AT721 Section 4:

Expansions, Quadrature and the Matrix Equation of Transfer

The last chapter introduced a form of the radiative transfer equation that integrates the source function through the atmosphere. This might appear to be a solution of our most general transport problems, but closer examination of the equation of transfer $(2.x)$ reveals the (virtual) source terms $(2.x)$ contain integrals of the intensity over the direction variable and thus contain part of the solution itself. In fact if it were not for this complication, the equation of transfer would be but a mere differential equation and the theory of multiple scattering would have been worked out and forgotten long ago. All methods of solution, either simple or complex, introduce some form of approximation to this integral source term. This approximation usually begins with the introduction of some form of quadrature scheme resulting in a general matrix form of equation. Construction of this matrix equation requires preliminary considerations of different types of expansions that are applied to approximate the radiance fields and other related quantities.

4.1 Radiance expansion

Both radiance quantity and the source term are functions of azimuth angle ϕ and as such repeat over the interval $[\phi_{\odot}, \phi_{\odot} + 2\pi]$. Given these circumstances it is convenient to write

$$
I(\vec{r}, \mu, \phi) = \sum_{m=0}^{M} I^{mc}(\vec{r}, \mu) \cos m(\phi - \phi_{\odot}) + I^{mc}(\vec{r}, \mu) \sin m(\phi - \phi_{\odot})
$$
(4.1)

where

$$
I^{mc}(\vec{r},\mu) = \frac{1}{(1+\delta_m)\pi} \int_{\phi_{\odot}}^{\phi_{\odot}+2\pi} I(\vec{r},\mu,\phi) \cos m\phi d\phi
$$
 (4.2)

$$
I^{mc}(z,\mu) = \frac{1}{\pi} \int_{\phi_{\mathcal{O}}}^{\phi_{\mathcal{O}}+2\pi} I(z,\mu,\phi) \sin m\phi d\phi
$$
 (4.3)

respectively for the 'even' and 'odd' coefficients. In this definition, δ_m is the Kroneckar delta function. Under the assumption of horizontal homogeneity, I is an even function of ϕ (i.e. it is symmetric about ϕ_{\odot}) and for a sun-based coordinate system, $\phi_{\odot} = 0$. Under these circumstances, it follows that

$$
I(\vec{r}, \mu, \phi) = \sum_{m=0}^{M} I^{m}(\vec{r}, \mu) \cos m(\phi)
$$
 (4.4)

add examples, illustrate the m=o mode, etc...

 \vert If we are only interested in hemispheric flux, then only the m=0 equation requires solution how might you show this]

4.2 Legendre Expansion of the Phase Function

Another expansion used in developing the solution to the radiative transfer equation is to represent the scattering phase function as a polynomial in scattering angle Θ or more precisely, $\cos \Theta$. As we will see, there are good reasons to do this, the principal reason being that certain quadrature schemes are exact when integrating of polynomial of related degree. The importance and relevance of this property is discussed below.

The phase function expansion is performed in the form of the following polynomial series,

$$
P(\cos \Theta) = \sum_{\ell=0}^{N} \chi_{\ell} P_{\ell}(\cos \Theta)
$$
\n(4.5)

where P_ℓ is the ℓ^{th} order Legendre polynomial and χ_ℓ are the associated expansion coefficients, defined as

$$
\chi_{\ell} = \frac{(2\ell+1)}{2} \int_{-1}^{1} P(\cos\Theta) P_{\ell}(\cos\Theta) d\cos\Theta.
$$
 (4.6)

A convenient form of the phase function often used in radiative transfer studies is the Henyey– Greenstein (HG) function given in Table 3.1. This function is is useful because the expansion of this function reduces to

$$
P_{HG}(\cos \Theta) = \sum_{\ell} (2\ell + 1) g^{\ell} P_{\ell}(\cos \Theta)
$$

Figure 4.1a provides a contrast of the expansion coefficients derived from Lorenz–Mie and the HG phase functions for a fair–weather–cumulus cloud model. Fig. 4.1b shows how the different truncation orders in the Legendre expansion affect the reproduction of the phase function.

Figure 4.1 Coefficients in the Legendre expansion for a Lorenz–Mie phase function as a function of size parameter (from Clark et al., 1957).

