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Effects of High Radial Velocities on Line Transfer in Extended Atmospheres

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ABSTRACT

The equation of radiative transfer in comoving frame has been solved for rapidly expanding gaseous medium in spherically symmetric extended stellar atmospheres. We have assumed a non-LTE two-level atom with Voigt profile function. The comoving terms in the radiative transfer are discretized in the frame work of discrete space theory of Grant. These terms simply reduce to a tri-diagonal matrix. The boundary conditions for the frequency derivative can be introduced through the elements of the first and last rows of this matrix. This seems to be quite stable for arbitrary velocities in the medium. We have considered maximum velocities up to 60 units of mean thermal velocities.

1. Introduction

The effect of high velocities on the formation of spectral lines in the outer layers of stars is very important. It is known that the matter moves at very high radial velocities in such diverse objects as Wolf-Rayet stars, quasars, novae, P Cygni, Planetary nebulae *etc.* The problem is complicated because the physical properties of the medium (*e.g.* absorption, emission, scattering characteristics) are affected by the local conditions of the moving matter. Several people attempted to solve the problem of transfer of line radiation by the moving media (Kunasz and Hummer 1974, Peraiah and Wehrse 1978, Wehrse and Peraiah 1979 and others). However, these calculations have been done in observer's frame and naturally restricted to small velocities. Therefore, to study the formation of lines in rapidly moving stellar atmospheres, one must study the solution of line transfer in the comoving frame. Chandrasekhar (1945) and Abhyankar (1964) made some of the earliest attempts. These methodes were restricted to assumptions such as coherent scattering, plane parallel atmospheres *etc.* Recently, Simmonneau (1973) has developed a method for the comoving frame solution of the line transfer which is restricted again to certain velocity laws. There is considerable amount of work done by Mihalas *et al.* (1975, 1976) on comoving frame calculations. However, these are iterative and, therefore, time consuming.

We shall develop a method to obtain a direct solution of line transfer in comoving frame of the gas in the frame work of discrete space theory (see Grant and Peraiah 1972). The comoving terms are discretized easily into a single tridiagonal matrix with the velocity and frequency boundary conditions prescribed in the elements of this matrix.

In the next section, we shall describe briefly the method and in section 3 a few samples of the results are presented.

2. Description of the Method

The comoving terms which appear in the transfer equation are (see Chandrasekhar 1945, Mihalas *et al.* 1975)

$$\left\{(1-\mu^2)\frac{V(r)}{r}+\mu^2\frac{\mathrm{d}V(r)}{\mathrm{d}r}\right\}\frac{\partial I(x,\mu,r)}{\partial x}, \tag{1}$$

where $I(x, \mu, r)$ is the specific intensity of the ray with frequency $x = (\nu-\nu_0)/\Delta_s$, Δ_s being some standard frequency interval, ν_0 is the central frequency of the line and ν is any frequency point in the line) making an angle $\cos^{-1}\mu$ with the radius vector at the radial point r. $V(r)$ is the velocity of the gas in mean thermal units at the radial point r. We shall incorporate the comoving terms given in Eq. (1) into the radiative transfer and write it (see Mihalas *et al.* 1975, 1976) for a Non-LTE two-level atom as,

$$\mu\frac{\partial I(x,\mu,r)}{\partial r}+\frac{1-\mu^2}{r}\frac{\partial I(x,\mu,r)}{\partial\mu} = K(x,r)S_L(r)+ +K_c(r)S_c(r)-[K(x,r)+K_c(r)]I(x,\mu,r)+ +\left\{(1-\mu^2)\frac{V(r)}{r}+\mu^2\frac{\mathrm{d}V(r)}{\mathrm{d}r}\right\}\frac{\partial I(x,\mu,r)}{\partial x}, \tag{2}$$

and for the oppositely directed beam,

$$-\mu\frac{\partial I(x,-\mu,r)}{\partial r}-\frac{1-\mu^2}{r}\frac{\partial I(x,-\mu,r)}{\partial\mu} = K(x,r)S_L(r)+ +K_c(r)S_c(r)-[K(x,r)+K_c(r)]I(x,-\mu,r)+ +\left\{(1-\mu^2)\frac{V(r)}{r}+\mu^2\frac{\mathrm{d}V(r)}{\mathrm{d}r}\right\}\frac{\partial I(x,-\mu,r)}{\partial x}, \tag{3}$$

where $K(x, r)$ and $K_c(r)$ are the absorption coefficients per unit frequency interval in the line and continuum respectively. The quantities $S_L(r)$ and $S_c(r)$ are the line and continuum source functions respectively and are given by

$$S_L(r) = \frac{(1-\varepsilon)}{2} \int_{-1}^{+1} \int_{-\infty}^{+\infty} dx \varphi(x) I(x, \mu, r) + \varepsilon B(r), \tag{4}$$

$$S_c(r) = \varrho(r) B(r), \tag{5}$$

$$K(x, r) = \varphi(x) K_L(r). \tag{6}$$

$K_L(r)$ is the absorption at line centre and $\varphi(x)$ is the line profile subjected to normalization such that

$$\int_{-\infty}^{+\infty} \varphi(x) dx = 1. \tag{7}$$

We have chosen Voigt profile given by

$$\varphi(a, x) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2} dy}{(x-y)^2 + a^2}. \tag{8}$$

The optical depth in the line is given by

$$\tau(x, r) = K(x, r) \Delta r = \frac{\pi^{1/2} e^2}{mc} \frac{N(r) f}{\Delta \nu_D} \varphi(a, x) \Delta r, \tag{9}$$

where $N(r)$ is the particle density. The quantity ε is the probability per scatter that a photon is lost by collisional de-excitation. The quantity $B(r)$ is the Planck function and $\varrho(r)$ is an arbitrary factor.

