ \\ \underline{r}^+ & \underline{r}^+ \end{bmatrix}^{-1}$$

$$\underline{r}^+ = \underline{\Delta}^+ \underline{S}^{+-}, \underline{r}^- = \underline{\Delta}^- \underline{S}^{-+}$$

$$\underline{\Delta}^+ = \left[ \underline{M} + \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} (\underline{I} - \underline{Q}_{n+\frac{1}{2}}^{++}) \right]^{-1}$$

$$\underline{\Delta}^- = \left[ \underline{M} + \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} (\underline{I} - \underline{Q}_{n+\frac{1}{2}}^{--}) \right]^{-1}$$

$$\underline{S}^{++} = \underline{M} - \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} (\underline{I} - \underline{Q}_{n+\frac{1}{2}}^{++})$$

$$\underline{S}^{--} = \underline{M} - \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} (\underline{I} - \underline{Q}_{n+\frac{1}{2}}^{--})$$

$$\underline{S}^{-+} = \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} \underline{Q}_{n+\frac{1}{2}}^{-+} \text{ and } \underline{S}^{+-} = \frac{1}{2} \underline{\tau}_{n+\frac{1}{2}} \underline{Q}_{n+\frac{1}{2}}^{+-}$$

$$\underline{Q}_{n+\frac{1}{2}}^{++} = \frac{1}{2} \omega \underline{p}^{++} \underline{c} - \rho \underline{\Lambda}^+ / \underline{\tau}_{n+\frac{1}{2}}$$

$$\underline{Q}_{n+\frac{1}{2}}^{--} = \frac{1}{2} \omega \underline{p}^{--} \underline{c} + \rho \underline{\Lambda}^- / \underline{\tau}_{n+\frac{1}{2}}$$

$$\underline{Q}_{n+\frac{1}{2}}^{-+} = \frac{1}{2} \omega \underline{p}^{-+} \underline{c} + \rho \underline{\Lambda}^- / \underline{\tau}_{n+\frac{1}{2}}$$

$$\underline{Q}_{n+\frac{1}{2}}^{+-} = \frac{1}{2} \omega \underline{p}^{+-} \underline{c} - \rho \underline{\Lambda}^+ / \underline{\tau}_{n+\frac{1}{2}}$$



Appendix AIII

$$\sigma = 1 - \epsilon, \quad \underline{Y} = \frac{1}{2} \sigma \left[ \underline{\phi} \underline{\phi}^t \underline{W} \right], \quad \underline{Z} = \underline{\phi} - \underline{Y}$$

$$\underline{Z}_+ = \underline{Z} + \rho_c \underline{\Lambda}^+ / \tau - \frac{M_1 d}{\tau}, \quad \underline{Y}_+ = \underline{Y} + \frac{\rho_c \underline{\Lambda}^-}{\tau}$$

$$\underline{Z}_- = \underline{Z} - \rho_c \underline{\Lambda}^+ / \tau - \frac{M_1 d}{\tau}, \quad \underline{Y}_- = \underline{Y} - \rho_c \underline{\Lambda}^- / \tau$$

$$\underline{\Delta}^\pm = \left[ \underline{M} + \frac{1}{2} \tau \underline{Z}_\pm \right]^{-1}, \quad \underline{\Gamma}^\pm = \left[ \underline{M} - \frac{1}{2} \tau \underline{Z}_\pm \right]$$

$$\underline{\beta}^{+-} = \frac{1}{2} \tau \underline{\Delta}^+ \underline{Y}_-, \quad \underline{\alpha}^{+-} = \left[ \underline{I} - \underline{\beta}^{+-} - \underline{\beta}^{-+} \right]^{-1}$$

Similarly  $\underline{\beta}^{-+}$  and  $\underline{\alpha}^{-+}$  are defined. Now we shall write the transmission and reflection matrices and the source vector as

$$t(n+1, n) = \underline{\alpha}^{+-} \left[ \underline{\Delta}^+ \underline{\Gamma}^+ + \underline{\beta}^{+-} - \underline{\beta}^{-+} \right]$$

$$r(n+1, n) = \underline{\alpha}^{-+} \underline{\beta}^{-+} \left[ \underline{I} + \underline{\Delta}^+ \underline{\Gamma}^+ \right]$$

$$\text{and } \underline{\Sigma}_{n+\frac{1}{2}}^+ = \tau \underline{\alpha}^{+-} \left[ \underline{\Delta}^+ + \underline{\beta}^{+-} - \underline{\Delta}^- \right] \underline{S}$$

The operators  $t(n, n+1)$ ,  $r(n, n+1)$  and  $\underline{\Sigma}_{n+\frac{1}{2}}^-$  are obtained by interchanging the + and - signs in the operators  $t(n+1, n)$ ,  $r(n, n+1)$  and  $\underline{\Sigma}_{n+\frac{1}{2}}^+$  respectively.

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