Figure 4.2 Double HG and single HG functions contrasted with the phase function of Takano and Liou (1989).

A shortcoming of the HG function is that it does not capture the peakiness of the forward scatter nor the typical increase in backscatter. A slight improvement of the HG function is provided by the double–HG function of the form

$$
P_{DHG} = bP_{HG}(g_1) + (1 - b)P_{HG}(g_2)
$$

where b is some arbitrary weight and $g_{1,2}$ are the values of the asymmetry parameters chosen. Figure 4.2 is an example of various double HG functions compared to a calculated phase function for hexagonal ice columns (the latter from Takano and Liou, 1989).

Table 4.1 presents a few phase functions commonly encountered in different scattering problems, together with their first four expansion coefficients. Figure 4.1a graphically presents the coefficients of a phase function derived from Lorenz–Mie theory and shows how the higher order coefficients contribute as the size parameter $x = 2\pi r/\lambda$ increases. This is a reflection of the general guideline that the larger the particle, and hence the more forward the scattering, the more polynomial terms are required to represent the true phase function (i.e. the larger is N). Simpler, analytic functions require fewer polynomial terms.

The expansion coefficients for the two analytic functions given in this table are expressed in terms of the asymmetry parameter g. This is a parameter of some importance to particle scattering problems and is defined as

$$
g = \frac{1}{3}\chi_1 = \frac{1}{2}\int_{-1}^{1} P(\cos\Theta)\cos\Theta d\cos\Theta
$$

An interpretation of this parameter is as follows:

- $q = 1$ for complete forward scattering,
- $g = -1$ for complete backward scattering, and
- $g = 0$ for isotropic or symmetric scattering (e.g. Rayleigh scattering).

For solar wavelengths and water droplet clouds, g is quasi–constant with an approximate value 0.85. Values of this parameter for irregular particles, like ice crystals, at solar wavelengths are less well known but are thought to be significantly different from the values associated with spherical particles that the multiple

Scatter type	Formula for $P(\Theta)$	Legendre Coefficients			
		χ_0	χ_1	χ_2	g
Isotropic	1	1	Ω	Ω	Ω
Rayleigh	$\frac{3}{4}(1+\cos^2\Theta)$	1	Ω	$\frac{1}{2}$	Ω
$Henyey-$	$\frac{1-g^2}{(1+g^2-2g\cos\Theta)^{3/2}}$	$\mathbf{1}$	3g	$5g^2$	g
Greenstein Forward [†] plus backward	$(1+g)\delta^+$ + $(1-g)\delta^-$	$\mathbf{1}$	3g	5	g

Table 4.1 First three Legendre coefficients of selected phase functions

scattering from such clouds differs from clouds composed of spherical particles of the same equivalent size. The spectrum of g illustrated in Fig. 4.3 is such that it is almost invariant with wavelength for $\lambda < 3\mu m$ and not too sensitive to the details of the particle–size distributions (suggested by the differences between cloud models). The asymmetry parameter is a very useful parameter when attempting to understand the bulk properties of multiple scattering media.

Before contemplating the expansion properties of other phase functions, let us consider further properties of the Legendre expansion. A most important property of the expansion derives from the addition theorem of spherical harmonics, from which it follows that

$$
P(\mu, \phi, \mu', \phi') = \sum_{m=0}^{M} \sum_{\ell=m}^{N} [2 - \delta(0, m)] \chi_{\ell} \frac{(\ell - m)!}{(\ell + m)!} P_{\ell}^{m}(\mu) P_{\ell}^{m}(\mu') \cos m(\phi - \phi')
$$
(4.7)

where $P_{\ell}^{m}(\mu)$ is the *associated* Legendre polynomial, N is some suitably chosen truncation (more to be said about this later). Through the addition theorem we are able to factor separately the dependencies of the phase function on μ , μ' and on the azimuthal difference $\phi - \phi'$ and, in turn, greatly reduce the dimensionality of the radiative transfer problem. From the numerical standpoint, however, it turns out to be more stable to write the expansion (3.7) in terms of re–normalized associated Legendre polynomials

$$
Y_{\ell}^{m}(\mu) = \left[\frac{(\ell - m)!}{(\ell + m)!}\right]^{1/2} P_{\ell}^{m}(\mu)
$$
\n(4.8)