We shall now integrate the line transfer Eqs. (2) and (3) along similar lines as shown in Peraiah and Grant (1973), Grant and Peraiah (1972), and Peraiah (1978) by incorporating the comoving terms. In discrete space theory, we approximate the integrals by the appropriate quadrature sums and the differentials by the weighted differences. For example the integration over angle variable is effected by the formula

$$\int_0^1 f(\mu) d\mu \simeq \sum_{j=1}^{J} c_j f(\mu_j), \quad \sum_{j=1}^{J} c_j = 1, \tag{10}$$

μ_j and c_j being the zeros and weights of a quadrature formula over $[0, 1]$, and J is the total number of angles. We shall define,

$$C = [c_j \delta_{jk}], \quad M_m = [\mu_j \delta_{jk}],$$

and corresponding specific intensities as

$$U^{+}_{i,n} = 4\pi r_n^2 \begin{bmatrix} I(\tau_n, \mu_1, x_i) \\ I(\tau_n, \mu_2, x_i) \\ \cdots\cdots \\ I(\tau_n, \mu_J, x_i) \end{bmatrix}, \tag{11}$$

and

$$U^{\pm}_{n} = [U^{\pm}_{1,n}, U^{\pm}_{2,n}, U_{3,n}, \ldots, U^{\pm}_{i,n}, \ldots, U^{\pm}_{I,n}]^T, \tag{12}$$

where T is transpose. Further, we shall write

$$\Phi_{n+1/2} = [\Phi_{kk'}]_{n+1/2} = (\beta+\varphi_k)_{n+1/2}\,\delta_{kk'}, \tag{13}$$

where

$$\beta = K_c/K_L,$$

and

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

i and j being the running indices of frequency and angle quadrature points and I is the total number of frequency points. The subscript $n+\frac{1}{2}$ represents the average of the parameter over the shell bounded by radii r_n and r_{n+1}. And write

$$\begin{aligned} \varphi_k &= \varphi(x_i, \mu_j), \\ S_{n+1/2} &= (\varrho\beta+\varepsilon\varphi_k)B'_{n+1/2}\,\delta_{kk'}, \\ B'_{n+1/2} &= 4\pi r^2_{n+1/2} B(r_{n+1/2}), \\ \varphi_i W_k &= a_i c_j, \\ a_i &= \frac{A_i\varphi_i}{\sum\limits_{i'=-I}^{I} A_{i'}\varphi(x_{i'})}, \end{aligned} \tag{14}$$

where A's are the quadrature weights for the frequency points. With the above definitions, Eqs (2) and (3) become after integration,

$$\begin{aligned} M[U^{+}_{n+1} - U^{+}_{n}] + \varrho_c[\Lambda^{+} U^{+}_{n+1/2} + \Lambda^{-} U^{-}_{n+1/2}] + \\ + \tau_{n+1/2}\Phi_{n+1/2} U^{+}_{n+1/2} = \tau_{n+1/2} S_{n+1/2} + \\ + \tfrac{1}{2}(1-\varepsilon)\,\tau_{n+1/2}[\Phi\Phi^T W][U^{+} + U^{-}]_{n+1/2} + \\ + M_1\, dU^{+}_{n+1/2}, \end{aligned} \tag{15}$$

Similarly,

$$\begin{aligned} M[U^{-}_{n} - U^{-}_{n+1}] - \varrho_c[\Lambda^{+} U^{-}_{n+1/2} + \Lambda^{-} U^{+}_{n+1/2}] + \tau_{n+1/2}\Phi_{n+1/2} U^{+}_{n+1/2} \\ = \tau_{n+1/2} S_{n+1/2} + \tfrac{1}{2}(1-\varepsilon)\,\tau_{n+1/2}[\Phi\Phi^T W][U^{+} + U^{-}] + M_1\, d\, U^{-}_{n+1/2} \end{aligned} \tag{16}$$

where

$$M = \begin{bmatrix} M_m & & & 0 \\ & M_m & & \\ & & \ddots & \\ 0 & & & M_m \end{bmatrix}, \quad \Lambda^{\pm} = \begin{bmatrix} \Lambda_m^{\pm} & & & 0 \\ & \Lambda_m^{\pm} & & \\ & & \ddots & \\ 0 & & & \Lambda_m^{\pm} \end{bmatrix} \tag{17}$$

$M_m = [\mu_j \delta_{jk}]$ and $\Lambda_m^{\pm}$ are the curvature matrices (see Peraiah and Grant 1973 for their derivation). The comoving terms given in (1) are represented by the term $M_1 dU_{n+1/2}^{\pm}$ in Eqs. (15) and (16). This is explained as follows:

$$M_1 = [M^1 \Delta V_{n+1/2} + M^2 \varrho_c V_{n+1/2}],$$

$$M^1 = \begin{bmatrix} M_m^1 & & & 0 \\ & M_m^1 & & \\ & & \ddots & \\ 0 & & & M_m^1 \end{bmatrix}, \quad M_m^1 = [\mu_j^2 \delta_{jl}],$$

$$M^2 = \begin{bmatrix} M_m^2 & & & 0 \\ & M_m^2 & & \\ & & \ddots & \\ 0 & & & M_m^2 \end{bmatrix}, \quad M_m^2 = [(1-\mu_j^2)\delta_{jl}], \tag{18}$$

$$j, l = 1, 2, \ldots, J, \qquad \Delta V_{n+1/2} = V_{n+1} - V_n.$$

$V_{n+1/2}$ is the average velocity over the shell bounded by the radii r_{n+1} and r_n. The matrix d is determined from the condition of flux conservation (see Appendix II) and is given by

$$d = \begin{bmatrix} -d_1 & d_1 & 0 & & & \\ -d_2 & 0 & d_2 & & 0 & \\ 0 & -d_3 & 0 & d_3 & & \\ & & \ddots & \ddots & \ddots & \\ 0 & & & & & d_{I-1} \\ & & & & -d_I & d_I \end{bmatrix}, \tag{19}$$

where

$$d_i = (x_{i+1} - x_{i-1})^{-1} \quad \text{for } i = 2, 3, \ldots, I-1, \tag{20}$$

and we shall set $d_1 = d_I = 0$.

The average intensities $U_{n+1/2}^{\pm}$ are approximated by the diamond scheme (see Grant 1968, Wiscombe 1976) given by,

$$(I - X_{n+1/2}) U_n^+ + X_{n+1/2} U_{n+1}^+ = U_{n+1/2}^+, \tag{21}$$
$$(I - X_{n+1/2}) U_{n+1}^- + X_{n+1/2} U_n^- = U_{n+1/2}^-,$$

with $X_{n+1/2} = \frac{1}{2}\mathbf{I}$, $\mathbf{I}$ being the unit matrix.

