1. Plane-parallel atmospheres with polarized scattering.

In the treatment by Chandrasekhar (1960, pp 38-50), the transfer equations are expressed in terms of I_l and I_r , the intensities in directions parallel and perpendicular to the meridian plane. In terms of Stokes parameters, this is $I = I_l + I_r$ and $Q = I_l - I_r$, where the meridian plane is the reference plane for Q. Because of the symmetry of the problem, the polarization can only be parallel or perpendicular to the meridian plane (Note: In an atmosphere where the temperature increases with depth, the emerging radiation will be most intense in the vertical direction. Then, if we are looking near the limb of the star, scattering will tend to polarize light perpendicular to the z-axis. This will make $I_r > I_l$, so that we will expect negative values of Q.)

We then find the radiation can be described by the following two transfer equations (Harrington, 1970):

$$\mu \frac{dI_{\nu}}{d\tau_{\nu}} = I_{\nu} - \left\{ s_{\nu}(\tau_{\nu}) + \left(\frac{1}{3} - \mu^2\right) p_{\nu}(\tau_{\nu}) \right\}$$
(1)

and

$$\mu \frac{dQ_{\nu}}{d\tau_{\nu}} = Q_{\nu} - \left\{ \left(1 - \mu^2 \right) p_{\nu}(\tau_{\nu}) \right\} \quad , \tag{2}$$

where we have defined two auxiliary functions, $s_{\nu}(\tau_{\nu})$ and $p_{\nu}(\tau_{\nu})$:

$$s_{\nu}(\tau_{\nu}) = (1 - \lambda_{\nu}) J_{\nu} + \lambda_{\nu} B_{\nu}(\tau_{\nu})$$
 (3)

$$p_{\nu}(\tau_{\nu}) = \frac{3}{8}(1 - \lambda_{\nu}) \left\{ (J_{\nu} - 3K_{\nu}) + 3 \left(J_{\nu}^{Q} - K_{\nu}^{Q} \right) \right\}$$
(4)

Here, J_{ν} and K_{ν} have their usual definitions:

$$J_{\nu} = \frac{1}{2} \int_{-1}^{1} I_{\nu} d\mu \qquad \qquad K_{\nu} = \frac{1}{2} \int_{-1}^{1} I_{\nu} \mu^{2} d\mu \quad , \qquad (5)$$

while we define

$$J_{\nu}^{Q} = \frac{1}{2} \int_{-1}^{1} Q_{\nu} d\mu \qquad \qquad K_{\nu}^{Q} = \frac{1}{2} \int_{-1}^{1} Q_{\nu} \mu^{2} d\mu \quad . \tag{6}$$

The quantity λ_{ν} is the ratio of pure absorption to extinction, and $(1 - \lambda_{\nu})$ the ratio of scattering to extinction. We then see that $s_{\nu}(\tau_{\nu})$ is just the usual source function for unpolarized radiation. We can regard $p_{\nu}(\tau_{\nu})$ as a sort of source function for the polarization. It will tend toward zero as τ_{ν} becomes large. Recalling Eddington's approximation, $3K_{\nu} \simeq J_{\nu}$, and we see that the first term of the r.h.s. of eq. (4) will vanish at depth. Since the second term depends only on Q_{ν} , and $Q_{\nu} = I_l - I_r$ will decrease as the radiation field becomes more isotropic, it will also vanish at depth.

We may use the formal solutions of the transfer equations to write the corresponding integral equations for $s_{\nu}(\tau_{\nu})$ and $p_{\nu}(\tau_{\nu})$ (Harrington, 1970):

$$s_{\nu}(\tau_{\nu}) = (1 - \lambda_{\nu}) \left[\Lambda_{\tau_{\nu}}(s_{\nu}) + \frac{1}{3} M_{\tau_{\nu}}(p_{\nu}) \right] + \lambda_{\nu} B_{\nu}(\tau_{\nu})$$
 (7)

$$p_{\nu}(\tau_{\nu}) = \frac{3}{8}(1 - \lambda_{\nu}) \left[M_{\tau_{\nu}}(s_{\nu}) + N_{\tau_{\nu}}(p_{\nu}) \right]$$
(8)

Here, Λ_{τ} is the familiar Λ -operator,

$$\Lambda_{\tau} \{ f(t) \} = \frac{1}{2} \int_0^\infty f(t) E_1(|t-\tau|) dt \quad .$$
(9)

If we ignore the term involving $M_{\tau}(p)$, we see that eq. (7) is just the familiar Schwarzschild-Milne equation for unpolarized radiation in a plane-parallel atmosphere. The new M_{τ} and N_{τ} operators (which have no relation to the $M_n(\tau)$ and $N_n(\tau)$ used in Kourganoff (1963) p. 259) are defined as

$$M_{\tau} \{f(t)\} = \int_{0}^{\infty} f(t) \left[\frac{1}{2}E_{1}(|t-\tau|) - \frac{3}{2}E_{3}(|t-\tau|)\right] dt$$
(10)

$$N_{\tau} \{f(t)\} = \int_{0}^{\infty} f(t) \left[\frac{5}{3} E_{1}(|t-\tau|) - 4E_{3}(|t-\tau|) + 3E_{5}(|t-\tau|) \right] dt$$
(11)

The kernels of all three operators have a logarithmic singularity at $t = \tau$. The kernel of the *M*-operator has a zero at $\tau_M = 0.30533216$; it is positive for $|t - \tau| < \tau_M$ and negative for $|t - \tau| > \tau_M$. Fig. 1 shows the behavior of this kernel. Thus the $M_{\tau_\nu}(s_\nu)$ term in eq. (8) is a measure of the anisotropy of the radiation at τ_ν . Radiation from layers with $|t - \tau| < \tau_M$ will be traveling horizontally, while radiation from layers with $|t - \tau| > \tau_M$ will be traveling vertically and will give a negative contribution to p_ν .

The kernel of the N-operator is always positive.

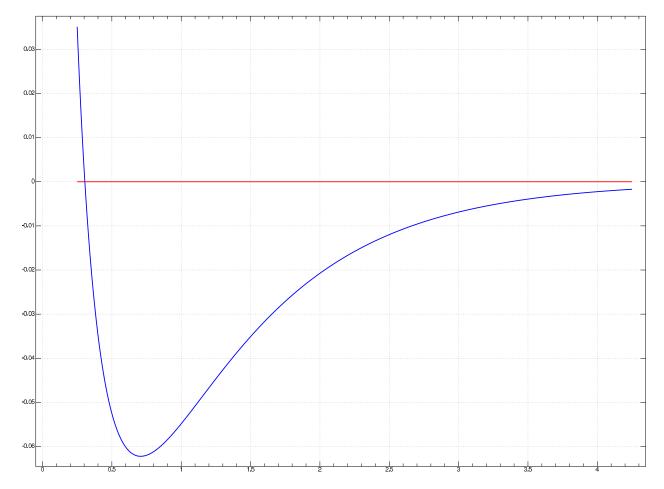


Fig. 1.— The kernel of the M-transform over $0.25 < \tau < 4.25.$

From the formal solutions of the transfer equations we then obtain the emergent radiation field:

$$I_{\nu}(0,\mu) = \int_{0}^{\infty} \left\{ s_{\nu}(\tau_{\nu}) + \left(\frac{1}{3} - \mu^{2}\right) p_{\nu}(\tau_{\nu}) \right\} e^{-\tau_{\nu}/\mu} \frac{d\tau_{\nu}}{\mu}$$
(12)

$$Q_{\nu}(0,\mu) = \int_{0}^{\infty} \left\{ \left(1-\mu^{2}\right) p_{\nu}(\tau_{\nu}) \right\} e^{-\tau_{\nu}/\mu} \frac{d\tau_{\nu}}{\mu}$$
(13)

2. The equations of the grey atmosphere problem.

In the grey atmosphere problem, where absorption and scattering are assumed not to vary with frequency, we can replace all the forgoing variables with those integrated over frequency, writing the integrated quantities without the ν subscript. In addition, in this case, the condition of radiative equilibrium is

$$\int_0^\infty j_\nu \, d\nu = \int_0^\infty \kappa \, B_\nu \, d\nu = \int_0^\infty \kappa \, J_\nu \, d\nu \quad , \tag{14}$$

where j_{ν} is the thermal emission coefficient. Kirchhoff's law provides the first equality. κ is the (frequency independent) coefficient of pure absorption (as opposed to scattering), so the second equality implies that B = J, and thus by eq. (3), J = s (But this does not imply that $J_{\nu} = s_{\nu}$!) This last result then reduces the frequency integrated form form of eq. (7) to

$$s(\tau) = \Lambda_{\tau}(s) + \frac{1}{3}M_{\tau}(p) \tag{15}$$

which we must solve along with the frequency integrated eq. (8):

$$p(\tau) = \frac{3}{8}(1-\lambda) \left[M_{\tau}(s) + N_{\tau}(p) \right] \quad .$$
 (16)

Now if $s(\tau)$ and $p(\tau)$ are solutions of equations (15) and (16), then for any constant c, $c \ s(\tau)$ and $c \ p(\tau)$ are also solutions. This follows from the linearity of the operators (see, Kourganoff, 1963, p 41). Thus any solution of eqns. (15) and (16) will have an arbitrary scale; to set the the scale, we may specify the emergent flux from the atmosphere. The operator that yields the flux for unpolarized radiation is the Φ -operator, defined as

$$\Phi_{\tau} \{ f(t) \} = 2 \int_{\tau}^{\infty} f(t) E_2(t-\tau) dt - 2 \int_{0}^{\tau} f(t) E_2(\tau-t) dt \quad .$$
 (17)

If we were dealing with the unpolarized problem, and the source function were $s(\tau)$, then Milne's second integral equation would hold: $\Phi_{\tau} \{s(t)\} = F$, where F is the net flux. Φ operating on any function $s(\tau)$ which is a solution of the grey problem, $\Lambda_{\tau} \{s(t)\} = s(\tau)$, must yield a value F which is the same for all values of τ . Furthermore, we see that the Φ -operator can set the scale of the solution since $\Phi_{\tau} \{c \ s(t)\} = c F$ for any constant c.