[Dave and Armstrong (1970; Computations of high–order associated Legendre Polynomials, JQRST, 10, 557–562]. Subroutine PLEG generates these normalized functions. Therefore the phase function expansion (4.7) becomes

$$
P(\mu, \phi, \mu', \phi') = \sum_{m=0}^{M} \sum_{\ell=m}^{N} \chi_{\ell}^{m} Y_{\ell}^{m}(\mu) Y_{\ell}^{m}(\mu') \cos m(\phi - \phi')
$$
(4.9)

where

$$
\chi_{\ell}^{m} = [2 - \delta(0, m)] \chi_{\ell}.
$$

Figure 4.2 The asymmetry factor as a function of wavelength for three hypothetical cloud models.

4.2.1 Examples of Phase Function expansions

4.3 Quadrature and Truncation

We are now left to introduce the procedures for integrating quantities over directional space. We do this using a quadrature scheme, of the general form

$$
\int_{-1}^{1} f(x)dx = \sum_{i=-n}^{n} f(x_i)w_i
$$
\n(4.10)

where x_i is referred to as the quadrature abscissa and w_i as the quadrature weight. There are several ways of choosing the abscissa and weights but for certain types of quadrature schemes, the integral is exact provided $f(x)$ is a polynomial of specified degree. This is most important as we have gone to some length to express the phase function as a polynomial of degree N and if we choose or quadrature carefully then we can ensure the phase function normalization condition $(2.x)$,

$$
\frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sum_{m=0}^M \sum_{\ell=m}^N \chi_\ell^m Y_\ell^m(\mu) Y_\ell^m(\mu') \cos m(\phi - \phi') d\mu' d\phi' = 1
$$

Figure 4.3 Comparison of Lorenz–Mie and HG functions for water cloud (left) and haze (right).

which reduces to the integral constraint

$$
\frac{1}{2} \int_{-1}^{1} \sum_{\ell=0}^{N} \chi_{\ell}^{m=0} P_{\ell}^{m=0}(\mu) P_{\ell}^{m=0}(\mu') d\mu' = 1.
$$
\n(4.11)

Two quadrature schemes of note are the Gaussian scheme which is exact for polynomials of degree N provided $N \leq 4n-1$ and the Lobatto scheme which is exact for polynomials of degree $N \leq 4n-3$. Given that the phase function can been expanded into a series of polynomial functions of maximum degree N, then by appropriately matching the number of streams $(2n)$ we use to characterize the radiance field to N according to the type of quadrature used, we can ensure energy conservation. For example, suppose we select $N = 31$, then the integral constraint is exact provided we select $n \leq 8$ which means we can divide the radiance field into a maximum 16 discrete angles (or less); 8 angles in the $+\mu$ direction and 8 angles in the $-\mu$ direction, (Fig. 4.4). This represents a compromise between the need to carry a large number of terms in the phase function expansions and while maintaining a practical number of quadrature points and a practical dimensionality to the transfer problem under consideration.

Figure 4.5a is an example of the distribution of Gaussian and Lobatto quadrature abscissae and weights provided by routines LOBATTO QUADRATURE and GAUSS LEGENDRE QUADRATURE. One of the advantages of the Lobatto scheme is the existence of weights at $\mu = \pm 1$. The Double–Gauss scheme is also commonly adopted because of the way it distributes its μ_i points. Double–Gauss simply refers to a quadrature rule in which the Gaussian formula is applied separately to the half ranges $0 < \mu < 1$ and $-1 < \mu < 0$. In this case, by choosing even ordered quadrature, the quadrature points are distributed evenly about $|\mu| = 0.5$ and clustered towards $\mu = 0$ and $\mu = \pm 1$.

Figure 4.2 (a) Coefficients for Lorenz–Mie and HG functions derived for a cumulus cloud model size distribution. (b) Comparison of the HG function and Legendre expansions of varying orders.