Introducing Eqs. (21) into Eqs. (15) and (16) and writing the resulting equations in the form of interaction principle (see Grant and Hunt 1969a, b)

$$\begin{bmatrix} \boldsymbol{M}+\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{+}+\frac{1}{2}\tau\boldsymbol{\Phi}-\frac{1}{4}\sigma\tau(\phi\phi^T\boldsymbol{W})-\frac{1}{2}\boldsymbol{M}_1\boldsymbol{d} & \frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{-}-\frac{1}{4}\sigma\tau(\phi\phi^T\boldsymbol{W}) \\ -\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{-}-\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W}) & \boldsymbol{M}-\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{+}+\frac{1}{2}\tau\boldsymbol{\Phi}-\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W})-\frac{1}{2}\boldsymbol{M}_1\boldsymbol{d}\end{bmatrix}\begin{bmatrix}\boldsymbol{U}^{+}_{n+1}\\ \boldsymbol{U}^{-}_{n}\end{bmatrix}$$
$$=\begin{bmatrix} \boldsymbol{M}-\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{+}-\frac{1}{2}\tau\boldsymbol{\Phi}+\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W})+\frac{1}{2}\boldsymbol{M}_1\boldsymbol{d} & -\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{-}+\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W}) \\ \frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{-}+\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W}) & \boldsymbol{M}+\frac{1}{2}\varrho_c\boldsymbol{\Lambda}^{+}-\frac{1}{2}\tau\boldsymbol{\Phi}+\frac{1}{4}\tau\sigma(\phi\phi^T\boldsymbol{W})+\frac{1}{2}\boldsymbol{M}_1\boldsymbol{d}\end{bmatrix}$$
$$\begin{bmatrix}\boldsymbol{U}^{+}_{n}\\ \boldsymbol{U}^{-}_{n+1}\end{bmatrix}+\tau\begin{bmatrix}\boldsymbol{S}\\ \boldsymbol{S}\end{bmatrix}, \qquad (22)$$

where $\sigma = 1-\varepsilon$, and $\tau = \tau_{n+1/2}$. A comparison of the Eqs. (22) with the interaction principle will give us the "cell" reflection and transmission matrices and source vectors. These are listed in Appendix I. One can calculate the diffuse radiation field by employing the scheme of Internal Field given in Peraiah and Grant (1973) and by calculating the transmission and reflection matrices in each cell. The optical and geometrical depths in each shell should be chosen such that unique and non-negative solution is obtained. This can be achieved by obtaining non-negative $\boldsymbol{r}$ and $\boldsymbol{t}$ matrices described in Appendix I. For this purpose the diagonal elements of $(\Delta^{\pm})^{-1}$ should be dominant and positive. This condition leads to the inequality

$$\tau_{k,k} < \left|\frac{2\mu_k \pm \varrho_c A^{+}_{k,k} - d_{kk}\{\mu^2_{kk}\,\Delta V_{n+1/2} + (1-\mu^2_{kk})\,\varrho_c V_{n+1/2}\}}{(\beta+\varphi_k)-\frac{1}{2}\sigma(\varphi\varphi^T W)_{kk}}\right|. \qquad (23)$$

Further, the off-diagonal elements of $[\Delta^{\pm}]^{-1}$ should be negative and this gives us

$$\tau_{k,k+1} < \left|\frac{2\varrho_c A^{+}_{k,k+1} - 2d_{k,k+1}\{\Delta V_{n+1/2}\,\mu^2_{k,k+1} + \varrho_c V_{n+1/2}(1-\mu^2_{k,k+1})\}}{\sigma(\varphi\varphi^T W)_{k,k+1}}\right|, \qquad (24)$$

for the upper diagonal elements and

$$\tau_{k+1,k} < \left|\frac{2\varrho_c A^{+}_{k+1,k} + 2d_{k+1,k}\{\Delta V_{n+1/2}\,\mu^2_{k+1,k} + \varrho_c V_{n+1/2}(1-\mu^2_{k+1,k})\}}{\sigma(\varphi\varphi^T W)_{k+1,k}}\right| \qquad (25)$$

for the lower diagonal elements.

We have to select $\tau_{crit} (= \tau_{CELL})$ such that

$$\tau_{crit} = \min\{\tau_{k,k},\ \tau_{k,k+1},\ \tau_{k+1,k}\}. \qquad (26)$$

We notice that the "cell" optical depth τ_{crit} depends on the number of cosines selected for the angle integration, the frequency differencing, the radial mesh, the differential velocity, the local velocity of the gas and the profile function. In the next section, we shall discuss briefly some of the computational aspects and present results.

3. Computational Procedure and Discussion of the Results

The radiation field that is obtained by comoving frame calculations will have to be transformed into (1) the star's rest frame or the observers frame and (2) the observers frame at the earth. The former calculation would give the spherically symmetric solution of the line transfer whereas the latter provides the fluxes received by the observer at earth which facilitates comparison with observations. The procedure is described in Peraiah (1978b, see also Figure 14.7 of Mihalas 1978). In this paper we shall present results which can be compared with observations.

There is a computational advantage in comoving frame calculations particularly with regard to the angle-frequency mesh. In the rest frame calculations, one has to cover the frequency mesh in the interval from $(-X-V_{max})$ to $(X+V_{max})$. When the velocity of the gas is large, we have to select a large number of angle-frequency points. This increases the size of the matrices and machines with large capacities are required. In comoving frame calculations, as we are computing the radiation field in the frame of reference of the gas there are no relative velocities. Consequently, we can employ the profile function corresponding to that of a static medium and we need to employ only a small number of frequency angle points. The program has been tested for several sets of frequency points. Trapezoidal equally spaced frequency points have been chosen with 9, 11, 13, 15 and 19 points, the odd numbers being selected for the sake of including the centre of the line at $x = 0$. The frequency independent source functions S_9, S_{11}, S_{13}, S_{15} and S_{19} have been calculated corresponding to the 9, 11, 13 15 and 17 frequency points. S_9 differs from others in the 4th to 5th place whereas S_{11}, S_{13}, S_{15} and S_{19} agree to about 9th figure. In order to save computer time and storage space one can easily select 11 frequency points and 4 angles. We have considered the line emission and continuum emission with parameters (1) $\varepsilon = 10^{-3}$ and $\beta = 0$ and (2) $\varepsilon = \beta = 10^{-3}$. The total optical depth at line centre is taken to be 10^4 and the damping constant is taken to be 10^{-3}.