In our case with polarization, if we integrate eqn. (1) over frequency and then integrate over μ , noting that in radiative equilibrium J - s = 0, and further that

$$\int_{-1}^{1} \left(\frac{1}{3} - \mu^2\right) d\mu = 0 \quad , \tag{18}$$

we have the result

$$\frac{d}{d\tau} \left\{ 2 \int_{-1}^{1} I \ \mu \ d\mu \right\} = 0 \qquad \longrightarrow \qquad 2 \int_{-1}^{1} I \ \mu \ d\mu = constant = F \tag{19}$$

Using equation (12) for I and reversing the order of integration results in the polarization analog of Milne's second equation:

$$\Phi_{\tau} \{ s(t) \} + \Phi_{\tau}^{(4)} \{ p(t) \} = F \qquad , \tag{20}$$

where we introduce another new operator

$$\Phi_{\tau}^{(4)}\left\{f(t)\right\} = 2\int_{\tau}^{\infty} f(t) \left\{\frac{1}{3}E_{2}(t-\tau) - E_{4}(t-\tau)\right\} dt$$
$$- 2\int_{0}^{\tau} f(t) \left\{\frac{1}{3}E_{2}(\tau-t) - E_{4}(\tau-t)\right\} dt \quad .$$
(21)

The kernel of $\Phi_{\tau}^{(4)}$ is zero at $\tau = 0$ and is otherwise negative. It reaches a minimum of -0.121137 at $\tau_M \simeq 0.3$, the zero of the *M*-transform. In figure 2 we show the kernel of Φ_{τ} with the kernel of $|\Phi_{\tau}^{(4)}|$ scaled up by a factor of 10.

3. Numerical solution of the grey atmosphere problem with polarization.

One method of solution is to lay down a grid of discrete points in τ : $\tau_1, \tau_2, ..., \tau_N$. Our solution will be represented by two vectors, $\vec{s} = s_1, s_2, ..., s_N$ and $\vec{p} = p_1, p_2, ..., p_N$ We will represent the Λ -, M-, N-, Φ - and $\Phi^{(4)}$ - operators of equations (15), (16) and (20) by $N \times N$ matrices. E.g., we will find a matrix Λ_{ij} such that for a vector $\vec{f} = f_1, f_2, ..., f_N$ of the values of some function $f(\tau)$ at our τ -points, the matrix product $\Lambda_{ij}\vec{f}$ gives the Λ transform of the function f at the τ points. We will show below how to compute such matrix representations based on spline approximations to the function.

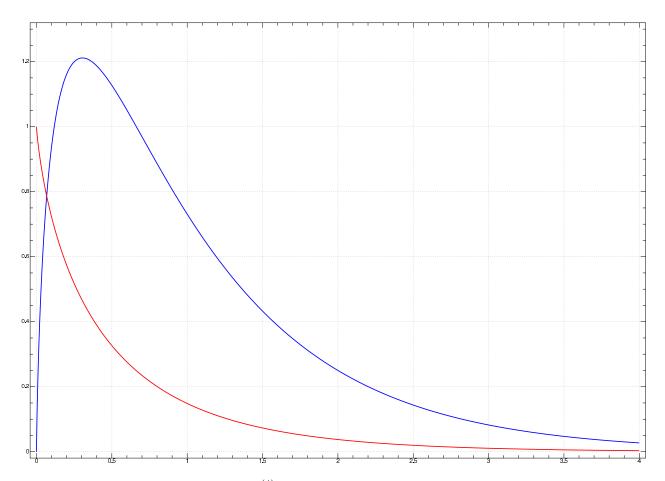


Fig. 2.— The kernel of Φ and of $-10*\Phi^{(4)}$ for $0<\tau<4.$

4. Spline approximation of the functions.

Following Press et al. "Numerical Recipes" (1992), consider a function y(x) for which we have tabulated values $y_i = y(x_i)$ for some $x_i, i = 1, 2, \dots, N$. The *linear* interpolation between any two points x_i and x_{i+1} is just

$$y(x) = A y_i + B y_{i+1}$$
 where $A = (x_{i+1} - x)/h_i$ and $B = 1 - A = (x - x_i)/h_i$ (22)

and h_i is the interval $h_i = x_{i+1} - x_i$. They show that the cubic spline interpolating polynomial can be written

$$y(x) = A y_i + B y_{i+1} + C y''_i + D y''_{i+1}$$
(23)

where y''_{i} and y''_{i+1} are the second derivatives of the tabulated function y(x) and C and D are

$$C = \frac{h_i^2}{6} \left(A^3 - A \right) \quad \text{and} \quad D = \frac{h_i^2}{6} \left(B^3 - B \right)$$
(24)

Thus, since A and B are linear in x, equation (23) gives y as a cubic polynomial in x. But what are the 2nd derivatives y''_i ? They are not the *actual* 2nd derivatives of y(x), which are of course unknown, but rather the 2nd derivatives of our cubic spline. It can be shown that to make the 1st derivative of the spline smooth across the interval boundaries x_i (and have the 2nd derivative continuous there), the y''_i must satisfy the following condition:

$$h_{i-1}y''_{i-1} + 2(h_{i-1} + h_i)y''_i + h_iy''_{i+1} = \frac{6}{h_{i-1}}y_{i-1} - \left[\frac{6}{h_{i-1}} + \frac{6}{h_i}\right]y_i + \frac{6}{h_i}y_{i+1} \quad (25)$$

for $i = 2, 3, \dots, N-1$. This gives, however, only N-2 equations for the N 2nd derivatives. A *natural cubic spline* is one with $y''_1 = y''_N = 0$. With this choice we have enough equations to find the remaining y''_i for $i = 2, \dots, N-1$.

These equations form a tridiagonal system which can be solved efficiently. However, for our purposes, we do not wish to solve the equations directly; rather, we want to express the y''_i formally in terms of the y_i . Let \vec{y} be the *N*-element column vector y_1, y_2, \dots, y_N , and let $\vec{y''}$ be the (N-2)-element column vector $y''_2, y''_3, \dots, y''_{N-1}$. Then equations (25) can be written as

$$\boldsymbol{A} \times \vec{y''} = \boldsymbol{B} \times \vec{y} \tag{26}$$

where \boldsymbol{A} is an $(N-2) \times (N-2)$ matrix and \boldsymbol{B} is an $(N-2) \times N$ matrix. We thus see that we can express the 2nd derivatives simply as

$$\vec{y''} = \boldsymbol{C} \times \vec{y}$$
 where $\boldsymbol{C} = \boldsymbol{A^{-1}} \times \boldsymbol{B}$, (27)

 A^{-1} being the inverse of A. The product C is an $(N-2) \times N$ matrix. With the row index $i = 2, \dots, (N-1)$ and column index $j = 1, \dots, N$, the non-zero elements of B are

$$\boldsymbol{B}_{i,i-1} = \frac{6}{h_{i-1}}$$
, $\boldsymbol{B}_{i,i} = -\left[\frac{6}{h_i} + \frac{6}{h_{i-1}}\right]$ and $\boldsymbol{B}_{i,i+1} = \frac{6}{h_i}$. (28)

Likewise, the elements of \boldsymbol{A} are

$$\mathbf{A}_{i,i-1} = h_{i-1}$$
 , $\mathbf{A}_{i,i} = 2(h_{i-1} + h_i)$ and $\mathbf{A}_{i,i+1} = h_i$, (29)

where the index $i = 2, \dots, (N-1)$, so that the elements $A_{2,1}$ and $A_{N-1,N}$ do not exist. Thus, given any array of points x_i , we can compute the matrix C. Then the 2nd derivatives for the spline fit of any function are given by the matrix multiplication (27).

Things are a bit more complex if, instead of natural splines, we want to impose a specific slope on the fit at one or both boundaries. The first derivative of expression (23) is

$$\frac{dy}{dx} = \frac{y_{i+1} - y_i}{h_i} - \frac{h_i}{6} \left\{ \left(3A^2 - 1 \right) y''_i - \left(3B^2 - 1 \right) y''_{i+1} \right\}$$
(30)

At the lower boundary, $x = x_1$, A = 0, B = 1 and we have

$$\left[\frac{dy}{dx}\right]_{x_1} = \frac{y_2 - y_1}{h_1} - \frac{h_1}{6} \left\{2 y''_1 + y''_2\right\}$$
(31)

and at the upper boundary, $x = x_N$, A = 1, B = 0 and

$$\left[\frac{dy}{dx}\right]_{x_N} = \frac{y_N - y_{N-1}}{h_{N-1}} + \frac{h_{N-1}}{6} \left\{ y''_{N-1} + 2 y''_N \right\}$$
(32)

which we write in the form of equations (25) as

$$2h_1 y''_1 + h_1 y''_2 = \left(-\frac{6}{h_1}\right) y_1 + \left(\frac{6}{h_1}\right) y_2 - 6\left[\frac{dy}{dx}\right]_{x_1}$$
(33)

and

$$h_{N-1}y''_{N-1} + 2h_{N-1}y''_{N} = \left(\frac{6}{h_{N-1}}\right)y_{N-1} + \left(-\frac{6}{h_{N-1}}\right)y_{N} + 6\left[\frac{dy}{dx}\right]_{x_{N}}$$
(34)

Our system of equations then become

$$\boldsymbol{A} \times \boldsymbol{y}^{\boldsymbol{y}} = \boldsymbol{B} \times \boldsymbol{y} + \boldsymbol{z} \tag{35}$$

where \vec{z} is a column vector $[z_0, z_1, \dots, z_{N-1}, z_N]$ with only two non-zero elements: $z_0 = -6[dy/dx]_{x_1}$ and $z_N = 6[dy/dx]_{x_N}$. Now, however, \boldsymbol{A} is an $N \times N$ matrix, as is \boldsymbol{B} . The elements of \boldsymbol{A} are still given by equation (29) for rows 2 through N-1, but now the elements $\boldsymbol{A}_{2,1}$ and $\boldsymbol{A}_{N-1,N}$ do exist. Further, the first row of \boldsymbol{A} is given by $[2h_1, h_1, 0, \dots, 0]$ and the last (Nth) row is $[0, \dots, h_{N-1}, 2h_{N-1}]$.

