A Direct Solution of the Spherical Harmonics Approximation to the Radiative Transfer Equation for an Arbitrary Solar Elevation.

Part I: Theory

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ABSTRACT

The spherical harmonics approximation to the transfer equation for an azimuth-dependent component of intensity of scattered radiation is reduced by finite differences to a block algebraic system of particularly simple structure. This algebraic system can be solved numerically for homogeneous or nonhomogeneous models of a plane-parallel atmosphere, using the finite-differences analogue of the simple-shooting technique based on initial-value problems or the multiple-shooting technique for the solution of two-point boundary-value problems.

1. Introduction

The spherical harmonics method is classic and was first suggested by Jeans (1917) in connection with problems of radiative transfer in stars. In the field of atmospheric radiative transfer, its development has been limited to obtaining analytic solutions which are generally applicable to homogeneous atmospheric models with isotropic, or mildly anisotropic, phase functions of scattering (Kourganoff, 1952; Guillemot, 1967). On the other hand, its most extensive development and applications have been in the field of neutron transport where one is interested in the transfer of neutrons in nonhomogeneous slabs with internal sources (e.g., Gelbard, 1968).

Canosa and Penafiel (1972) developed a direct method for the solution of the spherical harmonics equations describing neutron transport in slab geometry, by reducing them by finite differences to a block algebraic system of equations of particularly simple structure. Since this specific neutron-transport problem is mathematically equivalent to the transfer of the azimuth-independent component \( I^0(\tau; \mu) \) of the intensity \( I(\tau; \mu, \phi) \) of the scattered radiation in plane-parallel models of planetary atmospheres, their method was quickly applied to flux-divergence calculations in homogeneous (Canosa and Penafiel, 1973), as well as nonhomogeneous, models of the terrestrial atmosphere with absorbing gases, aerosol and water drops (Dave and Canosa, 1974; Dave and Braslau, 1975). The parameter \( \tau \) represents the optical depth of a level within the atmosphere, \( \mu \) is the cosine of the zenith angle (\( \theta \)) measured with respect to the negative \( \tau \) axis following Chandrasekhar's (1950) convention, and \( \phi \) is the azimuthal angle referred to an arbitrarily chosen meridian plane.

Use of Canosa and Penafiel's approach to computations of \( I(\tau; \mu, \phi) \) required in several applications such as remote sensing of the atmosphere, is not completely straightforward. First, because of the fundamental nature of the spherical harmonics method, a given \( I^0(\tau; \mu) \) vs \( \theta \) curve for a reasonably finite Legendre representation of \( I^0(\tau; \mu) \) is too oscillatory to be useful in practical applications (Dave and Canosa, 1974). Recently, Dave and Armstrong (1974) have shown that a relatively smooth and reliable \( I^0(\tau; \mu) \) vs \( \theta \) curve can be obtained after applying mathematically sound smoothing procedures to the spherical harmonics results. Second, the quantities \( I^0(\tau; \mu) \) and \( I(\tau; \mu, \phi) \) are equivalent for the overhead (\( \theta_0 = 0^0 \)) sun only. Because of the azimuthal asymmetry, evaluation of \( I(\tau; \mu, \phi) \) for \( \theta_0 > 0^0 \) requires values of the azimuth-dependent components \( I(\tau; \mu) \), \( I^0(\tau; \mu) \), etc., as well as of the azimuth-independent component \( I^0(\tau; \mu) \).

Obviously, the spherical harmonics approximation for the transfer of the 9th azimuth-dependent component \([I^9(\tau; \mu)]\) of the intensity requires a more general treatment than that involved in the transfer of the azimuth-independent component \( I^0(\tau; \mu) \). Furthermore, the form of the spherical harmonics approximation to the transfer equation as available in the literature (Guillemot, 1967) for analytic solutions, is not appropriate for arriving at a block algebraic system of equations suitable for the direct numerical solution (Canosa and Penafiel, 1972, 1973; Dave and Canosa, 1974). In what follows, we shall therefore derive the spherical harmonics approximation to the equation of radiative
transfer for the $n$th component $[I^n(\tau; \mu), n \geq 0]$ for a plane-parallel atmosphere, in a form suitable for applying the direct method of solution.

In Part II of this paper, we will discuss representative results of our numerical investigations for plane-parallel, non-absorbing, homogeneous models with Rayleigh phase function, and with mildly as well as strongly anisotropic phase functions representing scattering of the solar radiation by aerosols and water drops, respectively.