We solve the problem subjected to two kinds of boundary conditions: (1) the radiation incident on either side of the atmosphere and (2) the frequency derivative term $\partial I/\partial x$ appearing in the comoving term. In the first case, we have not given any incident radiation on either side of the atmosphere or

$$U^-_{N+1}(x_i, \tau = T, \mu_j) = 0, \qquad U^+_1(x_i, \tau = 0, \mu_j) = 0. \tag{27}$$

In the second case, we shall assume that in the continuum $\partial I/\partial x = 0$. This leads us to

$$[\boldsymbol{dU}^{\pm}_{n+1/2}]_{i=1\,\mathrm{and}\,I} = 0. \tag{28}$$

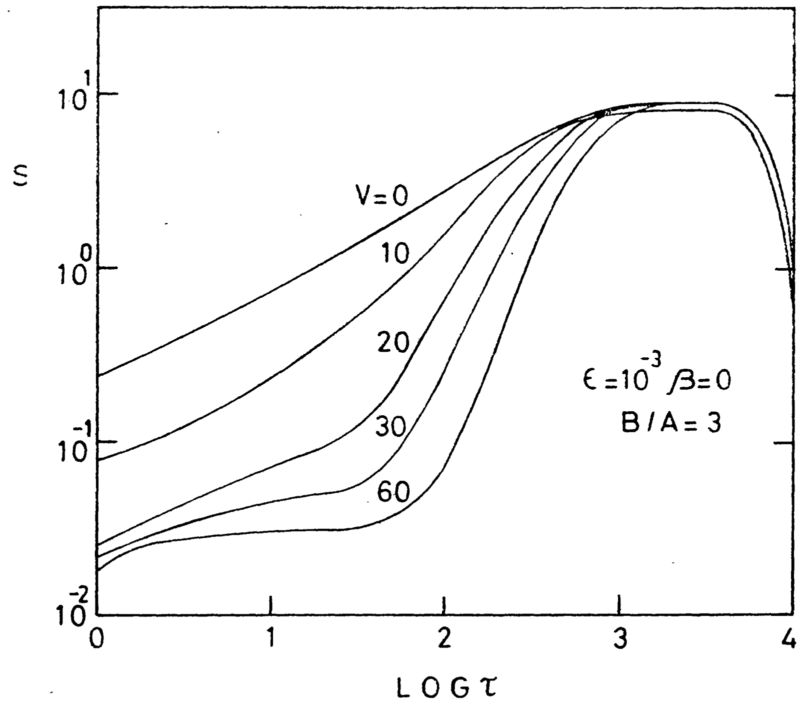

Fig. 1. Frequency independent line source functions for $\varepsilon = 10^{-3}$, $\beta = 0$, $B/A = 3$, are plotted against optical depth.

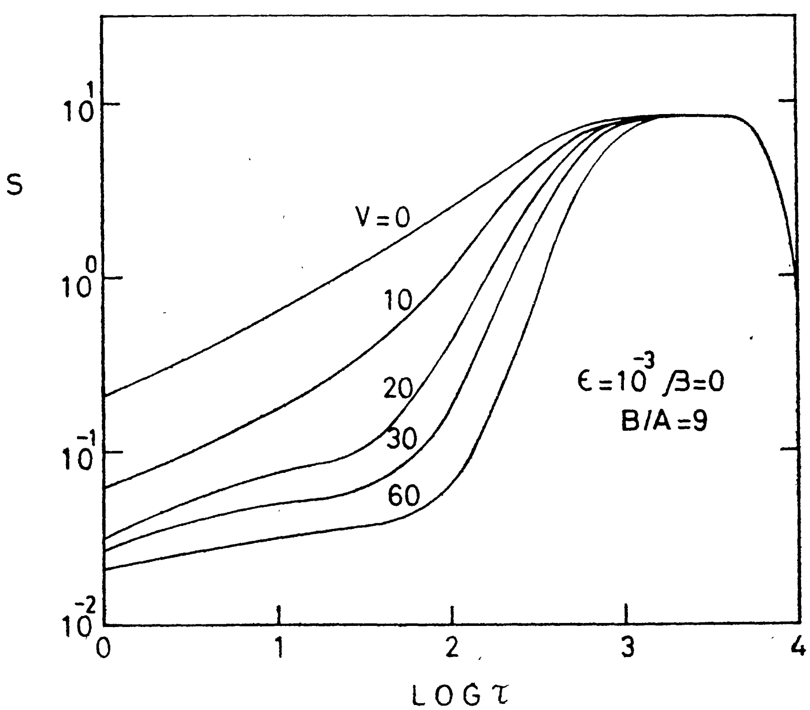

Fig. 2. Same as in those given in Fig. 1 with $B/A = 9$.

In addition to these we have to choose a velocity law which should include the boundary condition of velocity at $n = N$ and $n = 1$. We shall use a linear velocity law given by

$$v(r) = v_A + \frac{v_B - v_A}{B - A}(r - A), \tag{29}$$

where $v(r)$ is the velocity at radius r and v_A and v_B are velocities at $r = A$ and $r = B$. We have selected $v_B = 0, 10, 20, 30$ and 60 and we have always set $v_A = 0$.

Results have been presented in Figs. (1)-(10). The frequency independent line source function S given by

$$S_n = \sum_{i=1}^{I} A_i \sum_{j=1}^{J} S(x_i, \mu_j, \tau_n) c_j,$$

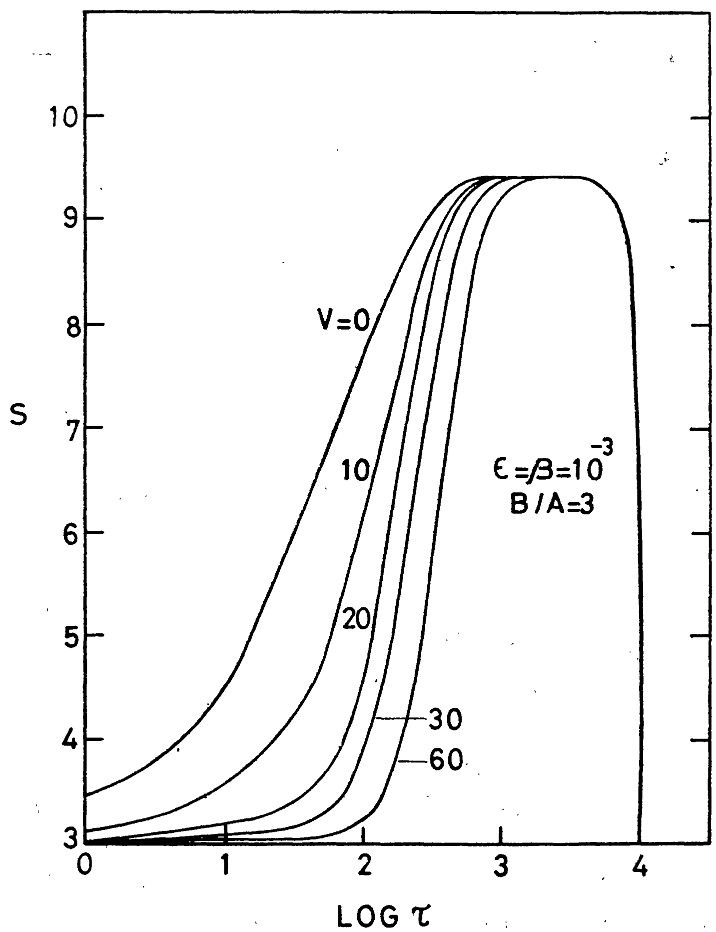

Fig. 3. Same as those given in Fig. 1 with $\varepsilon = 10^{-3} = \beta$ and $B/A = 3$.