The elements of \boldsymbol{B} are as given in equation (28) for rows 2 through N-1, while the first and last rows of \boldsymbol{B} are $[(-6/h_1), (6/h_1), 0, \dots, 0]$ and $[0, \dots, (6/h_{N-1}), (-6/h_{N-1})]$. Then, multiplying through by \boldsymbol{A}^{-1} we obtain the desired result

$$\vec{y''} = C \times \vec{y} + \vec{d}$$
, where $C = A^{-1} \times B$ and $\vec{d} = A^{-1} \times \vec{z}$. (36)

Our ultimate aim is to integrate the product of a kernel function and the spline fit to an arbitrary function y(x). To do this we have to expand equation (23) to isolate the powers of x. After some algebra we see that, over the interval $x_i \leq x \leq x_{i+1}$,

$$C = C_0 + C_1 x + C_2 x^2 + C_3 x^3 (37)$$

where

$$C_0 = \frac{x_{i+1}(x_{i+1}^2 - h_i^2)}{6h_i} \quad , \quad C_1 = -\frac{3x_{i+1}^2 - h_i^2}{6h_i} \quad , \quad C_2 = \frac{x_{i+1}}{2h_i} \quad , \quad C_3 = -\frac{1}{6h_i}$$
(38)

while for the coefficient D

$$D_0 = -\frac{x_i(x_i^2 - h_i^2)}{6h_i} \quad , \quad D_1 = \frac{3x_i^2 - h_i^2}{6h_i} \quad , \quad D_2 = -\frac{x_i}{2h_i} \quad , \quad D_3 = \frac{1}{6h_i} \tag{39}$$

We thus can write the cubic spline fit as

$$y(x) = (a_i + \alpha_i) + (b_i + \beta_i) x + \gamma_i x^2 + \delta_i x^3$$
 for $x_i \le x \le x_{i+1}$ (40)

where the coefficients are

$$a_{i} = \frac{1}{h_{i}} \left[x_{i+1}y_{i} - x_{i}y_{i+1} \right] , \quad \alpha_{i} = \frac{1}{6h_{i}} \left[x_{i+1}(x_{i+1}^{2} - h_{i}^{2})y''_{i} - x_{i}(x_{i}^{2} - h_{i}^{2})y''_{i+1} \right] , \quad (41)$$

$$b_{i} = \frac{1}{h_{i}} \left[-y_{i} + y_{i+1} \right], \quad \beta_{i} = \frac{1}{6h_{i}} \left[-(3x_{i+1}^{2} - h_{i}^{2})y''_{i} + (3x_{i}^{2} - h_{i}^{2})y''_{i+1} \right], \quad (42)$$

$$\gamma_i = \frac{1}{2h_i} \left[x_{i+1} y''_i - x_i y''_{i+1} \right] \quad \text{and} \quad \delta_i = \frac{1}{6h_i} \left[-y''_i + y''_{i+1} \right] \quad .$$
(43)

At this point, recall from equation (27) or (36) that each of the y''_i can be obtained as a weighted sum over all the y_k :

$$y''_{i} = \sum_{k=1}^{N} C_{i,k} \cdot y_{k}$$
 or $y''_{i} = \sum_{k=1}^{N} C_{i,k} \cdot y_{k} + d_{i}$. (44)

This means that each of the factors α , β , γ and δ of equation (40) can be expressed as a sum over the y_i multiplied by coefficients whose value can be pre-computed based only on the choice of the x_i grid.

Suppose we wish to evaluate the integral of y(x) times some kernel $\mathcal{K}(x)$ over the interval x_i to x_{i+1} . We see this becomes

$$T_{i} = \int_{x_{i}}^{x_{i+1}} y(x) \mathcal{K}(x) dx = (a_{i} + \alpha_{i}) \mathcal{I}_{i}^{(0)} + (b_{i} + \beta_{i}) \mathcal{I}_{i}^{(1)} + \gamma_{i} \mathcal{I}_{i}^{(2)} + \delta_{i} \mathcal{I}_{i}^{(3)} , \quad (45)$$

where

$$\mathcal{I}_{i}^{(n)} = \int_{x_{i}}^{x_{i+1}} x^{n} \mathcal{K}(x) \, dx \quad .$$
(46)

Note that for a given x-grid the $\mathcal{I}_i^{(n)}$ are just numbers that need be evaluated only once. As the simplest possible example, consider just the integral of y(x), which corresponds to $\mathcal{K}(x) = 1$. Then

$$\mathcal{I}_{i}^{(0)} = x_{i+1} - x_{i} , \quad \mathcal{I}_{i}^{(1)} = \frac{1}{2}(x_{i+1}^{2} - x_{i}^{2}) , \quad \mathcal{I}_{i}^{(2)} = \frac{1}{3}(x_{i+1}^{3} - x_{i}^{3}) , \quad \mathcal{I}_{i}^{(3)} = \frac{1}{4}(x_{i+1}^{4} - x_{i}^{4})$$
(47)

and hence

$$a_i \mathcal{I}_i^{(0)} = [x_{i+1}y_i - x_iy_{i+1}], \quad \alpha_i \mathcal{I}_i^{(0)} = \frac{1}{6} \left[x_{i+1}(x_{i+1}^2 - h_i^2)y''_i - x_i(x_i^2 - h_i^2)y''_{i+1} \right], \quad (48)$$

$$b_{i} \mathcal{I}_{i}^{(1)} = \frac{1}{2} (x_{i+1} + x_{i}) \left[-y_{i} + y_{i+1} \right], \quad \beta_{i} \mathcal{I}_{i}^{(1)} = \frac{1}{12} (x_{i+1} + x_{i}) \left[-(3x_{i+1}^{2} - h_{i}^{2})y''_{i} + (3x_{i}^{2} - h_{i}^{2})y''_{i+1} \right], \quad (49)$$

$$\gamma_i \,\mathcal{I}_i^{(2)} = \frac{x_{i+1}^3 - x_i^3}{6h_i} \left[x_{i+1} y''_i - x_i y''_{i+1} \right] \,, \tag{50}$$

$$\delta_i \mathcal{I}_i^{(3)} = \frac{x_{i+1}^4 - x_i^4}{24h_i} \left[-y''_i + y''_{i+1} \right]$$
(51)

We now add these and regroup to obtain

$$T_{i} = \frac{1}{2}h_{i} (y_{i} + y_{i+1}) + U_{i} y''_{i} + V_{i} y''_{i+1}$$
(52)

where

$$U_{i} = \frac{1}{6} \left\{ x_{i+1}(x_{i+1}^{2} - h_{i}^{2}) - \frac{1}{2}(x_{i+1} + x_{i})(3x_{i+1}^{2} - h_{i}^{2}) + \frac{x_{i+1}}{h_{i}}(x_{i+1}^{3} - x_{i}^{3}) - \frac{1}{4h_{i}}(x_{i+1}^{4} - x_{i}^{4}) \right\}$$
(53)

and

$$V_{i} = -\frac{1}{6} \left\{ x_{i}(x_{i}^{2} - h_{i}^{2}) - \frac{1}{2}(x_{i+1} + x_{i})(3x_{i}^{2} - h_{i}^{2}) + \frac{x_{i}}{h_{i}}(x_{i+1}^{3} - x_{i}^{3}) - \frac{1}{4h_{i}}(x_{i+1}^{4} - x_{i}^{4}) \right\}$$
(54)

After tedious manipulation it turns out that

$$U_i = V_i = -\frac{1}{24}(x_{i+1} - x_i)^3 = -\frac{1}{24}h_i^3 \quad !!$$
(55)

So, recalling equation (44), we finally obtain

$$T_{i} = \frac{h_{i}}{2}(y_{i} + y_{i+1}) - \frac{1}{24}h_{i}^{3}\left[y''_{i} + y''_{i+1}\right] = \frac{h_{i}}{2}(y_{i} + y_{i+1}) - \frac{h_{i}^{3}}{24}\sum_{k=1}^{N}\left[\boldsymbol{C}_{i,k} + \boldsymbol{C}_{i+1,k}\right]y_{k} \quad (56)$$

The first term is just the result of integrating a linear fit to points y_i and y_{i+1} ; the remaining part is the integral of the spline correction to the linear fit. The bottom line is that we have expressed the integral T_i in the form

$$T_{i} = \sum_{k=1}^{N} W_{ik} y_{k} , \text{ where } W_{ik} = \frac{h_{i}}{2} \left(\delta_{ii} + \delta_{i,i+1} \right) - \frac{h_{i}^{3}}{24} \left[\boldsymbol{C}_{i,k} + \boldsymbol{C}_{i+1,k} \right]$$
(57)

and the range of *i* is $i = 1, \dots, (N - 1)$. Here, δ_{ij} stands for the Kronecker delta. The elements W_{ik} are independent of the y_k and can be computed from the x_k alone.