2. Equation of radiative transfer

The transfer of monochromatic radiation through a non-emitting plane-parallel atmosphere of infinite extent in the horizontal directions, but of finite extent in the vertical direction, is represented by

$$dJ(\tau; \mu, \phi) \over d\tau = I(\tau; \mu, \phi) - J(\tau; \mu, \phi). \quad (1)$$

The intensity $I(\tau; \mu, \phi)$ of the scattered radiation and associated parameters are defined in Section 1. The quantity $J(\tau; \mu, \phi)$ is the source function representing virtual emission per unit mass, per unit wavelength interval, at a level $\tau$ in a cone of unit solid angle with axis along the direction $\mu, \phi$; it is given by

$$J(\tau; \mu, \phi) = \frac{1}{4\pi} P(\tau; \mu, \phi; -\mu_0, \phi_0) \exp{-\tau/\mu_0} + \frac{1}{4\pi} \int_{-1}^{+1} \int_{0}^{\pi} P(\tau; \mu, \phi; \mu', \phi') I(\tau; \mu', \phi') d\mu' d\phi', \quad (2)$$

when the atmospheric model is illuminated from above ($\tau=0$) by a unidirectional beam of monochromatic radiation of strength $\pi \mu F$ per unit area normal to its direction of propagation given by $-\mu_0, \phi_0$.

The normalized scattering phase function $P(\tau; \mu, \phi; \mu', \phi')$ can be expressed in a Fourier series whose argument is $\phi' - \phi$, the difference between azimuth angles of the directions of incidence and scattering. Accordingly,

$$P(\tau; \mu, \phi; \mu', \phi') = \sum_{n=0}^{N} P^n(\tau; \mu, \mu') \cos(n(\phi' - \phi)). \quad (3)$$

The upper limit $N$ of this series required for a given accuracy depends upon the composition of the unit volume at the level $\tau$ and the wavelength $\lambda$ of the monochromatic radiation under investigation. The coefficients $P^n(\tau; \mu, \mu')$ appearing in (3) are expressible in the form (Chandrasekhar, 1950; Section 48)

$$P^n(\tau; \mu, \mu') = (2 - \delta_{n,0}) \sum_{i=-n}^{N} \Lambda_i(\tau) Y^i(\mu) Y^i(\mu'), \quad (4)$$

where $\delta_{n,0}$ is the Kronecker delta function given by $\delta_{n,0} = 1$ for $n = 0$ and otherwise zero, and $\Lambda_i(\tau)$ are the height-dependent Legendre coefficients representing scattering and/or absorbing nonhomogeneity in the vertical (Dave, 1974). The functions $Y^i(\mu)$ are the re-normalized associated Legendre polynomials (Dave and Armstrong, 1970) which are expressible in terms of the well-known associated Legendre polynomials $P^i(\mu)$ as follows:

$$Y^i(\mu) = \frac{(-1)^i}{(i+n)!} P^i(\mu). \quad (5)$$

Finally, the two-point boundary conditions corresponding to no incidence of the scattered radiation from above the top ($\tau=0$) and from below the bottom ($\tau=\tau_b$) are given by

$$I(\tau; -\mu, \phi) = 0, \quad I(\tau_b; +\mu, \phi) = 0. \quad (6)$$

With the Fourier series representation of the phase function [Eq. (3)], the intensity $I(\tau; \mu, \phi)$ can also be expressed in a Fourier series as

$$I(\tau; \mu, \phi) = \sum_{n=0}^{N} \sum_{m=0}^{N} I^n(\tau; \mu, \phi) \cos(n\phi - m\phi). \quad (7)$$

Hence, the double integral appearing on the right-hand side of (2) can be evaluated analytically over $\phi'$ after making use of the following orthogonality relationships for the trigonometric functions:

$$\int_{0}^{2\pi} \cos(n\phi - m\phi') \cos(n\phi - m\phi') d\phi' = \begin{cases} 0, & if \ n \neq m \\ (1 + \delta_{n,0}) \pi \cos(m\phi), & if \ n = m \\ \end{cases} \quad (8)$$

Because of this, Eq. (1) can be reduced to the following system of uncoupled integro-differential equations for values of $n$ given by $n = O(1)$:

$$dI^n(\tau; \mu) \over d\tau = I^n(\tau; \mu) - \frac{1}{4} \int_{-1}^{+1} P^n(\tau; \mu, \mu') I^n(\tau; \mu, \mu') d\mu', \quad (9)$$

with the boundary conditions given by

$$I^n(0; -\mu) = 0, \quad I^n(\tau_b; +\mu) = 0. \quad (10)$$

This system of equations is to be solved for each value of $n$, one at a time.

3. Spherical harmonics approximation

If Eq. (4) is substituted in Eq. (9), and the resulting expression is multiplied by $Y^i(\mu)$, we can then integrate each term on both sides over $\mu$ in the range $-1$ to $+1$,
and obtain
\[ d \int_{-1}^{+1} I^n(\tau; \mu) Y_l^m(\mu) d\mu \]
\[ = \int_{-1}^{+1} I^n(\tau; \mu) Y_l^m(\mu) d\mu \]
\[- \frac{1}{2} F e^{-r/m} \int_{-1}^{+1} Y_l^m(\mu)(2 - \delta_{0,n}) \]
\[ \times \sum_{l=0}^{N} \Lambda_l(\tau) Y_l^m(\mu) Y_l^m(-\mu) d\mu \]
\[ - \int_{-1}^{+1} Y_l^m(\mu) (1 + \delta_{0,n})(2 - \delta_{0,n}) \]
\[ \times \int_{-1}^{+1} \sum_{l=0}^{N} \Lambda_l(\tau) Y_l^m(\mu) Y_l^m(\mu') I^n(\tau; \mu') d\mu' d\mu. \] \tag{11}