and is plotted in Figs. (1)-(4) for various values of the parameters ε, β, B/A and V_B. As there is no radiation incident on either side of the medium, there is a drop in the source functions at $\tau = \tau_{max} (= 10^4)$ and at $\tau = 0$. These results look similar to those of Mihalas *et al.* (1975) although slightly different physical situations are treated here. The line source function

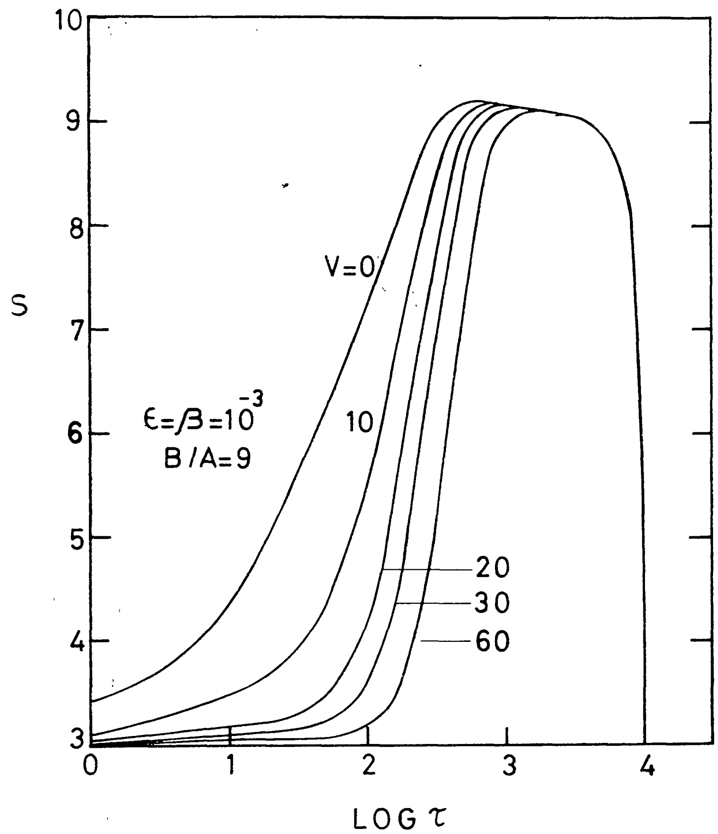

Fig. 4. Same as those given in Fig. 3 with $B/A = 9$.

for a higher velocity fall below the one for a smaller velocity. In Figs. (5) and (6) we have plotted the frequency integrated mean intensities against the optical depth. The same tendency as seen in Figs. (1)-(4) is to be noticed here. We have not shown the mean intensities for $B/A = 9$ for $\varepsilon = 10^{-3}$, $\beta = 0$ and $\varepsilon = \beta = 10^{-3}$ because these do not give any new information. In Figs. (7)-(10), we have plotted the line profiles at the observer's point, corresponding to the line source functions given in Figs. (1)-(4). These are narrow emission lines similar to those observed in quasars (see Baldwin 1975, Baldwin and Netzer 1978). As the velocity increases, the lines become narrow but with extended wings, and this becomes increasingly apparent for larger geometrical extensions.

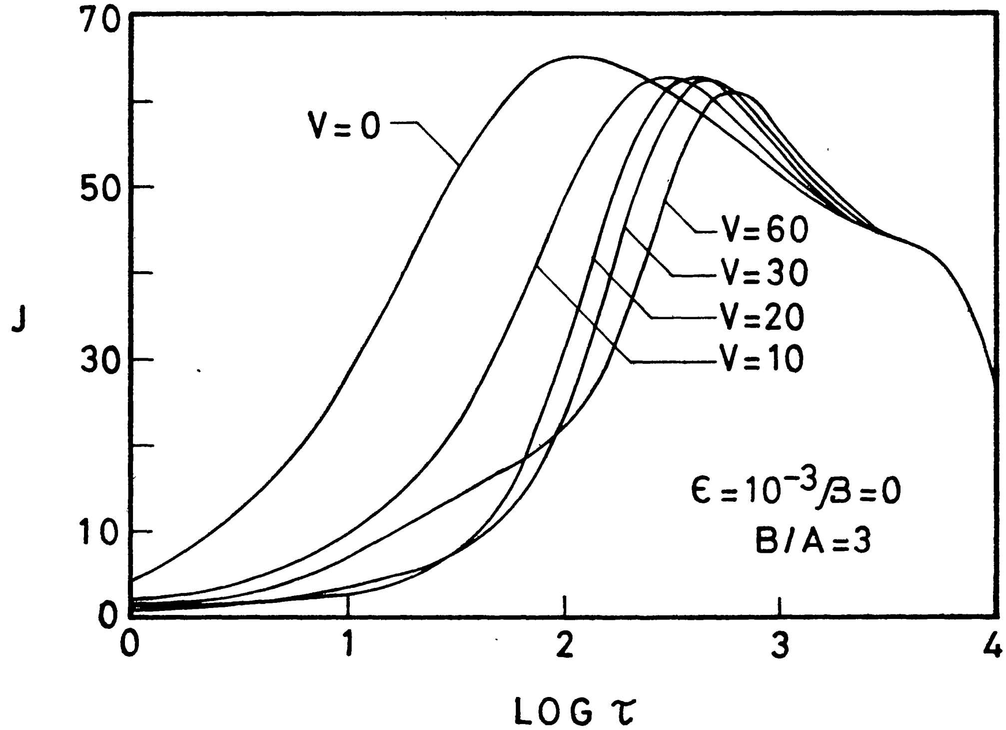

Fig. 5. Total mean intensities in the line are plotted against optical depth for $\varepsilon = \beta = 10^{-3}$.