4.4 The Matrix Equation of Transfer

We begin by writing the radiative transfer equation (2.25) as

$$
\mu \frac{dI(\tau; \mu, \phi)}{d\tau} = I(\tau; \mu, \phi) - \frac{\varpi_o}{4\pi} \int_0^{2\pi} \int_{-1}^1 P(\tau; \mu, \phi, \mu', \phi') I(\tau; \mu', \phi') d\mu' d\phi'
$$

-S(\tau; \mu, \phi), (4.12)

where $\mu = \cos \theta$ and the source term is

$$
S(\tau;\mu,\phi) = \frac{\varpi_o}{4\pi} F_{\odot} P(\tau;\mu,\phi,-\mu_{\odot},\phi_{\odot}) e^{-\tau/\mu_{\odot}} + (1-\varpi_o) \mathcal{B}(\tau)
$$

where as above F_{\odot} is the monochromatic flux at the top of the atmosphere ($\tau = 0$), $d\tau = -\sigma_{ext}dz$. Note also that the frequency or wavelength dependence has been omitted and μ ranges from 1 to 0 for upward intensities and -1 to 0 for downward intensities.

Figure 4.4 An example of the discrete μ –radiance space.

Carrying out the integral transform (4.2) with $\phi_{\odot} = 0$ on each term separately leads to

LHS:
$$
\mu \frac{dI(\tau; \mu, \phi)}{d\tau} \to \mu \frac{dI^m(\tau; \mu)}{d\tau}
$$

First term RHS: $I(\tau; \mu, \phi) \to I^m(\tau; \mu)$

Second term RHS: In this case we write this term under the integral transform as

$$
\frac{1}{(1+\delta_m)\pi}\int_0^{2\pi}\cos m\phi d\phi \frac{\varpi_o}{4\pi}\int_0^{2\pi}\int_{-1}^1 P(\tau,\mu,\phi,\mu',\phi')I(\tau,\mu',\phi')d\mu'd\phi'
$$

Introducing the phase function expansion (4.9) into this expression yields

$$
\frac{1}{(1+\delta_m)\pi} \int_0^{2\pi} \cos m\phi d\phi \frac{\varpi_o}{4\pi} \int_0^{2\pi} \int_{-1}^1 \sum \sum \chi_\ell^{m'} Y_\ell^{m'}(\mu) Y_\ell^{m'}(\mu') \cos m'(\phi - \phi')
$$

$$
\times \sum_{m''} I^{m''}(\mu') \cos m''(\phi') d\mu' d\phi'
$$

which produces integrals of the form

$$
\int_0^{2\pi} [\cdots] \cos m'(\phi - \phi') \cos m'' \phi' d\phi' = 2\pi [\cdots] \cos m' \phi
$$

so we can write the second term as

$$
\frac{1}{(1+\delta_m))\pi}\int_0^{2\pi}\frac{\varpi_o}{2}\int_{-1}^1\sum_{m'}\left[\sum_{\ell}\chi_{\ell}^{m'}Y_{\ell}^{m'}(\mu)Y_{\ell}^{m'}(\mu')\right]I^{m'}(\mu')d\mu'\cos m'\phi\cos m\phi d\phi.
$$

or as

$$
(1+\delta_m)\frac{\varpi_o}{4}\sum_{\ell=m}\chi_\ell^mY_\ell^m(\mu)\int_{-1}^1Y_\ell^m(\mu')I^m(\mu')d\mu'
$$

Figure 4.7 (a) Comparison of Gaussian and Lobatto quadrature. (b) Double-Gaussian versus single Gaussian quadrature.

Source terms RHS: Since the Planck emission is isotropic, it follows that

$$
(1 - \varpi_o) \mathcal{B} \to \delta_m (1 - \varpi_o) \mathcal{B}
$$

and for the direct source (as an exercise show this)

$$
\frac{\varpi_o}{4} F_{\odot} e^{-\tau/\mu_{\odot}} \sum_{\ell=m} \chi_\ell^m Y_\ell^m(\mu) Y_\ell^m(-\mu_{\odot})
$$

Grouping terms we obtain

$$
\mu \frac{dI^{m}(\tau;\mu)}{d\tau} = I^{m}(\tau;\mu) - (1+\delta_{0,m}) \frac{\varpi_{o}}{4} \sum_{\ell=m}^{N} \chi_{\ell}^{m} Y_{\ell}^{m}(\mu) \int_{-1}^{1} Y_{\ell}^{m}(\mu') I^{m}(\tau;\mu') d\mu'
$$

$$
- \frac{\varpi_{o}}{4\pi} F_{\odot} \sum_{\ell=m}^{N} \chi_{\ell}^{m} Y_{\ell}^{m}(\mu) Y_{\ell}^{m}(-\mu_{\odot}) e^{-\tau/\mu_{\odot}} - \delta_{m} (1-\varpi_{o}) \mathcal{B}(\tau) \tag{4.13}
$$

Key point is that (4.13) is a system of *uncoupled* equations in m such that the solutions for the $m = 0, 1, \ldots, M$ modes proceed independently of each other and the final radiance solution constructed from the expansion (4.4).