Further, (1 + \delta_{0,n})(2 - \delta_{0,n}) = 2 for all values of \( n \).
Hence, for the \( k = l \) case, Eq. (11) can be rewritten as
\[ d \int_{-1}^{+1} I^n(\tau; \mu) \]
\[ = \int_{-1}^{+1} I^n(\tau; \mu) Y_l^m(\mu) d\mu \]
\[ = \int_{-1}^{+1} I^n(\tau; \mu) Y_l^m(\mu) d\mu \]
\[ - \frac{2 - \delta_{0,n}}{2(2l+1)} F e^{-r/m} \Lambda_l(\tau) Y_l^m(-\mu) \]
\[ = \int_{-1}^{+1} I^n(\tau; \mu') Y_l^m(\mu') d\mu' \] \tag{14}

then after some rearranging of terms, Eqs. (14) can be rewritten as
\[ \frac{[(l-n+1)(l+n+1)]^l}{2l+1} \frac{df_{l+1}(\tau)}{d\tau} + \sigma_{l}(\tau) f_{l+1}^{n}(\tau) \]
\[ + \frac{[(l-n)(l+n)]^l}{2l+1} \frac{df_{l-1}(\tau)}{d\tau} = s_{l}^{n}(\tau), \] \tag{17}

where
\[ \sigma_{l}(\tau) = \frac{\Lambda_l(\tau)}{2l+1} - 1, \] \tag{18}

and \( l = n, n+1, n+2, \ldots, L_n \). This is the spherical harmonics approximation for the \( n \)th Fourier component of the equation of radiative transfer which can be explicitly rewritten as
\[ \frac{(2n+1)^l}{2n+3} \frac{df_{l+1}(\tau)}{d\tau} + \sigma_{l+1}(\tau) f_{l+1}^{n}(\tau) + \frac{(2n+1)^l}{2n+3} \frac{df_{l+1}(\tau)}{d\tau} = s_{l+1}^{n}(\tau) \] \tag{19}
It should be noted that the $f_{n+1}^{n}(\tau)$ moment in the last equation of Eqs. (19) has been neglected so as to obtain a determined system of $L_n-n+1$ equations in the $L_n-n+1$ unknowns for the $n$th Fourier component. Eqs. (19) consist of $L_n-n+1$ inhomogeneous ordinary differential equations. The general solution, therefore, consists of $L_n-n+1$ arbitrary constants of integration, which must be determined by imposing $L_n-n+1$ suitable boundary conditions (see Section 5).

\[
A^n = \begin{pmatrix}
\frac{1}{(2n+1)^3} & 0 & 2(n+1)^3 & 0 \\
\frac{2(n+1)^3}{2n+3} & 0 & \frac{2(n+1)^3}{2n+3} & 0 \\
\frac{2(n+1)^3}{2n+5} & 0 & \frac{[3(2n+3)]^3}{2n+5} & 0 \\
\frac{[L_n-n-1](L_n-1-n-1)^3}{2L_n-1} & 0 & \frac{[L_n-n](L_n+n+1)^3}{2L_n-1} & 0 \\
0 & \frac{[L_n-n](L_n+n+1)^3}{2L_n+1} & 0 & 0 \\
\end{pmatrix}
\]

(21)

the diagonal matrix $C^n(\tau)$ is given by

\[
C^n(\tau) = \begin{pmatrix}
\sigma_n(\tau) & 0 & 0 \\
\sigma_{n+1}(\tau) & 0 & 0 \\
\sigma_{n+2}(\tau) & 0 & 0 \\
\vdots & \vdots & \vdots \\
\sigma_{L_n-1}(\tau) & 0 & 0 \\
\sigma_{L_n}(\tau) & 0 & 0 \\
\end{pmatrix}
\]

(22)

and the one-column vectors $f^n(\tau)$ and $s^n(\tau)$ of length $L_n-n+1$ are given by

\[
f^n(\tau) = \begin{pmatrix}
f_n^{n}(\tau) \\
f_{n+1}^{n}(\tau) \\
f_{n+2}^{n}(\tau) \\
\vdots \\
f_{L_n}^{n}(\tau)
\end{pmatrix}
\]

(23)

\[
s^n(\tau) = \begin{pmatrix}
s_n^{n}(\tau) \\
s_{n+1}^{n}(\tau) \\
s_{n+2}^{n}(\tau) \\
\vdots \\
s_{L_n-1}^{n}(\tau) \\
s_{L_n}^{n}(\tau)
\end{pmatrix}
\]

(24)

4. Compact form

Eqs. (19) representing the spherical harmonics approximation to the $n$th Fourier component of the transfer equation can be rewritten in the matrix form:

\[
\frac{dI^n(\tau)}{d\tau} + C^n(\tau)f^n(\tau) = s^n(\tau),
\]