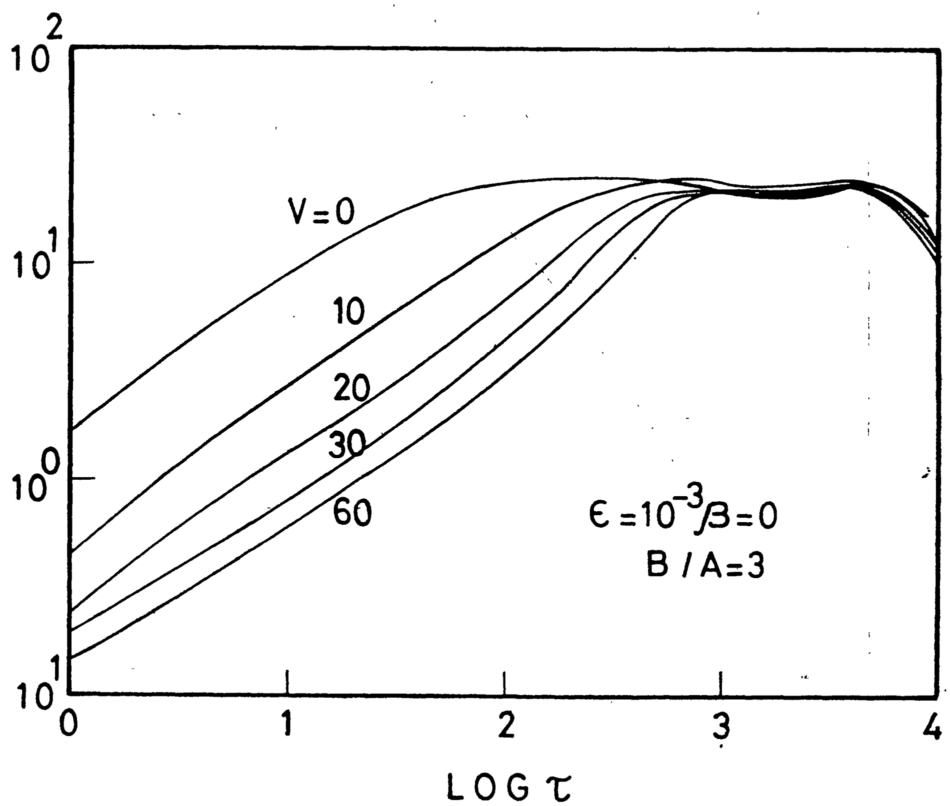

Fig. 6. Same as those given in Fig. 5 with $\varepsilon = 10^{-3}$ and $\beta = 0$.

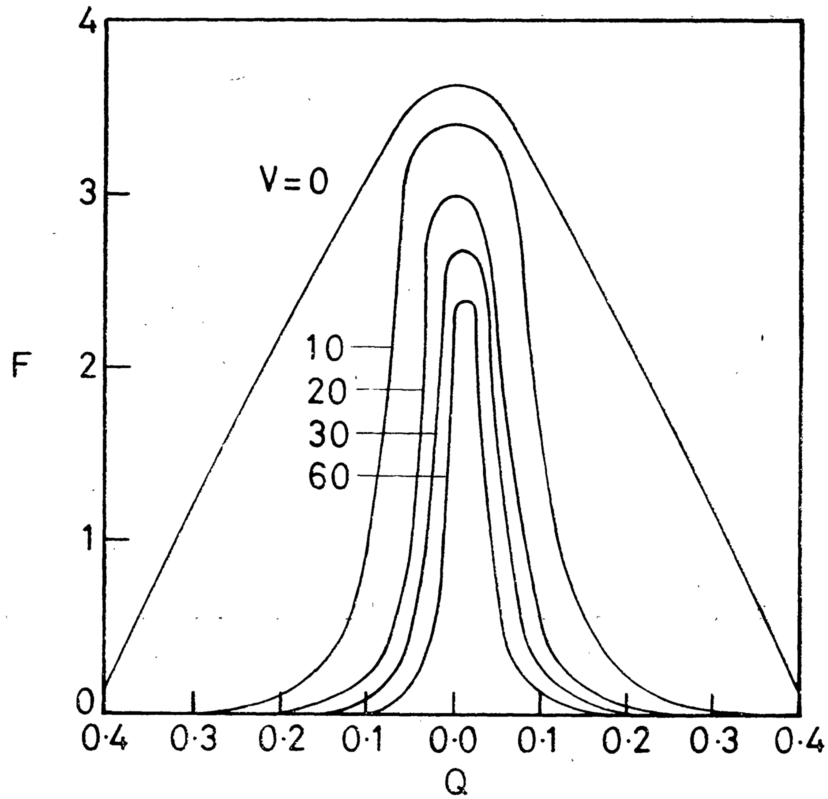

Fig. 7. Line profiles at the observer's point for the source functions given in Fig. 1. $Q(X) = \text{Flux}\,(X)/\text{Flux}\,(X_{max})$.

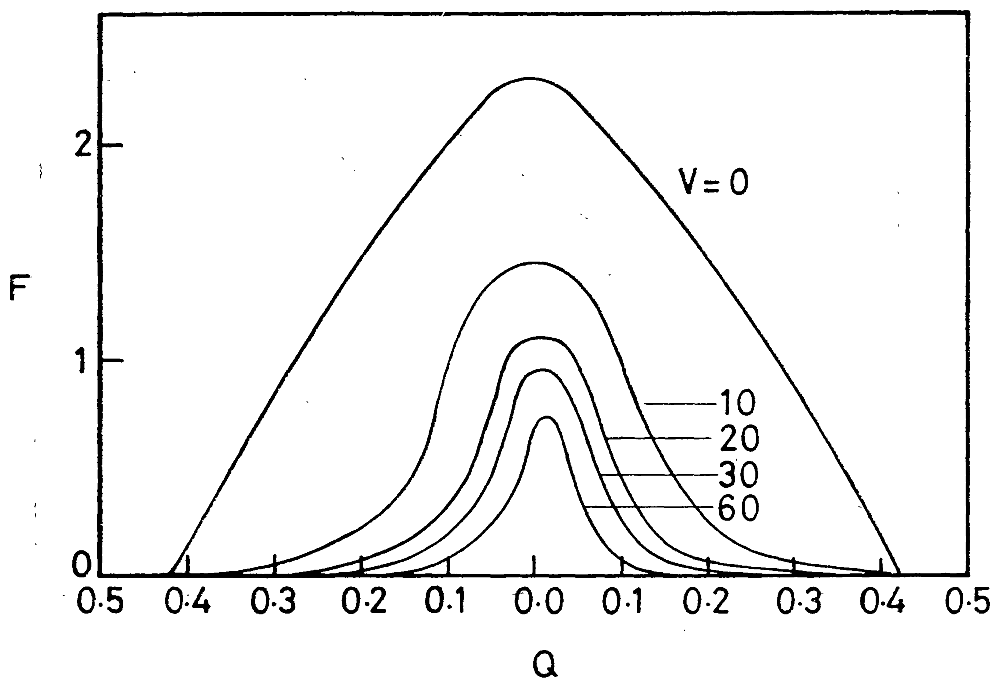

Fig. 8. Line profiles at the observer's point corresponding to the source functions given in Fig. 2.