Finally, the total integral of y(x) over the range $[x_1, x_N]$ is just

$$T = \sum_{i=1}^{N-1} T_i = \sum_{k=1}^{N} \bar{W}_k \cdot y_k \quad \text{, where the vector} \quad \bar{W}_k = \sum_{i=1}^{N-1} W_{ik} \quad .$$
(58)

For example, on the interval [0,1] with $x = 0, 0.1, 0.2, \dots, 1.0$, we get $\overline{W} = 0.0394337, 0.113398, 0.0964088, 0.100967, 0.0997238, 0.100138, 0.100138, 0.0997238, 0.100967, 0.0964088, 0.113398, 0.039433.$

In case, instead of natural splines, we wish to specify the slope of the spline fit at the boundary, equations (57) and (58) become

$$T_i = D_i + \sum_{k=1}^N W_{ik} y_k$$
, where $D_i = -\frac{h_i^3}{24} (d_i + d_{i+1})$ (59)

and

$$T = \bar{D} + \sum_{k=1}^{N} \bar{W}_k \cdot y_k \quad \text{, where } \quad \bar{D} = \sum_{i=1}^{N-1} D_i = -\frac{h_i^3}{24} \left[\left(2\sum_{i=1}^{N} d_i \right) - \left(d_1 + d_N \right) \right] \quad . \tag{60}$$

If we have information on y' at x_1 and/or x_N , then this will improve the fit. Consider the following cubic polynomial:

$$y(x) = 4 - 3x + 2x^2 - x^3$$
 with derivative $y'(x) = -3 + 4x - 3x^2$ (61)

Let's integrate it over the interval [-1,3]. The integral of y(x) over this range is exactly 2 $\frac{2}{3}$. Let us choose an x-grid of 5 evenly spaced values: [-1,0,1,2,3]. If we assume a natural spline fit with this grid we obtain $\overline{W}_i = [0.392857, 1.14286, 0.928571, 1.14286, 0.392857]$. We then see that

$$T = \sum_{k=1}^{N} \bar{W}_k \cdot y_k = 2.57143 \text{ , an error of } 3.6\%$$
(62)

We might expect an exact fit to a cubic polynomial, but note that y'' = 4 - 6x which is at odds with y'' = 0 at x = -1 and x = 3. If instead we force y'(-1) = -10 and y'(3) = -18, then we obtain $\bar{W}_i = [0.5, 1, 1, 1, 0.5]$ and $\bar{D} = 2/3$. This leads to

$$T = \bar{D} + \sum_{k=1}^{N} \bar{W}_k \cdot y_k = \frac{2}{3} + 2 = 2\frac{2}{3} \quad , \tag{63}$$

the exact result, as expected. If we were to consider a higher order polynomial for y(x), neither would give the exact result, but the weights based use of $y'(x_1)$ and $y'(x_N)$ would be significantly more accurate.

5. Matrix representation of the integral operators.

To compute the matrix representations of the Λ , M, N, Φ , and $\Phi^{(4)}$ operators where the function to be transformed is represented by a cubic spline, we must have the integrals of $1, x, x^2$ and x^3 against the exponential integral functions E_1, E_2, E_3, E_4 , and E_5 . These are:

$$\int E_1(x)dx = -E_2(x) \int x E_1(x)dx = E_3(x) - e^{-x} \int x^2 E_1(x)dx = -2E_4(x) - x e^{-x} \int x^3 E_1(x)dx = 6E_5(x) - e^{-x} (3 + x + x^2) \int E_2(x)dx = -E_3(x) \int x E_2(x)dx = 2E_4(x) - e^{-x} \int x^2 E_2(x)dx = 24E_6(x) - e^{-x} (1 - x) \int x^3 E_2(x)dx = 24E_6(x) - e^{-x} (6 + x^2) \int E_3(x)dx = -E_4(x) \int x E_3(x)dx = 3E_5(x) - e^{-x} \int x^2 E_3(x)dx = -12E_6(x) + e^{-x}(2 - x) \int x^3 E_3(x)dx = 60E_7(x) - e^{-x} (11 - x + x^2) \int E_4(x)dx = -E_5(x) \int x E_4(x)dx = 4E_6(x) - e^{-x} \int x^2 E_4(x)dx = -20E_7(x) + e^{-x}(3 - x) \int x^3 E_4(x)dx = 120E_8(x) - e^{-x} (18 - 2x + x^2) \int E_5(x)dx = -E_6(x) \int x E_5(x)dx = 5E_7(x) - e^{-x} \int x^2 E_5(x)dx = -30E_8(x) + e^{-x}(4 - x) \int x^3 E_5(x)dx = 210E_9(x) - e^{-x} (27 - 3x + x^2)$$

If we then consider $\mathcal{M}(x) = \frac{1}{2}E_1(x) - \frac{3}{2}E_3(x)$, we find that

$$\int \mathcal{M}(x)dx = -\frac{1}{2}E_2(x) + \frac{3}{2}E_4(x)$$

$$\int x \ \mathcal{M}(x)dx = \frac{1}{2}E_3(x) - \frac{9}{2}E_5(x) + e^{-x}$$

$$\int x^2 \ \mathcal{M}(x)dx = -E_4(x) + 18E_6(x) - e^{-x} (3-x)$$

$$\int x^3 \ \mathcal{M}(x)dx = 3E_5(x) - 90E_7(x) + e^{-x} (15 - 2x + x^2)$$

while with $\mathcal{N}(x) = \frac{5}{3}E_1(x) - 4E_3(x) + 3E_5(x)$ we obtain

$$\int \mathcal{N}(x)dx = -\frac{5}{3}E_2(x) + 4E_4(x) - 3E_6(x)$$

$$\int x \,\mathcal{N}(x)dx = \frac{5}{3}E_3(x) - 12E_5(x) + 15E_7(x) - \frac{2}{3}e^{-x}$$

$$\int x^2 \,\mathcal{N}(x)dx = -\frac{10}{3}E_4(x) + 48E_6(x) - 90E_8(x) + \frac{2}{3}e^{-x} (6-x)$$

$$\int x^3 \,\mathcal{N}(x)dx = 10E_5(x) - 240E_7(x) + 630E_9(x) - \frac{2}{3}e^{-x} (63 - 5x + x^2)$$

and for $\Phi^{(4)}(x) = \frac{2}{3}E_2(x) - 2E_4(x)$ we have

$$\int \Phi^{(4)}(x) dx = -\frac{2}{3}E_3(x) + 2E_5(x)$$

$$\int x \Phi^{(4)}(x) dx = \frac{4}{3}E_4(x) - 8E_6(x) + \frac{4}{3}e^{-x}$$

$$\int x^2 \Phi^{(4)}(x) dx = -4E_5(x) + 40E_7(x) - \frac{4}{3}e^{-x}(4-x)$$

$$\int x^3 \Phi^{(4)}(x) dx = 16E_6(x) - 240E_8(x) + \frac{4}{3}e^{-x}(24 - 3x + x^2)$$

We assume a grid of optical depths $[\tau_0, \tau_1, \cdots, \tau_{N-1}]$, at which the functions are known and at which we want to evaluate the transforms. Usually, $\tau_0 = 0$, while τ_{N-1} may be the central plane of a slab, or the far surface (so that $\tau_{N-1} = 0$ also), or perhaps $\tau_{N-1} >> 1$ for a semi-infinite atmosphere.

To form the matrix representation of the Λ -operator we will thus need to evaluate the integrals Λ_{ik} which give the contribution at τ_i due to the emission from the material in the layers between τ_k and τ_{k+1} :

$$\Lambda_{ik} = \frac{1}{2} \int_{\tau_k}^{\tau_{k+1}} f(\tau) E_1(|\tau - \tau_i|) d\tau = \frac{1}{2} \int_{\tau_k - \tau_i}^{\tau_{k+1} - \tau_i} f(\tau_i + x) E_1(x) dx \quad , \tag{64}$$

for the case where $\tau_k \geq \tau_i$, while if $\tau_{k+1} \leq \tau_i$ we have

$$\Lambda_{ik} = \frac{1}{2} \int_{\tau_k}^{\tau_{k+1}} f(\tau) E_1(|\tau - \tau_i|) d\tau = \frac{1}{2} \int_{\tau_i - \tau_{k+1}}^{\tau_i - \tau_k} f(\tau_i - x) E_1(x) dx \quad , \tag{65}$$