(20)

where the bi-diagonal matrix $A^n$ of the order $(L_n-n+1)$ is given by

5. Boundary conditions

In order to obtain the $n$th azimuth-dependent component $I^n(\tau;\mu)$ of the intensity from computed values of $f^n(\tau)$ given by Eq. (15), we can expand $I^n(\tau;\mu)$ in a finite series of the renormalized associated Legendre polynomials with $L_n-n+1$ terms as follows. (This may be referred to as the $L_n$th spherical harmonics approximation to the $n$th azimuth-dependent component of the transfer equation.)

\[
I^n(\tau;\mu) = \sum_{l=0}^{L_n} \Phi_l^n(\tau) Y_l^m(\mu).
\]

(25)

For determining the values of the unknown coefficients $\Phi_l^n(\tau)$, we have to substitute (25) in (15), and then make use of (13). Accordingly,

\[
I^n(\tau;\mu) = \sum_{l=0}^{L_n} \frac{2l+1}{2} \Phi_l^n(\tau) Y_l^m(\mu).
\]

(26)
The spherical harmonics approximation to the $n$th Fourier component of the equation of radiative transfer [Eqs. (19) or (29)] is a system of $L_n - n + 1$ inhomogeneous ordinary differential equations. Hence, its general solution has $L_n - n + 1$ arbitrary constants of integration, which must be determined by imposing $L_n - n + 1$ suitable boundary conditions.

The physical boundary conditions for the transfer equation are that no scattered radiation is incident on the top or the bottom of the atmosphere from outside [Eq. (6) or Eq. (10)]. These same boundary conditions are associated with some problems in neutron transport, and are called "vacuum" boundary conditions, i.e., no neutrons are scattered from a vacuum into a multiplying medium. It is clear that boundary conditions as given by Eq. (10) cannot be satisfied exactly by any finite expansion such as Eq. (26), because in such a representation the intensity can at most vanish at $L_n - n$ discrete points whose positions depend upon the parameters $L_n$ and $n$, and the atmospheric model under investigation. This problem has been discussed in many articles in the neutron transport literature (Gelbard, 1968) and at other places (Dave and Canosa, 1974) where an implicit form of Marshak's matrix elements for $n = 0$ is given in terms of certain half-range integrals of the Legendre polynomials.

After making use of Eq. (26), the boundary conditions for an arbitrary integer value of $n$ and corresponding to the bottom ($\mu > 0$) of the atmosphere [second equation in Eq. (10)] can be rewritten as

$$\sum_{l=n}^{L_n} \frac{2l+1}{2} f_l^\mu (\tau_b) Y_l^\mu (\mu) = 0. \tag{27}$$

Since this condition cannot be exactly satisfied for all $\mu > 0$ with a finite value of $L_n - n$, we will follow a procedure similar to the one recommended by Marshak (1947) for the $n = 0$ case, and multiply Eq. (27) by $f_m^\mu (\mu)$ with $m = n - \delta_n + 1, n - \delta_n + 3, n - \delta_n + 5, \ldots, L_n$ (i.e., $m$ is always chosen to be odd), and integrate the resultant expressions over the lower hemisphere. Accordingly, we have,

$$\sum_{l=n}^{L_n} C_{ml}^n f_l^\mu (\tau_b) = 0, \tag{28}$$

where

$$C_{ml}^n = \frac{2l+1}{2} \int_0^1 Y_m^\mu (\mu) Y_l^\mu (\mu) d\mu, \tag{29}$$

with $l = n, n+1, n+2, \ldots, L_n$, and $m = n - \delta_n + 1, n - \delta_n + 3, n - \delta_n + 5, \ldots, L_n$.

If the system of equations given by Eq. (28) is explicitly written down after transferring the terms involving even values of the subscript $l$ to the right-hand side, we have the following matrix equation where $\nu = n - \delta_n$ and $\eta = n + \delta_n$:

$$\begin{bmatrix}
C_{n+1,n+1} & C_{n+1,n+3} & \cdots & C_{n+1,L_n - \delta_n} \\
C_{n+3,n+1} & C_{n+3,n+3} & \cdots & C_{n+3,L_n - \delta_n} \\
\vdots & \vdots & \ddots & \vdots \\
C_{L_n - \delta_n,n+1} & C_{L_n - \delta_n,n+3} & \cdots & C_{L_n - \delta_n,L_n - \delta_n}
\end{bmatrix}
\begin{bmatrix}
f_{n+1}^\mu (\tau_b) \\
f_{n+3}^\mu (\tau_b) \\
\vdots \\
f_{L_n - \delta_n}^\mu (\tau_b)
\end{bmatrix}
= 
\begin{bmatrix}
C_{n+1,n} & C_{n+1,n+1+2} & \cdots & C_{n+1,L_n - \delta_n - 1 + \delta_n} \\
C_{n+3,n} & C_{n+3,n+1+2} & \cdots & C_{n+3,L_n - \delta_n - 1 + \delta_n} \\
\vdots & \vdots & \ddots & \vdots \\
C_{L_n - \delta_n,n} & C_{L_n - \delta_n,n+1+2} & \cdots & C_{L_n - \delta_n,L_n - \delta_n - 1 + \delta_n}
\end{bmatrix}
\begin{bmatrix}
f_{n+1}^\eta (\tau_b) \\
f_{n+3}^\eta (\tau_b) \\
\vdots \\
f_{L_n - \delta_n}^\eta (\tau_b)
\end{bmatrix}. \tag{30}$$