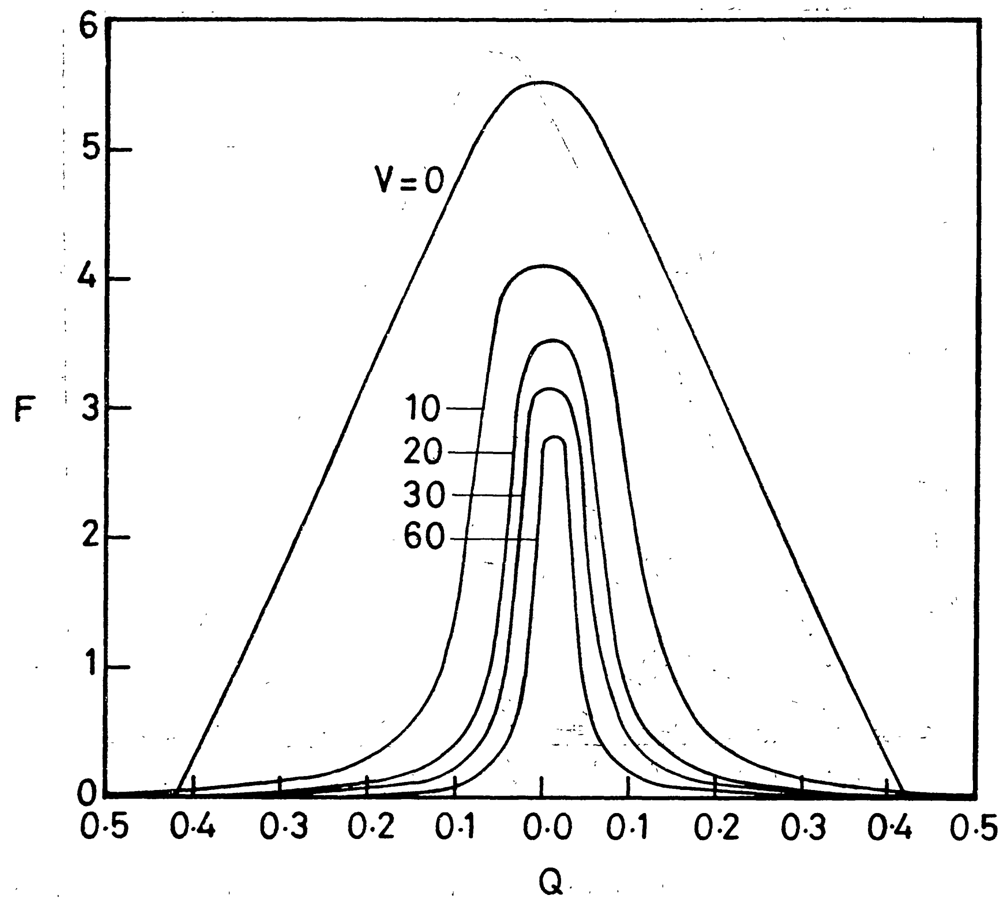

Fig. 9. Line profiles at the observer's point corresponding to the source functions given in Fig. 3.

4. Conclusions

We have presented a method to solve line transfer in comoving frame. This method is stable and can be subjected to rigorous numerical analysis.

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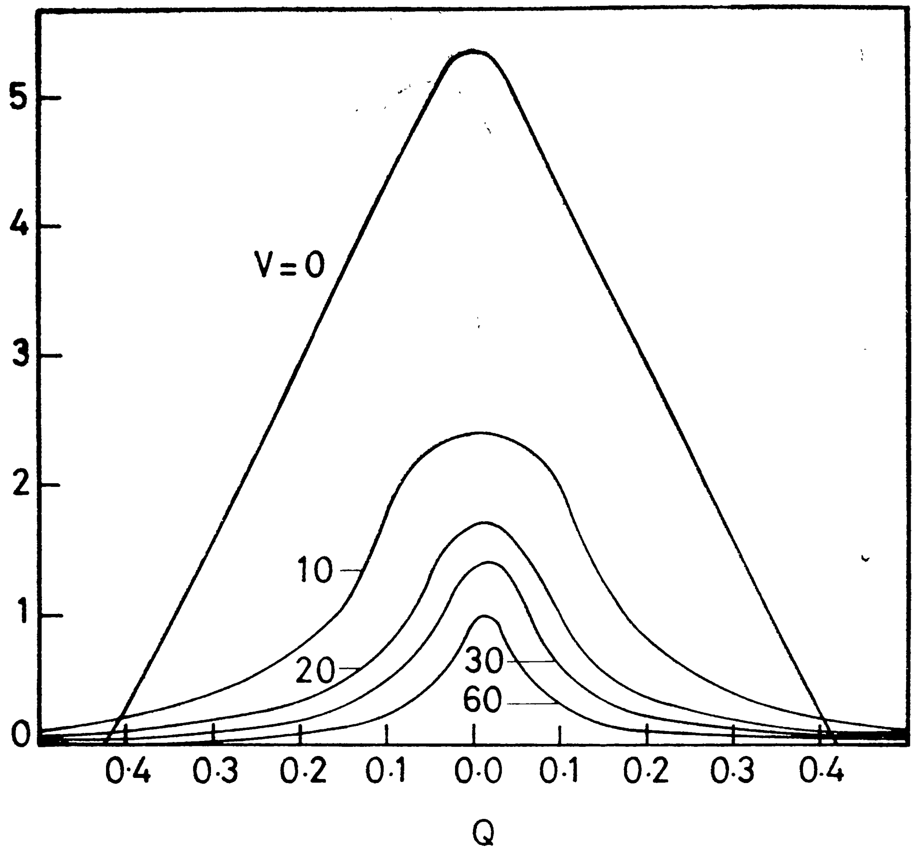

Fig. 10. Line profiles at the observer's point corresponding to the source functions given in Fig. 4.