Now from equation (40) we see that

$$f(\tau_i + x) = (a_k + \alpha_k) + (b_k + \beta_k)(\tau_i + x) + \gamma_k(\tau_i + x)^2 + \delta_k(\tau_i + x)^3$$
(66)

so that equation (64) can be written as

$$\Lambda_{ik} = (a'_k + \alpha'_k) \mathcal{I}^{(0)}_{ik} + (b_k + \beta'_k) \mathcal{I}^{(1)}_{ik} + \gamma'_k \mathcal{I}^{(2)}_{ik} + \delta_k \mathcal{I}^{(3)}_{ik} .$$
(67)

where we have indicated the integrals by

$$\mathcal{I}_{ik}^{(n)} = \pm \frac{1}{2} \int_{|\tau_k - \tau_i|}^{|\tau_{k+1} - \tau_i|} x^n E_1(x) dx \quad \text{where the } (+) \text{ sign is for this } (\tau_k \ge \tau_i) \text{ case,} \quad (68)$$

and, after expanding eqn (66), we see that the primed coefficients are given by

$$a'_{k} = a_{k} + \tau_{i}b_{k} , \quad \alpha'_{k} = \alpha_{k} + \tau_{i}\beta_{k} + \tau_{i}^{2}\gamma_{k} + \tau_{i}^{3}\delta_{k} ,$$

$$\beta'_{k} = \beta_{k} + 2\tau_{i}\gamma_{k} + 3\tau_{i}^{2}\delta_{k} , \quad \gamma'_{k} = \gamma_{k} + 3\tau_{i}\delta_{k} .$$
(69)

Likewise, equation (65) can be written as

$$\Lambda_{ik} = (a_k^* + \alpha_k^*) \mathcal{I}_{ik}^{(0)} + (b_k^* + \beta_k^*) \mathcal{I}_{ik}^{(1)} + \gamma_k^* \mathcal{I}_{ik}^{(2)} + \delta_k^* \mathcal{I}_{ik}^{(3)} , \qquad (70)$$

but for this case, where $\tau_{k+1} \leq \tau_i$, equation (68) requires the lower (minus) sign:

$$\frac{1}{2} \int_{\tau_i - \tau_{k+1}}^{\tau_i - \tau_k} x^n E_1(x) dx = -\frac{1}{2} \int_{|\tau_k - \tau_i|}^{|\tau_{k+1} - \tau_i|} x^n E_1(x) dx = \mathcal{I}_{ik}^{(n)} , \qquad (71)$$

which is why we used \pm in eqn (68). (We cannot just take the absolute value of the integral because some kernels, like $\mathcal{M}(x)$, may take negative values.) Now the coefficients are

$$a_k^* = a_k', \ \alpha_k^* = \alpha_k', \ b_k^* = -b_k, \ \beta_k^* = -\beta_k', \ \gamma_k^* = \gamma_k', \ \delta_k^* = -\delta_k.$$
 (72)

From equations (41), (42) and (43), and defining $\Delta_k = \tau_{k+1} - \tau_k$, we see that

$$a'_{k} = \frac{1}{\Delta_{k}} (\tau_{k+1} - \tau_{i}) y_{k} - \frac{1}{\Delta_{k}} (\tau_{k} - \tau_{i}) y_{k+1} ,$$

$$\alpha'_{k} = \frac{1}{6\Delta_{k}} \left\{ \tau_{k+1} (\tau_{k+1}^{2} - \Delta_{k}^{2}) - \tau_{i} (3\tau_{k+1}^{2} - \Delta_{k}^{2}) + 3\tau_{i}^{2}\tau_{k+1} - \tau_{i}^{3} \right\} y_{k}^{"} + \frac{1}{6\Delta_{k}} \left\{ -\tau_{k} (\tau_{k}^{2} - \Delta_{k}^{2}) + \tau_{i} (3\tau_{k}^{2} - \Delta_{k}^{2}) - 3\tau_{i}^{2}\tau_{k} + \tau_{i}^{3} \right\} y_{k+1}^{"}$$
(73)

$$b_{k} = \left(-\frac{1}{\Delta_{k}}\right)y_{k} + \left(\frac{1}{\Delta_{k}}\right)y_{k+1},$$

$$\beta_{k}' = \frac{1}{6\Delta_{k}}\left\{-\left(3\tau_{k+1}^{2} - \Delta_{k}^{2}\right) + 6\tau_{i}\tau_{k+1} - 3\tau_{i}^{2}\right\}y_{k}'' + \frac{1}{6\Delta_{k}}\left\{\left(3\tau_{k}^{2} - \Delta_{k}^{2}\right) - 6\tau_{i}\tau_{k} + 3\tau_{i}^{2}\right\}y_{k+1}''$$
(74)

$$\gamma'_{k} = \frac{1}{2\Delta_{k}} \{\tau_{k+1} - \tau_{i}\} y_{k}^{"} + \frac{1}{2\Delta_{k}} \{-\tau_{k} + \tau_{i}\} y_{k+1}^{"}$$
(75)

$$\delta_{k} = -\frac{1}{6\Delta_{k}} y_{k}^{"} + \frac{1}{6\Delta_{k}} y_{k+1}^{"}$$
(76)

Now we want to arrange this in the form

$$\Lambda_{ik} = X_{ik} y_k + Y_{ik} y_{k+1} + U_{ik} y_k'' + V_{ik} y_{k+1}''$$
(77)

From equations (67), (70) and (73)-(76) we see that X, Y, U and V are given by

$$X_{ik} = \Delta_k^{-1} \left[(\tau_{k+1} - \tau_i) \mathcal{I}_{ik}^{(0)} \mp \mathcal{I}_{ik}^{(1)} \right] , \quad Y_{ik} = -\Delta_k^{-1} \left[(\tau_k - \tau_i) \mathcal{I}_{ik}^{(0)} \mp \mathcal{I}_{ik}^{(1)} \right]$$
(78)

$$(6\Delta_{k}) U_{ik} = \left[\tau_{k+1} (\tau_{k+1}^{2} - \Delta_{k}^{2}) - \tau_{i} (3\tau_{k+1}^{2} - \Delta_{k}^{2}) + 3\tau_{i}^{2}\tau_{k+1} - \tau_{i}^{3} \right] \mathcal{I}_{ik}^{(0)} \mp \left[(3\tau_{k+1}^{2} - \Delta_{k}^{2}) - 6\tau_{i}\tau_{k+1} + 3\tau_{i}^{2} \right] \mathcal{I}_{ik}^{(1)} + 3 \left[\tau_{k+1} - \tau_{i} \right] \mathcal{I}_{ik}^{(2)} \mp \mathcal{I}_{ik}^{(3)}$$
(79)

$$(6\Delta_k) V_{ik} = -\left[\tau_k(\tau_k^2 - \Delta_k^2) - \tau_i(3\tau_k^2 - \Delta_k^2) + 3\tau_i^2\tau_k - \tau_i^3\right]\mathcal{I}_{ik}^{(0)} \\ \pm \left[(3\tau_k^2 - \Delta_k^2) - 6\tau_i\tau_k + 3\tau_i^2\right]\mathcal{I}_{ik}^{(1)} - 3\left[\tau_k - \tau_i\right]\mathcal{I}_{ik}^{(2)} \pm \mathcal{I}_{ik}^{(3)}$$
(80)

Here, the upper sign of the \pm and \mp pair applies when $\tau_k \ge \tau_i$ and the lower when $\tau_{k+1} \le \tau_i$.

The integral Λ_{ik} can thus be expressed as

$$\Lambda_{ik} = \sum_{n=1}^{N} L_n^{(ik)} y_n \quad \text{where} \quad L_n^{(ik)} = X_{ik} \delta_{nk} + Y_{ik} \delta_{n,k+1} + U_{ik} \boldsymbol{C}_{k,n} + V_{ik} \boldsymbol{C}_{k+1,n}$$
(81)

But this is only the contribution to the transform from the material between τ_k and τ_{k+1} . To find the Λ -transform at τ_i , we need the sum over all k from k = 1 to k = N - 1:

$$\Lambda_{i} = \sum_{k=1}^{N-1} \Lambda_{ik} = \sum_{k=1}^{N-1} \sum_{n=1}^{N} L_{n}^{(ik)} y_{n} = \sum_{n=1}^{N} \left(\sum_{k=1}^{N-1} L_{n}^{(ik)} \right) y_{n} = \sum_{n=1}^{N} L_{n}^{(i)} y_{n}$$
(82)

where, carrying out the sum over k we have

$$L_{n}^{(i)} = X_{i,n} + Y_{i,n-1} + \sum_{k=1}^{N-1} U_{i,k} C_{k,n} + \sum_{k=1}^{N-1} V_{i,k} C_{k+1,n}$$
(83)

where for n = 1, $Y_{i,n-1}$ is absent, and for n = N, $X_{i,n}$ is absent. The X and Y terms alone give the transform which results from a linear approximation to the function $f(\tau)$.

We thus see that if we construct the matrix $\Lambda_{i,n} = L_n^{(i)}$, where each row is evaluates the transform at the $i = 1, \dots, N$ values of τ_i , then $\Lambda_{i,n}$ is the matrix approximation to the Λ -transform that we require. Further, this result extends immediately to the M- and N-transforms by use of the appropriate functions for the $\mathcal{I}_{ik}^{(n)}$ integrals.

The Φ and $\Phi^{(4)}$ -transforms are slightly different. Consider the partial contribution to the Φ -transform at point τ_i by radiation from the layers between τ_k and τ_{k+1} . If $\tau_k \geq \tau_i$, then we see from equation (17) that

$$\Phi_{ik} = 2 \int_{\tau_k}^{\tau_{k+1}} f(\tau) E_2(\tau - \tau_i) d\tau = 2 \int_{\tau_k - \tau_i}^{\tau_{k+1} - \tau_i} f(\tau_i + x) E_2(x) dx$$
(84)

On the other hand, when $\tau_{k+1} \leq \tau_i$, we have

$$\Phi_{ik} = -2 \int_{\tau_k}^{\tau_{k+1}} f(\tau) E_2(\tau_i - \tau) d\tau = -2 \int_{\tau_i - \tau_{k+1}}^{\tau_i - \tau_k} f(\tau_i - x) E_2(x) dx$$
(85)

If we now define the integrals $\mathcal{I}_{ik}^{(n)}$ by the expression

$$\mathcal{I}_{ik}^{(n)} = 2 \int_{|\tau_k - \tau_i|}^{|\tau_{k+1} - \tau_i|} x^n E_2(x) dx$$
(86)

we see that $\mathcal{I}_{ik}^{(n)} > 0$ for $\tau_k \geq \tau_i$ but $\mathcal{I}_{ik}^{(n)} < 0$ for $\tau_{k+1} \leq \tau_i$, as required. Note that this differs from the form of the earlier equation (68) only in that we do not reverse the sign for $\tau_{k+1} \leq \tau_i$. With this definition of the $\mathcal{I}_{ik}^{(n)}$, equations (78) through (83) also can be applied to the Φ -transform, and the $\Phi^{(4)}$ -transform is analogous.