If we note that the subscript $\nu$ always assumes an even value, elements of the matrix appearing on the left-hand side of (30) always have odd values for their subscripts. From the integral properties of the associated Legendre polynomials (Stegun, 1964), we find that all off-diagonal elements of the matrix on the left-hand side of Eq. (30) vanish, while all elements along the diagonal of this matrix have a fixed value of $1$. Thus, the square matrix of the order $(L_n - n + 1)/2$ appearing on the left-hand side of Eq. (29) reduces to a unit matrix multiplied by a scalar factor. Hence, Eq. (30) can be rewritten as

$$f_{\text{odd}}^\mu (\tau_b) = \mathbf{G}^n f_{\text{even}}^\mu (\tau_b), \tag{31}$$

where $f_{\text{odd}}^\mu$ is a column vector formed by the odd components of $f^\mu$, i.e., $f_{n+1}^\mu, f_{n+3}^\mu, \cdots, f_{L_n - \delta_n}^\mu$, and $f_{\text{even}}^\mu$ by the even components, $f_{n}^\mu, f_{n+2}^\mu, \cdots, f_{L_n - 1 + \delta_n}^\mu$. Explicitly,

$$f_{\text{odd}}^\mu (\tau_b) = \begin{bmatrix}
f_{n+1}^\mu (\tau_b) \\
f_{n+3}^\mu (\tau_b) \\
\vdots \\
f_{L_n - \delta_n}^\mu (\tau_b)
\end{bmatrix}, \quad f_{\text{even}}^\mu (\tau_b) = \begin{bmatrix}
f_{n}^\mu (\tau_b) \\
f_{n+2}^\mu (\tau_b) \\
\vdots \\
f_{L_n - 1 + \delta_n}^\mu (\tau_b)
\end{bmatrix}. \tag{32, 33}$$

Finally, the $G_{ml}^n$ element of the $(L_n - n + 1)/2$-order matrix $\mathbf{G}^n$ is given by

$$G_{ml}^n = - \frac{(2l+1)}{2} \int_0^1 Y_m^\mu (\mu) Y_l^\mu (\mu) d\mu, \tag{34}$$
with \( m = n - \delta_n + 1, \ n - \delta_n + 3, \cdots, \ L_0, \) and \( \ell = n + \delta_n, \ n + \delta_n + 2, \cdots, \ L_0 - 1 + 2\delta_n. \)

One can follow the procedure outlined above to arrive at the following expression for the boundary conditions at the top of the atmosphere:

\[
\left. f_{\text{out}}(0) \right|_{0} = -G_n^m f_{\text{in}}(0). \tag{35}
\]

It can be seen that each of Eqs. (31) and (35) represents exactly \((L_n - n + 1)/2\) conditions, so that both equations together provide us with the required \(L_n - n + 1\) conditions for determining the \(L_n - n + 1\) arbitrary constants of integration appearing in the system of equations represented by (19) or (20).

Finally, the elements \(G_{m,i}^n\) of the boundary-condition matrix \(G^n\) [Eq. (34)] can be evaluated analytically by making use of the following expressions based on an integral relationship for the associated Legendre polynomials given by Robin (1958):

1. For odd values of \( m \) and \( n \)

\[
G_{m,i}^n = \frac{(2l+1)(l-n)!(l+n+1)!(l)!Y_m^n(0)V^{\ell+1}_m(0)}{(l-m)!(l+m+1)!} \tag{36}
\]

2. For odd values of \( m \), but for even values of \( n \)

\[
G_{m,i}^n = \frac{-(2l+1)(m-n)!(m+n+1)!(l)!Y_m^n(0)V^{\ell+1}_m(0)}{(l-m)!(l+m+1)!} \tag{37}
\]

Since tables of \(V^n_m(0)\) may not be readily available, one can consider using the following recurrence relationships which provide an efficient procedure for machine computations of \(G_{m,i}^n\):

1. For odd values of \( n \), the first element of the first row of the \(G^n\) matrix is given by

\[
G_{1,1}^{n+1,2,n+3} = \frac{(2n+7)(2n+1)(2n+5)!}{(2n+4)(2n+6)!} G_{1,1}^{n+1,2,n+3}, \tag{38}
\]

with

\[
G_{1,1}^{n+1,2,n+3} = \frac{5\sqrt{3}}{8}. \tag{39}
\]