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APPENDIX I

First we shall define,

$$\boldsymbol{Y} = \tfrac{1}{2}\sigma[\boldsymbol{\varphi}\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{W}], \quad \boldsymbol{Z} = \boldsymbol{\Phi}-\boldsymbol{Y},$$

$$\boldsymbol{Z}_{+} = \boldsymbol{Z}+\frac{\varrho_c\boldsymbol{\Lambda}^{+}}{\tau}-\frac{\boldsymbol{M}_1\boldsymbol{d}}{\tau}, \quad \boldsymbol{Y}_{+} = \boldsymbol{Y}+\frac{\varrho_c\boldsymbol{\Lambda}^{-}}{\tau},$$

$$\boldsymbol{Z}_{-} = \boldsymbol{Z}-\frac{\varrho_c\boldsymbol{\Lambda}^{+}}{\tau}-\frac{\boldsymbol{M}_1\boldsymbol{d}}{\tau}, \quad \boldsymbol{Y}_{-} = \boldsymbol{Y}-\frac{\varrho_c\boldsymbol{\Lambda}^{-}}{\tau},$$

$$\boldsymbol{\Delta}^{\pm} = [\boldsymbol{M}+\tfrac{1}{2}\tau\boldsymbol{Z}_{\pm}]^{-1}, \quad \boldsymbol{\Gamma}^{\pm} = [\boldsymbol{M}-\tfrac{1}{2}\tau\boldsymbol{Z}_{\pm}],$$

$$\boldsymbol{\beta}^{+-} = \tfrac{1}{2}\tau\boldsymbol{\Delta}^{+}\boldsymbol{Y}_{-}, \quad \boldsymbol{a}^{+-} = [\boldsymbol{I}-\boldsymbol{\beta}^{+-}\beta^{-+}]^{-1}$$

(similarly $\boldsymbol{\beta}^{-+}$ and $\boldsymbol{a}^{-+}$ are written by interchanging the signes), and we shall write the transmission and reflection matrices as

$$\boldsymbol{T}(n+1, n) = \boldsymbol{a}^{+-}[\boldsymbol{\Delta}^{+}\boldsymbol{\Gamma}^{+}+\boldsymbol{\beta}^{+-}\boldsymbol{\beta}^{-+}],$$

$$\boldsymbol{T}(n, n+1) = \boldsymbol{a}^{-+}[\boldsymbol{\Delta}^{-}\boldsymbol{\Gamma}^{-}+\boldsymbol{\beta}^{-+}\beta^{+-}],$$

$$\boldsymbol{R}(N+1, n) = \boldsymbol{a}^{-+}\boldsymbol{\beta}^{-+}[\boldsymbol{I}+\boldsymbol{\Delta}^{+}\boldsymbol{\Gamma}^{+}],$$

$$\boldsymbol{R}(n, n+1) = \boldsymbol{a}^{+-}\boldsymbol{\beta}^{+-}[\boldsymbol{I}+\boldsymbol{\Delta}^{-}\boldsymbol{\Gamma}^{-}],$$

and the cell source vectors are given by

$$\boldsymbol{\Sigma}^{+}_{n+1/2} = \tau\boldsymbol{a}^{+-}[\boldsymbol{\Delta}^{+}+\boldsymbol{\beta}^{+-}\boldsymbol{\Delta}^{-}]\boldsymbol{S},$$

$$\boldsymbol{\Sigma}^{-}_{n+1/2} = \tau\boldsymbol{a}^{-+}[\boldsymbol{\Delta}^{-}+\boldsymbol{\beta}^{-+}\boldsymbol{\Delta}^{+}]\boldsymbol{S}.$$

APPENDIX II

The nature of the elements of the $\boldsymbol{d}$ matrix can be derived from the condition of flux conservation. In a conservative medium energy is neither created nor destroyed. We shall employ this principle and follow closely the procedure given in Grant and Hunt (1969a, b). In this case the infinitesimal generators are given by,

$$\boldsymbol{G}^{++} = \boldsymbol{M}^{-1}\left[\boldsymbol{\Phi}-\tfrac{1}{2}\sigma(\boldsymbol{\varphi}\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{W})+\frac{\varrho_c\boldsymbol{\Lambda}^{+}}{\tau}-\frac{\boldsymbol{M}_1\boldsymbol{d}}{\tau}\right],$$

and

$$\boldsymbol{G}^{-+} = \boldsymbol{M}^{-1}\left[\tfrac{1}{2}\sigma(\boldsymbol{\varphi}\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{W})+\frac{\varrho_c\boldsymbol{\Lambda}^{-}}{\tau}\right].$$

If we assume that τ is the critical optical depth in the "cell", then the $\boldsymbol{r}$ and $\boldsymbol{t}$ operators are given by,

$$\boldsymbol{t}(n+1, n) = \boldsymbol{I}-\tau\boldsymbol{G}^{++}, \qquad \boldsymbol{r}(n+1, n) = \tau\boldsymbol{G}^{-+}. \tag{A1}$$

For a conservative case, we must have

$$\|\boldsymbol{t}(n+1, n)+\boldsymbol{r}(n+1, n)\| = 1+O(\tau), \tag{A2}$$

where $\|\cdot\|$ is the radiometric flux norm defined by (see Grant and Hunt 1969b).

$$\|\boldsymbol{P}\| = \max_{k'} \boldsymbol{\Sigma}|HPH^{-1}|_{kk'}, \tag{A3}$$

where $\boldsymbol{H} = 2\pi\boldsymbol{MW}$.

The norm of **r** and **t** operators is

$$\|\boldsymbol{t}(n+1, n)+\boldsymbol{r}(n+1), n)\| = \max_{k'} \sum_{k=1}^{K} \left| 2\pi\boldsymbol{MW}\left\{\boldsymbol{I}-\tau\boldsymbol{M}^{-1}\left[\boldsymbol{\Phi}-\sigma(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{W})+\frac{\varrho_c}{\tau}(\boldsymbol{\Lambda}^{+}+\boldsymbol{\Lambda}^{-})-\right.\right.\right. \left.\left.\left. -\frac{\boldsymbol{M}_1\boldsymbol{d}}{\tau}\right\}\right](2\pi\boldsymbol{MW})^{-1}_{kk'}. \tag{A4}$$

In a purely scattering media $\varepsilon = 0$ and, therefore, $\sigma = 1$ and $\beta = 0$, hence $\boldsymbol{\Phi}$ reduces to φ. Furthermore, the normalization of the line profile gives us that

$$\int_{-\infty}^{+\infty} \varphi(x)\,\mathrm{d}x = 1, \tag{A5}$$

or, in discrete form,

$$\boldsymbol{\Sigma} W_k\varphi_k = 1, \tag{A6}$$

and the curvature matrices should satisfy the identity

$$\sum_{j=1}^{T} c_j(\boldsymbol{\Lambda}_{jl}^{+} - \Lambda_{jl}^{-}) = 0 \qquad \text{for all } l = 1, \ldots, J \tag{A7}$$

With the aid of (A6) and (A7), (A4) reduces to

$$\|\boldsymbol{t}(n+1, n)+\boldsymbol{r}(n+1, n)\| = 1+\Sigma d_i a_i+O(\tau). \tag{A8}$$

Therefore, for flux conservation we must have $\Sigma d_i a_i = 0$, or the weighted columm sum of the $\boldsymbol{d}$-matrix should identically be zero.