A special case of (4.13) is the $m = 0$ equation corresponding to the azimuthally averaged intensity. For this case, it follows that

$$
\mu \frac{dI^{m=0}(\tau;\mu)}{d\tau} = I^{m=0}(\tau;\mu) - \frac{\varpi_o}{2} \sum_{\ell=0}^{N} \chi_{\ell} P_{\ell}(\mu) \int_{-1}^{1} P_{\ell}(\mu') I^{m=0}(\tau;\mu') d\mu' -\frac{\varpi_o}{4} F_{\odot} \sum_{\ell=0}^{N} \chi_{\ell} P_{\ell}(\mu) P_{\ell}(-\mu_{\odot}) e^{-\tau/\mu_{\odot}} - (1 - \varpi_o) \mathcal{B}(\tau)
$$
(4.14)

4.5 Quadrature and the matrix equation

With the introduction of quadrature we can replace the integrals in (4.13) and (4.14) by finite summations thus producing a fully discrete from the the transfer equation which can be written in a very compact form as a matrix equation. Let the upward and downward intensities defined at the fixed quadrature points be grouped into upward (+) and downward (−) intensity vectors as follows

$$
{}^{m}\mathbf{I}^{+} = \begin{pmatrix} I^{m}(\tau;\mu_{1}) \\ \vdots \\ I^{m}(\tau;\mu_{n}) \end{pmatrix} \text{ and } {}^{m}\mathbf{I}^{-} = \begin{pmatrix} I^{m}(\tau;-\mu_{1}) \\ \vdots \\ I^{m}(\tau;-\mu_{n}) \end{pmatrix}
$$

where I^m 's are the intensity amplitudes and $1, \ldots, n$ refer to quadrature points $\mu_i, 1, \ldots, n$. When $m = 0$, ${}^{0}I^{+}$ and ${}^{0}I^{-}$ are the azimuthally averaged intensity vectors. We can also construct scattering matrices from the scattering phase functions. The $n \times n$ forward (+) and backward (-) bidirectional phase function matrices can be written as

$$
{}^{m}\mathbf{P}^{\pm} = \begin{pmatrix} P^{m}(\pm \mu_{1}, \mu_{1}) & \cdots & P^{m}(\pm \mu_{1}, \mu_{n}) \\ \vdots & \ddots & \vdots \\ P^{m}(\pm \mu_{n}, \mu_{1}) & \cdots & P^{m}(\pm \mu_{n}, \mu_{n}) \end{pmatrix}
$$
(4.15)

respectively, where the forward scatter refers to he angle pair μ_i, μ_j of the same sign and backscatter refers to angle pairs of opposite sign. Similarly, the forward and backward phase function matrices for single scatter of the direct beam are $\overline{}$ \mathbf{r}

$$
{}^{m}\mathbf{P}_{\odot}^{\pm} = \begin{pmatrix} P^{m}(\mp \mu_{1}, -\mu_{\odot}) \\ \cdot \\ P^{m}(\mp \mu_{n}, -\mu_{\odot}) \end{pmatrix}
$$
(4.16)