The remaining elements in the first row of the \(G^n\) matrix are then obtained by making use of the relationship

\[
G_{m,i+2}^n = \frac{(m-l)(l+1)!(l+n+1)!}{(2l+1)(l+n+3)!} \left[ \frac{(l+n+1)(l+n+2)!}{(l-n+1)(l-n+2)!} \right] G_{m,i}^n \tag{40}
\]

and all elements except the first one, of a given column, are obtained by making use of the relationship

\[
G_{m+2,i}^n = \frac{(m-l)(m+l+1)}{(l-m-2)(l+m+3)} \times \left[ \frac{(m+n+1)(m-n+1)!}{(m+n+2)(m-n+2)!} \right] G_{m,i}^n. \tag{41}
\]

2. For even values of \( n \), the first element of the first row of the \(G^n\) matrix is given by

\[
G_{1,1}^{n+1,2,n+3} = \frac{(2n+3)(2n+5)!}{(2n+4)(2n+6)!} G_{1,1}^{n+1,2,n+3}, \tag{42}
\]

with

\[
G_{1,1}^{n+1,2,n+3} = -\frac{3}{8}. \tag{43}
\]

The remaining elements in the first row of the \(G^n\) matrix are then obtained by making use of the relationship

\[
G_{m+1,i+2}^n = \frac{(m-l)(m+l+1)}{(l-m-2)(l+m+3)} \times \left[ \frac{(m+n+2)(m-n+2)!}{(m+n+1)(m+n+1)!} \right] G_{m,i}^n \tag{44}
\]

and all elements except the first one, of a given column, are obtained by making use of the relationship

\[
G_{m+2,i}^n = \frac{(m-l)(m+l+1)}{(l-m-2)(l+m+3)} \times \left[ \frac{(m+n+2)(m-n+2)!}{(m+n+1)(m+n+1)!} \right] G_{m,i}^n. \tag{45}
\]

6. The algebraic problem

From our discussion in Sections 4 and 5, we find that a direct solution of the spherical harmonics approximation corresponding to the \(n\)th Fourier component of the transfer equation requires \(L_n - n + 1\) inhomogeneous differential equations [Eq. (20)] with \(L_n - n + 1\) unknowns. This is a two-point boundary-value problem with \((L_n - n + 1)/2\) conditions for determining \((L_n - n + 1)/2\) arbitrary constants of integration given by Eq. (31), and the remaining \((L_n - n + 1)/2\) arbitrary constants of integration given by Eq. (35).

For nonhomogeneous atmospheric models, a usual approximation is to divide the atmospheric model into several layers of constant optical properties, i.e., within each layer, elements \(\sigma_i(r)\) given by Eq. (18) of the \(C_i(r)\) matrix [see Eq. (22)] can be assumed to be constant. Thus, if we integrate Eq. (20) between two optical levels \(r_{j-1}\) and \(r_j\), \((j = 1, 2, \cdots, J)\) corresponding to the top of the atmosphere) and use the trapezoidal rule of integration, after some rearrangement of terms, we have

\[
(A^n + \frac{1}{2} \Delta r_{j-1}, C^n_{j-1}) F^n_{j-1} + (A^n + \frac{1}{2} \Delta r_{j-1}, C^n_{j-1}) F_j = w_{j-1}, \tag{46}
\]

where

\[
\Delta r_{j-1} = r_j - r_{j-1}, \tag{47}
\]

\[
C^n_{j-1} = C^n(r_{j-1} + \frac{1}{2} \Delta r_{j-1}), \tag{48}
\]

\[
w_{j-1} = \frac{1}{2} \Delta r_{j-1}(s^n_{j-1} + s^n_{j}), \tag{49}
\]

\[
\Delta r_{j-1} = r_j - r_{j-1}, \tag{47}
\]

\[
C^n_{j-1} = C^n(r_{j-1} + \frac{1}{2} \Delta r_{j-1}), \tag{48}
\]

\[
w_{j-1} = \frac{1}{2} \Delta r_{j-1}(s^n_{j-1} + s^n_{j}), \tag{49}
\]

\[
\Delta r_{j-1} = r_j - r_{j-1}, \tag{47}
\]

\[
C^n_{j-1} = C^n(r_{j-1} + \frac{1}{2} \Delta r_{j-1}), \tag{48}
\]

\[
w_{j-1} = \frac{1}{2} \Delta r_{j-1}(s^n_{j-1} + s^n_{j}), \tag{49}
\]
It may be noted that \( C^r_{j-1} \) is the matrix \( C^n(\tau) \) evaluated at the midpoint of the layer between \( \tau_{j-1} \) and \( \tau_j \). With these centered differences, we know that the finite-difference approximation to our problem as given by Eqs. (20), (31) and (35) has second-order accuracy, i.e., the truncation errors \( |f_j^n - f^n(\tau_j)| \) are of the order of \( \Delta \tau^2 \), where \( \Delta \tau \) is the largest mesh width used (Keller, 1968).

The boundary conditions at the top and bottom of the atmosphere given by Eqs. (31) and (33) become, in discrete form,

\[
(f^i_t)_{\text{odd}} = -G^n(f^i_t)_{\text{even}},
\]

\[
(f^i_j)_{\text{odd}} = G^n(f^i_j)_{\text{even}},
\]

respectively. The parameter \( J \) stands for the serial number of the bottom-most level of the atmosphere.