We now have prescriptions for evaluating the matrix approximations of the transforms for a slab extending from τ_1 to τ_N . However, in the treatment of a semi-infinite atmosphere, we must include the contributions to the integrals of material below the last point, τ_N . To do this we must make some assumption about the behavior of the function $f(\tau)$ over the interval $[\tau_N, \infty]$. One simple possibility would to be to assume the function constant over this interval: $f(\tau) = f(\tau_N)$. However, we know that in the unpolarized grey case, the asymptotic behavior of the source function is linear in τ . Thus, let us suppose that we can write

$$f(\tau) = f(\tau_N) + \left[\frac{df}{d\tau}\right]_{\tau_N} (\tau - \tau_N) \qquad \text{for} \quad \tau > \tau_N .$$
(87)

Now, from eqn (32), the derivative of the spline fit to f at τ_N is

$$\left[\frac{df}{d\tau}\right]_{\tau_N} = \frac{f_N - f_{N-1}}{\Delta_{N-1}} + \left(\frac{\Delta_{N-1}}{6}\right) \left[f''_{N-1} + 2f''_N\right] \quad . \tag{88}$$

in terms of f and the 2nd derivatives f''. The first term is just the extrapolated linear fit to the last two points. Let us define the integrals

$$\mathcal{I}_{iN}^{(0)} = \frac{1}{2} \int_{\tau_N}^{\infty} E_1(|\tau - \tau_i|) \, d\tau = \frac{1}{2} \int_{\tau_N - \tau_i}^{\infty} E_1(x) \, dx = \frac{1}{2} E_2(\tau_N - \tau_i) \tag{89}$$

and

$$\mathcal{I}_{iN}^{(1)} = \frac{1}{2} \int_{\tau_N - \tau_i}^{\infty} x \ E_1(x) \ dx = \frac{1}{2} \left[e^{-(\tau_N - \tau_i)} - E_3(\tau_N - \tau_i) \right] . \tag{90}$$

We then see that

$$\frac{1}{2} \int_{\tau_N}^{\infty} (\tau - \tau_N) E_1(|\tau - \tau_i|) d\tau = \left[\tau_i \mathcal{I}_{iN}^{(0)} + \mathcal{I}_{iN}^{(1)} \right] - \tau_N \mathcal{I}_{iN}^{(0)} = \mathcal{I}_{iN}^{(1)} - (\tau_N - \tau_i) \mathcal{I}_{iN}^{(0)}$$
(91)

In this case, since $2E_3(x) = e^{-x} - xE_2(x)$, this simplifies further:

$$\mathcal{I}_{iN}^{(1)} - (\tau_N - \tau_i)\mathcal{I}_{iN}^{(0)} = \mathcal{I}_{iN}^{(*)} = \frac{1}{2}E_3(\tau_N - \tau_i) \quad .$$
(92)

We thus see that we can write the contribution to the Λ -transform at τ_i due to emission from $\tau > \tau_N$, using eqns (87)-(92), as

$$\Lambda_{iN} = \left(-\frac{\mathcal{I}_{iN}^{(*)}}{\Delta_{N-1}}\right) f_{N-1} + \left(\mathcal{I}_{iN}^{(0)} + \frac{\mathcal{I}_{iN}^{(*)}}{\Delta_{N-1}}\right) f_N + \left(\frac{\Delta_{N-1}}{6} \,\mathcal{I}_{iN}^{(*)}\right) \left[f''_{N-1} + 2f''_N\right] \,. \tag{93}$$

Thus, as in eqn (81) we can write the contribution from beyond τ_N as

$$\Lambda_{iN} = \sum_{n=1}^{N} L_n^{(iN)} y_n \quad \text{where now the elements of} \quad L_n^{(iN)} \quad \text{are}$$

$$L_n^{(iN)} = \left(-\frac{\mathcal{I}_{iN}^{(*)}}{\Delta_{N-1}} \right) \delta_{n,N-1} + \left(\mathcal{I}_{iN}^{(0)} + \frac{\mathcal{I}_{iN}^{(*)}}{\Delta_{N-1}} \right) \delta_{n,N}$$

$$+ \left(\frac{\Delta_{N-1}}{6} \mathcal{I}_{iN}^{(*)} \right) \boldsymbol{C}_{N-1,n} + \left(\frac{\Delta_{N-1}}{3} \mathcal{I}_{iN}^{(*)} \right) \boldsymbol{C}_{N,n}$$
(95)

For "natural splines", $y''_{N} = 0$ so the $C_{N,n} = 0$ and the last term vanishes.

So we then must add the vector $L_n^{(iN)}$ to each $L_n^{(i)}$ of eqn (83) to account for the radiation from below τ_N .

6. Boundary conditions for a finite slab.

In addition to the semi-infinite atmosphere, another important problem is that of a finite slab. For this case, we may simply take a grid of points through the whole slab and then use the "natural" y'' = 0 conditions at both boundaries. But this problem may be symmetric about the central plane (but not always: e.g., if the slab is illuminated from one side). If we do have symmetry, we will only need half half as many points if our grid is defined to cover $0 \le \tau \le \tau_N$, where the optical thickness of the whole slab is $2\tau_N$. In this case, we will want to specify the first derivative at τ_N , since τ_N is the mid-plane of a slab and thus $y'_N = 0$ by symmetry. (This does not mean that $y''_N = 0$, however.)

In the case where we set $y'_N = 0$, z_N of eqn (35) is also zero and as a result \vec{d} of eqn (36) vanishes and hence does not complicate the expression for y''. Now the function $f(\tau)$) (e.g., $s(\tau)$ and $p(\tau)$) will be symmetric about τ_N so that $f(\tau) = f(2\tau_N - \tau)$. The transform at some τ_i will now have contributions from both the layer between τ_k and τ_{k+1} and the corresponding layer on the far side between $(2\tau_N - \tau_k)$ and $(2\tau_N - \tau_{k+1})$ – where the function $f(\tau)$ is described by the same spline fit. So for the Λ -transform, we have

$$\Lambda_{ik} = \frac{1}{2} \int_{\tau_k}^{\tau_{k+1}} f(\tau) E_1(|\tau - \tau_i|) d\tau + \frac{1}{2} \int_{2\tau_N - \tau_{k+1}}^{2\tau_N - \tau_k} f(2\tau_N - \tau) E_1(\tau - \tau_i) d\tau \quad .$$
(96)

Note that for the second term, $(\tau - \tau_i)$ will always be positive. We let $x = \tau - \tau_i$ and define $\tau_i^* = 2\tau_N - \tau_i$. We then see that the far-side contribution can be written as

$$\Lambda_{ik}^{(f)} = \frac{1}{2} \int_{\tau_i^* - \tau_{k+1}}^{\tau_i^* - \tau_k} f(\tau_i^* - x) E_1(x) dx \quad .$$
(97)

By analogy with eqn (66), the spline approximation to $f(\tau)$ over this interval can be written as

$$f(\tau_i^* - x) = (a_k + \alpha_k) + (b_k + \beta_k)(\tau_i^* - x) + \gamma_k(\tau_i^* - x)^2 + \delta_k(\tau_i^* - x)^3$$
(98)

and after expanding and collecting coefficients of powers of x, as with eqn (67) and eqn (70), we can write

$$\Lambda_{ik}^{(f)} = (a_k^{(f)} + \alpha_k^{(f)}) \mathcal{I}_{ik}^{(f,0)} + (b_k^{(f)} + \beta_k^{(f)}) \mathcal{I}_{ik}^{(f,1)} + \gamma_k^{(f)} \mathcal{I}_{ik}^{(f,2)} + \delta_k^{(f)} \mathcal{I}_{ik}^{(f,3)}$$
(99)

where now the coefficients are

$$a_{k}^{(f)} = a_{k} + \tau_{i}^{*}b_{k} , \quad b_{k}^{(f)} = -b_{k} , \quad \alpha_{k}^{(f)} = \alpha_{k} + \tau_{i}^{*}\beta_{k} + \tau_{i}^{*2}\gamma_{k} + \tau_{i}^{*3}\delta_{k} ,$$

$$\beta_{k}^{(f)} = -\beta_{k} - 2\tau_{i}^{*}\gamma_{k} - 3\tau_{i}^{*2}\delta_{k} , \quad \gamma_{k}^{(f)} = \gamma_{k} + 3\tau_{i}^{*}\delta_{k} , \quad \delta_{k}^{(f)} = -\delta_{k} .$$
(100)

and the integrals are

$$\mathcal{I}_{ik}^{(f,n)} = \frac{1}{2} \int_{\tau_i^* - \tau_{k+1}}^{\tau_i^* - \tau_k} x^n E_1(x) dx \quad .$$
 (101)