Given these definitions, the set of transfer equations for the upward and downward intensity fields can be written in matrix form as

$$
\pm \frac{d^m \mathbf{I}^\pm}{d\tau} = \mathbf{M}^{-1m} \mathbf{I}^\pm - (1 + \delta_m) \frac{\tilde{\omega}}{4} \left[\mathbf{M}^{-1m} \mathbf{P}^\pm \mathbf{C}^m \mathbf{I}^+ + \mathbf{M}^{-1m} \mathbf{P}^\mp \mathbf{C}^m \mathbf{I}^- \right]
$$

$$
-\frac{\tilde{\omega}}{4}F_{\odot}\mathbf{M}^{-1m}\mathbf{P}_{\odot}^{\mp}e^{-\tau/\mu_{\odot}} - (1-\varpi_{o})\mathbf{M}^{-1m}\mathbf{U}\mathcal{B}, \qquad m = 0, 1, 2, ..., M \qquad (4.17)
$$

where the column vector m **U** has each element specified by δ_m and,

$$
\mathbf{C} = \begin{pmatrix} w_1 & 0 \\ & \ddots & \\ 0 & w_n \end{pmatrix}, \qquad \mathbf{M} = \begin{pmatrix} \mu_1 & 0 \\ & \ddots & \\ 0 & \mu_n \end{pmatrix} \tag{4.18}
$$

and w's are the quadrature weights. At this point it is convenient to introduce the bidirectional reflectance and transmittance matrices and this topic will be discussed in much more detail in chapter 5. These functions describe the local reflection and transmission properties of the medium. They are defined as follows

$$
\mathbf{r}^{m} = (1 + \delta_{m}) \frac{\tilde{\omega}}{4} \mathbf{M}^{-1m} \mathbf{P}^{-} \mathbf{C}
$$
 (4.19*a*)

and

$$
\mathbf{t}^{m} = \mathbf{M}^{-1} - (1 + \delta_{m}) \frac{\tilde{\omega}}{4} \mathbf{M}^{-1m} \mathbf{P}^{+} \mathbf{C}.
$$
 (4.19b)

Using these definitions, the set of matrix equations (4.17) may be rewritten in a more compact form as

$$
\frac{d}{d\tau}\begin{pmatrix}{}^{m}\mathbf{I}^{+}\\{}^{m}\mathbf{I}^{-}\end{pmatrix} = \begin{pmatrix} \mathbf{t}^{m} & -\mathbf{r}^{m}\\{}^{m} & -\mathbf{t}^{m}\end{pmatrix} \begin{pmatrix}{}^{m}\mathbf{I}^{+}\\{}^{m}\mathbf{I}^{-}\end{pmatrix} + \begin{pmatrix}{}^{m}\Sigma^{+}\\{}^{m}\Sigma^{-}\end{pmatrix}, \qquad m = 0, 1, 2, ..., 2n - 1 \qquad (4.20)
$$

where the source vectors are

$$
{}^{m}\Sigma^{\pm} = \frac{\varpi_o}{4\pi} F_{\odot} \mathbf{M}^{-1} {}^{m} \mathbf{P}_{\odot}^{\mp} e^{-\tau/\mu_{\odot}} + (1 - \varpi_o) \mathcal{B} \mathbf{M}^{-1} {}^{m} \mathbf{U}
$$
(4.21)

This general equation can be further written as

$$
\frac{d}{d\tau}\mathbf{I} = \mathbf{AI} + \Sigma \tag{4.22}
$$

where the vectors I and Σ are of length 2n and the attenuation matrix A is $2n \times 2n$. We will see that all forms of solution discussed below, simple or complex, reduce the equation of transfer to the form (4.22).

4.6 The general solution

If we consider the solution to (4.22) as an initial value problem, then the general solution to the equation

$$
\frac{d}{d\tau}\mathbf{I} = \mathbf{AI}
$$

may be written in the form

$$
\mathbf{I}(\tau) = \exp[\mathbf{A}\tau]\mathbf{I}(0)
$$

This is, however, only a solution in principle as the evaluation of the exponential of a matrix quantity is not straight forward¹. In fact much of the discussion of the first half of this book is about this topic. Two notable approaches to the evaluation of the quantity $\exp[A\tau]$ are introduced here:

¹ 1. Moler and Van Laon, 1978; Nineteen dubious ways to compute the exponential of a matrix, SAIM rev., 20, 801-xxx

The expansion: $\,$

$$
\exp[\mathbf{A}\tau] = \mathbf{E} + \tau \mathbf{A} + \tau^2 \frac{\mathbf{A}}{2!} + \dots
$$

The diagonal Matrix; For this case,

$$
\exp[\mathbf{A}\tau] = \begin{pmatrix} \exp(a_{11}\tau) & 0 \\ 0 & \exp(a_{nn}\tau) \end{pmatrix}
$$