The boundary conditions given by Eqs. (51) and (52) separate sharply the even from the odd components of \( f^i_j \) at the top and bottom of the atmosphere. It is therefore convenient to rearrange the solution vectors \( f^i_j \), putting the even and odd components at the top and bottom halves, respectively, in all the spatial grid. We thus define the following additional \( (L_n-n+1) \)-component vector, and \( (L_n-n+1) \)-order matrices:

\[
G^n_i = \begin{pmatrix} 
(f^i_t)_{\text{even}} \\
(f^i_j)_{\text{odd}}
\end{pmatrix},
\]

\[
D^n_{j-1,i-1} = \text{Column}[ -A^n + \frac{1}{2} \Delta \tau_{j-1} C^r_{j-1}],
\]

\[
D^n_{j-1,i} = \text{Column}[ A^n + \frac{1}{2} \Delta \tau_{j-1} C^r_{j-1}],
\]

where “Column” is a column operator denoting a rearrangement of the columns of a matrix depending upon the value of the superscript \( n \). For even values of the superscript \( n \), the first half of the columns of the resulting matrix are the 1st, 3rd, 5th, \ldots, \((L_n-n)\)th columns of the matrix inside the parentheses, and the second half the 2nd, 4th, \ldots, \((L_n-n+1)\)st columns. For odd values of the superscript \( n \), the first half of the columns of the resulting matrix are the 2nd, 4th, \ldots, \((L_n-n+1)\)st columns of the matrix inside the parentheses, and the second half the 1st, 3rd, \ldots, \((L_n-n)\)th columns.

After making use of Eqs. (53) to (55), we finally write, in full, the block algebraic system given by Eqs. (46), (51), and (52), as follows:

\[
\begin{align*}
D^n_{i} g^n_i + D^n_{i} g^n_i &= w^n_i \\
D^n_{2i} g^n_i + D^n_{2i} g^n_i &= w^n_i \\
D^n_{j-1,i} g^n_{j-1,i} + D^n_{j-1,i} g^n_{j-1,i} &= w^n_{j-1,i}
\end{align*}
\]

\[
\begin{align*}
\begin{bmatrix} g^n_i \\ g^n_{j-1,i} 
\end{bmatrix} &= -G^n \begin{bmatrix} g^n_i \\ g^n_{j-1,i} 
\end{bmatrix} \\
\begin{bmatrix} g^n_i \\ g^n_{j-1,i} 
\end{bmatrix} &= G^n \begin{bmatrix} g^n_i \\ g^n_{j-1,i} 
\end{bmatrix}
\end{align*}
\]

where the superscripts \( b \) and \( t \) designate the bottom and top half of the vector inside the parentheses. In fact, \( g^n_{i} = (f^i_t)_{\text{even}} \), and \( g^n_{j-1,i} = (f^i_j)_{\text{odd}} \), and so on [see Eq. (53)].

It should be pointed out that the form of the algebraic system [Eq. (56)] is independent of the nature of the phase function, and/or nonhomogeneity of the atmosphere.

The block algebraic system of equations represented by Eq. (56) can be solved for each value of \( n \), one at a time by using the procedures discussed elsewhere (Canosa and Penañel, 1972, 1973; Dave and Canosa, 1974; Dave, 1974).

7. Smoothing of intensity versus \( \theta \) curves

It is well known that an \( I^n(\tau;\mu) \) vs \( \mu \) (or \( \theta \)) curve obtained with Eq. (26) will be oscillatory in character with the amplitude and frequency of oscillations depending upon the parameter \( L_n-\nu_n \) and position of the level under investigation with respect to the top or bottom of the atmosphere. Dave and Armstrong (1974) pointed out that the values of \( I^n(\tau;\mu) \) accurate within \( \pm 0.1\% \) can be obtained for all possible directions of observation from computed values of \( f^n(\tau) \) by making use of the integration-of-the-source-function method recommended by Kourganoff (1952). If we substitute Eq. (26) in the last term on the right-hand side of Eq. (9) and make use of Eq. (13), the \( n \)th Fourier component of the source function given by the last two terms on the right-hand side of Eq. (9) can be written as

\[
J^n(\tau;\mu) = \frac{(2-\delta_{\theta,n})}{4} Fe^{-r_{\theta}u_n} \sum_{i=n}^{N} \Lambda_i(\tau)M_i(\mu)M_i(\mu) + \frac{i}{2} \sum_{i=n}^{L_n} \Lambda_i(\tau)M_i(\mu)M_i(\mu) .
\]

Values of \( I^n(\tau;\mu) \), the \( n \)th Fourier component of the intensity of the scattered radiation \( I(\tau;\mu,\phi); \text{see Eq. (7)} \) can then be computed by making use of the equations

\[
I^n(\tau;\mu) = \int_{0}^{r} J^n(t;\mu) e^{-(r-t)\mu dt},
\]

\[
I^n(\tau;\mu) = \int_{0}^{r} J^n(t;\mu) e^{-(r-t)\mu dt}.
\]