Once again, we go back to eqns (41)-(43), collecting the coefficients of y_k , y_{k+1} , y''_k , and y''_{k+1} to express the far-side contribution in the form

$$\Lambda_{ik}^{(f)} = X_{ik}^{(f)} y_k + Y_{ik}^{(f)} y_{k+1} + U_{ik}^{(f)} y_k^{"} + V_{ik}^{(f)} y_{k+1}^{"}$$
(102)

where now

$$X_{ik}^{(f)} = \Delta_k^{-1} \left[(\tau_{k+1} - \tau_i^*) \mathcal{I}_{ik}^{(f,0)} + \mathcal{I}_{ik}^{(f,1)} \right] , \quad Y_{ik}^{(f)} = -\Delta_k^{-1} \left[(\tau_k - \tau_i^*) \mathcal{I}_{ik}^{(f,0)} + \mathcal{I}_{ik}^{(f,1)} \right]$$
(103)

$$(6\Delta_{k}) U_{ik}^{(f)} = \left[\tau_{k+1} (\tau_{k+1}^{2} - \Delta_{k}^{2}) - \tau_{i}^{*} (3\tau_{k+1}^{2} - \Delta_{k}^{2}) + 3\tau_{i}^{*2} \tau_{k+1} - \tau_{i}^{*3} \right] \mathcal{I}_{ik}^{(f,0)} + \left[(3\tau_{k+1}^{2} - \Delta_{k}^{2}) - 6\tau_{i}^{*} \tau_{k+1} + 3\tau_{i}^{*2} \right] \mathcal{I}_{ik}^{(f,1)} + 3 \left[\tau_{k+1} - \tau_{i}^{*} \right] \mathcal{I}_{ik}^{(f,2)} + \mathcal{I}_{ik}^{(f,3)}$$
(104)

$$(6\Delta_{k}) V_{ik}^{(f)} = -\left[\tau_{k}(\tau_{k}^{2} - \Delta_{k}^{2}) - \tau_{i}^{*}(3\tau_{k}^{2} - \Delta_{k}^{2}) + 3\tau_{i}^{*2}\tau_{k} - \tau_{i}^{*3}\right] \mathcal{I}_{ik}^{(f,0)} - \left[(3\tau_{k}^{2} - \Delta_{k}^{2}) - 6\tau_{i}^{*}\tau_{k} + 3\tau_{i}^{*2}\right] \mathcal{I}_{ik}^{(f,1)} - 3\left[\tau_{k} - \tau_{i}^{*}\right] \mathcal{I}_{ik}^{(f,2)} - \mathcal{I}_{ik}^{(f,3)}$$
(105)

Finally, eqn (44) is used for the y'', and the contribution from the far half of the slab has exactly the same form as eqn (83). We then add the near and far sides to get the total $\Lambda_{i,n}$ matrix transform. The $\Phi_{i,n}$ and $\Phi^{(4)}_{i,n}$ -transforms are not special cases here since the radiation from the far side is traveling upwards (positive) for all near-side layers.

7. The emergent radiation.

From equations (12) and (13), we have the emergent radiation in terms of the source terms $s(\tau)$ and $p(\tau)$:

$$I(0,\mu) = \int_0^\infty s(\tau) \ e^{-\tau/\mu} \ \frac{d\tau}{\mu} + \left(\frac{1}{3} - \mu^2\right) \int_0^\infty \ p(\tau) \ e^{-\tau/\mu} \ \frac{d\tau}{\mu}$$
(106)

$$Q(0,\mu) = (1-\mu^2) \int_0^\infty p(\tau) \ e^{-\tau/\mu} \ \frac{d\tau}{\mu}$$
(107)

We can define a transform E_{μ} as

$$E_{\mu}\{f(t)\} = \int_{0}^{\infty} f(t) \ e^{-t/\mu} \ \frac{dt}{\mu}$$
(108)

so that the emergent radiation is given by

$$I(0,\mu) = E_{\mu}(s) + \left(\frac{1}{3} - \mu^2\right) E_{\mu}(p) \quad ; \qquad Q(0,\mu) = \left(1 - \mu^2\right) E_{\mu}(p) \tag{109}$$

To evaluate E_{μ} based on the values of s and p at the grid points τ_i , we will need to find $E_{\mu,k}$ for $k = 1, \dots, (N-1)$:

$$E_{\mu,k} = \int_{\tau_k}^{\tau_{k+1}} f(\tau) \ e^{-\tau/\mu} \ \frac{d\tau}{\mu} = \int_{x_k}^{x_{k+1}} f(\mu x) \ e^{-x} \ dx \tag{110}$$

where $x_i = \tau_i/\mu$ and $f(\mu x_i) = f(\tau_i) = f_i$. As before, we assume the function is represented by a cubic spline. Then, going back to eqn (40),

$$f(\mu x) = (a_k + \alpha_k) + (b_k + \beta_k)\mu x + \gamma_k \ \mu^2 x^2 + \delta_k \ \mu^3 x^3$$
(111)

so we can write

$$E_{\mu,k} = (a_k + \alpha_k) \mathcal{E}_{\mu,k}^{(0)} + (b_k + \beta_k) \mathcal{E}_{\mu,k}^{(1)} + \gamma_k \mathcal{E}_{\mu,k}^{(2)} + \delta_k \mathcal{E}_{\mu,k}^{(3)}$$
(112)

it terms of the integrals

$$\mathcal{E}_{\mu,k}^{(n)} = \mu^n \int_{x_k}^{x_{k+1}} x^n \ e^{-x} \ dx \quad \text{where} \quad x_k = \tau_k / \mu \ , \quad x_{k+1} = \tau_{k+1} / \mu \ , \tag{113}$$

and the integrals against e^{-x} are:

$$\int e^{-x} dx = -e^{-x}$$

$$\int x e^{-x} dx = -e^{-x} (1+x)$$

$$\int x^2 e^{-x} dx = -e^{-x} (2+2x+x^2)$$

$$\int x^3 e^{-x} dx = -e^{-x} (6+6x+3x^2+x^3)$$

We next write $E_{\mu,k}$ as

$$E_{\mu,k} = X_{\mu,k} f_k + Y_{\mu,k} f_{k+1} + U_{\mu,k} f_k'' + V_{\mu,k} f_{k+1}''$$
(114)

Referring to eqn (41)-(43), we see that

$$X_{\mu,k} = \Delta_k^{-1} \left(\tau_{k+1} \, \mathcal{E}_{\mu,k}^{(0)} - \, \mathcal{E}_{\mu,k}^{(1)} \right) \,, \quad Y_{\mu,k} = -\Delta_k^{-1} \left(\tau_k \, \mathcal{E}_{\mu,k}^{(0)} - \, \mathcal{E}_{\mu,k}^{(1)} \right) \tag{115}$$

$$(6\Delta_k)U_{\mu,k} = \tau_{k+1}(\tau_{k+1}^2 - \Delta_k^2) \ \mathcal{E}_{\mu,k}^{(0)} - (3\tau_{k+1}^2 - \Delta_k^2) \ \mathcal{E}_{\mu,k}^{(1)} + 3\tau_{k+1} \ \mathcal{E}_{\mu,k}^{(2)} - \mathcal{E}_{\mu,k}^{(3)}$$
(116)

$$(6\Delta_k)V_{\mu,k} = -\tau_k(\tau_k^2 - \Delta_k^2) \ \mathcal{E}_{\mu,k}^{(0)} + (3\tau_k^2 - \Delta_k^2) \ \mathcal{E}_{\mu,k}^{(1)} - 3\tau_k \ \mathcal{E}_{\mu,k}^{(2)} + \mathcal{E}_{\mu,k}^{(3)}$$
(117)

and thus, using eqn (44),

$$E_{\mu,k} = \sum_{n=1}^{N} \{ X_{\mu,k} \ \delta_{nk} + Y_{\mu,k} \ \delta_{n,k+1} + U_{\mu,k} \ \boldsymbol{C}_{k,n} + V_{\mu,k} \ \boldsymbol{C}_{k+1,n} \} \ f_n$$
(118)

Finally, just as with eqns (81)-(83), our transformation is approximated by

$$E_{\mu}(f) = \sum_{k=1}^{N-1} E_{\mu,k} = \sum_{n=1}^{N} E_n^{(\mu)} f_n$$
(119)

where

$$E_{n}^{(\mu)} = X_{\mu,n} + Y_{\mu,n-1} + \sum_{k=1}^{N-1} U_{\mu,k} \boldsymbol{C}_{k,n} + \sum_{k=1}^{N-1} V_{\mu,k} \boldsymbol{C}_{k+1,n}$$
(120)

and, once again, for $n = 1, Y_{\mu,n-1}$ is absent, while for $n = N, X_{\mu,n}$ is absent.

Thus, having chosen a set of M angles μ_m , we can compute the $E_n^{(\mu_m)}$ for each of them. Then, the emergent intensity and polarization are obtained from

$$I(0,\mu_m) = \sum_{n=1}^{N} E_n^{(\mu_m)} s_n + \left(\frac{1}{3} - \mu^2\right) \sum_{n=1}^{N} E_n^{(\mu_m)} p_n$$
(121)

$$Q(0,\mu_m) = (1-\mu^2) \sum_{n=1}^{N} E_n^{(\mu_m)} p_n$$
(122)

In the case of a slab with symmetric sources, where the last grid point τ_N is the midpoint of the slab, we must add the contributions from the far side. From each slab we have a contribution

$$E_{\mu,k}^{(f)} = \int_{\tau^* - \tau_{k+1}}^{\tau^* - \tau_k} f(\tau) \ e^{-\tau/\mu} \ \frac{d\tau}{\mu} , \quad \text{where} \quad \tau^* = 2\tau_N \tag{123}$$

By the symmetry of the function f , $\ f(\tau^*-\tau)=f(\tau).$ Let $x=\tau/\mu$. Then we can write

$$E_{\mu,k}^{(f)} = \int_{\mu x^* - \mu x_{k+1}}^{\mu x^* - \mu x_k} f(\mu x^* - \mu x) \ e^{-x} \ dx \ . \tag{124}$$

The cubic spline representation of f is of the form

$$f(\mu x^* - \mu x) = (a_k + \alpha_k) + (b_k + \beta_k)\mu(x^* - x) + \gamma_k \ \mu^2(x^* - x)^2 + \delta_k \ \mu^3(x^* - x)^3 \quad (125)$$

The point of this is that at the edges of the interval, $f(\mu x^* - \mu x_k) = f(\tau_k) = f_k$. The moment integrals we then need are just

$$\mathcal{E}_{\mu,k}^{(f,n)} = \mu^n \int_{x^* - x_{k+1}}^{x^* - x_k} x^n \ e^{-x} \ dx \ , \ \text{where} \quad x^* = 2\tau_N/\mu \ , \ x_k = \tau_k/\mu \ , \ \text{etc.}$$
(126)

and we then write

$$E_{\mu,k}^{(f)} = (a_k^{(f)} + \alpha_k^{(f)}) \mathcal{E}_{\mu,k}^{(f,0)} + (b_k^{(f)} + \beta_k^{(f)}) \mathcal{E}_{\mu,k}^{(f,1)} + \gamma_k^{(f)} \mathcal{E}_{\mu,k}^{(f,2)} + \delta_k^{(f)} \mathcal{E}_{\mu,k}^{(f,3)}$$
(127)

where now (with $\tau^* = 2\tau_N$) the coefficients are

$$a_{k}^{(f)} = a_{k} + \tau^{*}b_{k} , \quad b_{k}^{(f)} = -b_{k} , \quad \alpha_{k}^{(f)} = \alpha_{k} + \tau^{*}\beta_{k} + \tau^{*2}\gamma_{k} + \tau^{*3}\delta_{k} ,$$

$$\beta_{k}^{(f)} = -\beta_{k} - 2\tau^{*}\gamma_{k} - 3\tau^{*2}\delta_{k} , \quad \gamma_{k}^{(f)} = \gamma_{k} + 3\tau^{*}\delta_{k} , \quad \delta_{k}^{(f)} = -\delta_{k} .$$
(128)

Proceeding as in section 6, we then write the partial contribution from the far side as

$$E_{\mu,k}^{(f)} = X_{\mu,k}^{(f)} y_k + Y_{\mu,k}^{(f)} y_{k+1} + U_{\mu,k}^{(f)} y_k^{"} + V_{\mu,k}^{(f)} y_{k+1}^{"}$$
(129)

where now

$$X_{\mu,k}^{(f)} = \Delta_k^{-1} \left[(\tau_{k+1} - \tau^*) \mathcal{E}_{\mu,k}^{(f,0)} + \mathcal{E}_{\mu,k}^{(f,1)} \right] , \quad Y_{\mu,k}^{(f)} = -\Delta_k^{-1} \left[(\tau_k - \tau^*) \mathcal{E}_{\mu,k}^{(f,0)} + \mathcal{E}_{\mu,k}^{(f,1)} \right]$$
(130)

$$(6\Delta_{k}) U_{\mu,i}^{(f)} = \left[\tau_{k+1} (\tau_{k+1}^{2} - \Delta_{k}^{2}) - \tau^{*} (3\tau_{k+1}^{2} - \Delta_{k}^{2}) + 3\tau^{*2}\tau_{k+1} - \tau^{*3} \right] \mathcal{E}_{\mu,k}^{(f,0)} + \left[(3\tau_{k+1}^{2} - \Delta_{k}^{2}) - 6\tau^{*}\tau_{k+1} + 3\tau^{*2} \right] \mathcal{E}_{\mu,k}^{(f,1)} + 3\left[\tau_{k+1} - \tau^{*}\right] \mathcal{E}_{\mu,k}^{(f,2)} + \mathcal{E}_{\mu,k}^{(f,3)}$$
(131)

$$(6\Delta_{k}) V_{\mu,k}^{(f)} = -\left[\tau_{k}(\tau_{k}^{2} - \Delta_{k}^{2}) - \tau^{*}(3\tau_{k}^{2} - \Delta_{k}^{2}) + 3\tau^{*2}\tau_{k} - \tau^{*3}\right] \mathcal{E}_{\mu,k}^{(f,0)} - \left[(3\tau_{k}^{2} - \Delta_{k}^{2}) - 6\tau^{*}\tau_{k} + 3\tau^{*2}\right] \mathcal{E}_{\mu,k}^{(f,1)} - 3\left[\tau_{k} - \tau^{*}\right] \mathcal{E}_{\mu,k}^{(f,2)} - \mathcal{E}_{\mu,k}^{(f,3)}$$
(132)

So finally, for the symmetric slab, equation (120) acquires additional terms:

$$E_{n}^{(\mu)} = \left(X_{\mu,n} + X_{\mu,n}^{(f)}\right) + \left(Y_{\mu,n-1} + Y_{\mu,n-1}^{(f)}\right) + \sum_{k=1}^{N-1} \left(U_{\mu,k} + U_{\mu,k}^{(f)}\right) \boldsymbol{C}_{k,n} + \sum_{k=1}^{N-1} \left(V_{\mu,k} + V_{\mu,k}^{(f)}\right) \boldsymbol{C}_{k+1,n}$$
(133)

8. Solution of some specific cases by the matrix transform method.

We now return to the grey problem that we abandoned in section 3. Let us consider this problem for the semi-infinite atmosphere. Combine the vectors \vec{s} and \vec{p} into one vector $\vec{sp} = s_1, s_2, ..., s_N, p_1, p_2, ..., p_N$ of length 2N. We then can express equations (15) and (16) as the following $2N \times 2N$ system:

$$\begin{bmatrix} \Lambda_{ij} - I_{ij} & \frac{1}{3}M_{ij} \\ \frac{3}{8}(1-\lambda)M_{ij} & \frac{3}{8}(1-\lambda)N_{ij} - I_{ij} \end{bmatrix} \begin{bmatrix} s_i \\ p_i \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
(134)

where I_{ij} is an $N \times N$ identity matrix. As it stands, we cannot solve this system since the r.h.s. is identically zero. But we can use the matrix form of the flux equation (20)

$$\Phi_{ij} \vec{s} + \Phi_{ij}^{(4)} \vec{p} = \vec{F}$$
(135)

This provides N equations. We can replace the first N equations with these and solve the system

$$\begin{bmatrix} \Phi_{ij} & \Phi_{ij}^{(4)} \\ \frac{3}{8}(1-\lambda)M_{ij} & \frac{3}{8}(1-\lambda)N_{ij} - I_{ij} \end{bmatrix} \begin{bmatrix} s_i \\ p_i \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix}$$
(136)

where the F on the right hand side represents an N-element column vector with each element equal to F. This works, but another method seems to give better values just near the surface. We only need to add any one of the flux equations to the first N equations of (134) to set the scale. A satisfactory approach seems to be to take the equation for the flux at the surface (the first equation, i = 1)

$$\sum_{n=1}^{N} \Phi_{1n} s_n + \sum_{n=1}^{N} \Phi_{1n}^{(4)} p_n = F$$
(137)

and add it to each of the first N equations (134):

$$\begin{bmatrix} \Lambda_{ij} - I_{ij} + \Phi_{1j} & \frac{1}{3}M_{ij} + \Phi_{1j}^{(4)} \\ \frac{3}{8}(1-\lambda)M_{ij} & \frac{3}{8}(1-\lambda)N_{ij} - I_{ij} \end{bmatrix} \begin{bmatrix} s_i \\ p_i \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix}$$
(138)

The resulting linear system can be solved by any standard numerical method.

All the foregoing have been implemented in J. The verb "tau_grid" constructs a logarithmic series of points $\tau = 0, \tau_1, \dots, \tau_N$ when provided with the arguments tau_grid τ_1, n, τ_N , where n is the number of points per decade. For example

 $tau_grid 0.1 5 3$

$0\ 0.1\ 0.158489\ 0.251189\ 0.398107\ 0.630957\ 1\ 1.58489\ 2.51189\ 3$

We provide some results for a fine grid: $\tau_1 = 0.0001, n = 20, \tau_N = 25$, which yields 110 grid points.

As opposed to the semi-infinite atmosphere, there is no grey solution for integrated radiation from a slab, since the equations have no source for the radiation (in the semiinfinite case, it streams in from beyond the lower boundary). Slabs must have an internal or external source added to the equations. Turning to the monochromatic case described by equations (7) and (8), we see that they lead to the following set of equations:

$$\begin{bmatrix} I_{ij} - (1 - \lambda_i)\Lambda_{ij} & -\frac{1}{3}(1 - \lambda_i)M_{ij} \\ -\frac{3}{8}(1 - \lambda_i)M_{ij} & I_{ij} - \frac{3}{8}(1 - \lambda_i)N_{ij} \end{bmatrix} \begin{bmatrix} s_i \\ p_i \end{bmatrix} = \begin{bmatrix} \lambda_i B_i \\ 0 \end{bmatrix}$$

where $B_i = B_{\nu}[T(\tau_i)]$ and we allow that λ_i , the fraction of opacity due to pure absorption, may vary with optical depth zone τ_i .

9. References.

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