Based on our experience for the \( n=0 \) case (Dave and Armstrong, 1974), we feel justified in assuming that the \( I^n(\tau;\mu) - \theta \) curves for non-vanishing values of the superscript \( n \) obtained by making use of Eqs. (57)–(59) will also be fairly smooth. If so, the curves of \( I(\tau;\mu,\phi) \) as a function of the zenith (or nadir) angle \( \theta \) or the azimuth angle \( \phi \) will be definitely smooth (e.g., Dave and Gadzad, 1970).
8. Selection of the parameter \( L_n \)

In Section 3, we defined a parameter \( L_n \) representing the order of the spherical harmonics approximation to the \( n \)th azimuth-dependent component of the transfer equation. This parameter is equal to \( L_0 + \delta_n \), where \( L_0 \) is the order of the approximation used in the numerical solution of the azimuth-independent term, and the quantity \( \delta_n \) is equal to zero or unity depending upon whether the superscript \( n \) is even or odd, respectively.

For a pure molecular atmosphere (Rayleigh’s law of scattering), the Legendre coefficient \( A_i(\tau) \) [see Eq. (4)] vanishes for all values of the subscript \( i > 2 \). It is therefore unnecessary to perform computations for the third and further high-order components of the intensity in this case. However, for obtaining a smooth \( I^2(\tau; \mu) \) vs \( \theta \) curve comparable in accuracy with that obtained with Chandrasekhar’s (1950) \( X \)- and \( Y \)-function method, Dave and Armstrong (1974) found that it is necessary to use a 19th (or higher) order of approximation for the numerical solution of the azimuth-independent component. Thus, even though the parameter \( N \) appearing in Eqs. (3) and (4) does not exceed 2 in theory for Rayleigh scattering, we set \( N = 19 \) (or higher) and \( L_0 = 19 \) (or higher) for a direct numerical solution of the spherical harmonics approximation. Computations of \( I^2(\tau; \mu) \), \( L^2(\tau; \mu) \) and \( I^2(\tau; \mu) \) with such an order of approximation does not pose any significant problem.

For the scattering of visible light by aerosol particles assumed spherical (Mie’s law of scattering), the upper upper limit \( N \) of the series defined by Eqs. (3) and (4) can assume any value in the range 50–150 depending upon the nature of the size distribution of aerosols, and wavelength under investigation. For the scattering of visible light by water drops in nonprecipitating clouds, this range is about 300–500. Hence, for such cases, we might require numerical solutions of several tens of azimuth-dependent components using fairly high orders of approximation. The numerical solution of the spherical harmonics approximation of such a large \( (\gtrsim 100) \) order is very time-consuming; consequently, it should be undertaken only if it is absolutely necessary.

With this in mind, we have terminated the first series on the right-hand side of Eq. (57) at \( N \) which is the total number of terms in the Legendre expansion [Eq. (3)] for an adequate reproduction of the phase function over the entire angular range. This term representing the scattering of the direct solar radiation, i.e., virtual emission due to primary scattering, can be evaluated for any value of \( N \) without much difficulty. On the other hand, the second series appearing on the right-hand side of Eq. (57) is terminated at \( L_n \) which is the order of the spherical harmonics approximation used in the numerical solution of the transfer equation. This second term representing the scattering of the atmospheric radiation can be expected to be less anisotropic than the first term. Hence, it is appropriate to perform several test calculations in the following manner before undertaking extensive radiation-transfer studies in hazy and cloudy atmospheric models: Let \( I_{L_n}(\tau; \mu, \phi) \) and \( I_{L_m}(\tau; \mu, \phi) \) represent the intensity of the scattered radiation computed with \( L_n \) and \( L_m \) orders of the spherical harmonics approximation for the second term in Eq. (57), but with all \( N \) terms for the first term in Eq. (57), respectively. We then define a ratio

\[
\rho(\tau; \mu, \phi; L_n/L_m) = I_{L_n}(\tau; \mu, \phi)/I_{L_m}(\tau; \mu, \phi),
\]

where \( L_n > L_m \). If the values of this ratio are found to be close to unity within the desired limit for the case under investigation (viz. size distribution of particles, wavelength, ranges of the parameters \( \mu \) and \( \mu_0 \), we can then use with reasonable confidence \( L_n \)-th order of approximation for all further investigations involving similar parameters.

9. Conclusion

In the preceding sections, we derived the spherical harmonics approximation to the equation of radiative transfer corresponding to any \( n \)th azimuth-dependent component of the intensity of the scattered radiation. Expressions were then derived for representing the boundary conditions of no incidence of the scattered radiation on the atmosphere from outside, in a discrete form consistent with the Legendre-series representation of intensity. This general spherical harmonics approximation was then reduced by finite differences to a block algebraic system of equations which can be solved by making use of the procedure developed by Canosa and Penafield (1972). Representative results of some extensive calculations for homogeneous atmospheric models with anisotropic phase functions of scattering, and obtained with the method discussed in this paper, will be presented in Part II of this paper.

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