TRANSPORT METHODS

In the previous chapter we discussed the multigroup diffusion methods and their numerical solution. Frequently, however, greater accuracy than that provided by the diffusion equation is demanded by the physical problem. To this end, one turns to a more accurate relation known as the Boltzmann transport equation. Unfortunately this equation is much more complex and time consuming to solve either analytically or numerically than the diffusion equation.

In this chapter we consider several special numerical methods for solving the transport equation. Most of the methods considered can be applied to either neutrons or photons. However, some of them will be discussed only for neutrons and others only for gamma rays. The development to follow is limited to one dimensional problems. This limitation does not alter the basic approach in any of the methods; however, geometries with several dimensions lead to algebraic complexity.

We first consider the one group model of the transport equation. We shall derive the spherical harmonics expansion of the transport equation which leads directly to the $P_N$ approximation. We then consider appropriate difference equations and alternative procedures for deriving the difference relations. The double $P_N$ method is then discussed. The multigroup transport equations are then derived and an elementary discussion of group cross sections presented. Methods for treating transient problems are then reviewed. Finally we conclude the chapter with a discussion of the moments method.

The Monte Carlo method is also a way to determine the flow of neutrons and gamma rays. However, this method may be related directly to the transport problem and need not be based directly on the Boltzmann equation. For this reason and because the approach in the Monte Carlo method is so very different from that in any of the methods discussed in this chapter, we defer its discussion to the next chapter.
5.1 The $P_N$ Approximation

The basic equation of neutron conservation is the linear Boltzmann equation.¹ For monoenergetic neutrons this equation is

$$\mathbf{\Omega} \cdot \nabla \phi(r, \mathbf{\Omega}) + \sigma_t(r) \phi(r, \mathbf{\Omega}) = \int_{\mathbf{\Omega}} d\Omega' \sigma_s(r, \mathbf{\Omega} \to \mathbf{\Omega}') \phi(r, \mathbf{\Omega}') + S(r, \mathbf{\Omega}),$$  

(5.1.1)

where $\phi(r, \mathbf{\Omega})$ is the number of neutrons crossing a unit surface at $r$ per unit time going in a unit solid angle centered in the direction $\mathbf{\Omega}$, $\sigma_t(r)$ is the total neutron cross section at $r$, $\sigma_s(r, \mathbf{\Omega} \to \mathbf{\Omega}')$ is the probability per unit length that a neutron at $r$ and going in a direction $\mathbf{\Omega}'$ will undergo a collision and emerge going in a unit solid angle centered at $\mathbf{\Omega}$, and $S(r, \mathbf{\Omega})$ is the number of neutrons created per unit volume at $r$ going in a unit solid angle centered at $\mathbf{\Omega}$.

Except for a very few special, idealized cases, the Boltzmann equation cannot be solved analytically. The term involving the integral is the prime source of difficulty. Accordingly, it behooves us to seek various approximate solutions. Because the integral term involves the angular variable, approximations concerning the angular dependence are suggested. We shall elaborate several of those which have been devised. In particular we shall consider analytic approximations to which numerical procedures may be readily applied.

A particularly useful approximation of the Boltzmann equation is the so-called $P_N$ or spherical harmonics approximation. The basis of the approximation is the expansion of all functions of the angular variable in terms of the spherical harmonics.² For one dimensional problems, a subset of the spherical harmonics, the Legendre polynomials, suffices. The Legendre polynomials are an orthogonal set of functions. The flux in the Boltzmann equation may be expanded in terms of these Legendre polynomials. The resulting set of equations separates into an infinite set of coupled differential equations. The spherical harmonic approximation is introduced by truncating the infinite set of differential equations at some order and treating them by either analytic or numerical methods. We shall illustrate the derivation for one dimensional plane geometry.

We first expand the scattering cross section, directional flux, and the source in Eq. (5.1.1). For an isotropic medium the scattering cross section is a function of only the angle between the vectors $\mathbf{\Omega}'$ and $\mathbf{\Omega}$, say $\theta_0$. It is convenient to consider the variable $\cos \theta_0 = \mu_0$, rather than

¹ For derivations and an elementary discussion, see Appendix A.
² For properties of the spherical harmonics, see Reference 4, pp. 1325–1328.
The scattering function can then be expanded in terms of the Legendre polynomials $P_n(\mu_0)$. Thus

$$\sigma_0(r, \Omega' \rightarrow \Omega) = \frac{1}{2\pi} \sum_{m} \frac{2m + 1}{2} \sigma_{s,m}(r) P_m(\mu_0), \quad (5.1.2)$$

the factor $(2m + 1)/4\pi$ being inserted for later convenience. From the orthogonality of the Legendre polynomials, we have

$$\sigma_{s,n}(r) = 2\pi \int_{-1}^{1} d\mu_0 \sigma_0(r, \Omega' \rightarrow \Omega) P_n(\mu_0). \quad (5.1.3)$$

In slab geometry the flux $\phi(r, \Omega)$ will be a function of position $x$ and, since the medium is assumed isotropic, the angle between the $x$ axis and $\Omega$, say $\theta$. It is again convenient to consider the variable $\cos \theta = \mu$. The directional flux is expanded in the form

$$\phi(x, \mu) = \sum_{n} \frac{2n + 1}{2} \phi_n(x) P_n(\mu), \quad (5.1.4)$$

with

$$\phi_n(x) = \int_{-1}^{1} d\mu \phi(x, \mu) P_n(\mu). \quad (5.1.5)$$

Likewise, for the source we have

$$S(x, \mu) = \sum_{n} \frac{2n + 1}{2} S_n(x) P_n(\mu), \quad (5.1.6)$$

with

$$S_n(x) = \int_{-1}^{1} d\mu S(x, \mu) P_n(\mu). \quad (5.1.7)$$

The expansions for the directional flux and directional source are functions of $\mu$, whereas the scattering function is a function of $\mu_0$. It is evident geometrically that $\mu$ and $\mu_0$ are related as shown by Fig. 5.1.1. The angles $\theta, \varphi$ refer to the coordinates of $\Omega$, whereas $\theta', \varphi'$ refer to the vector $\Omega'$. The unit vectors $\Omega$ and $\Omega'$ may be written in terms of the unit coordinate vectors as

$$\Omega = \cos \theta \hat{i} + \sin \theta \cos \varphi \hat{j} + \sin \theta \sin \varphi \hat{k}, \quad (5.1.8a)$$

See Appendix D (Eq. D.7) or Reference 3 or 4.
and
\[ \Omega' = \cos \theta' \mathbf{i} + \sin \theta' \cos \phi' \mathbf{j} + \sin \theta' \sin \phi' \mathbf{k}. \quad (5.1.8b) \]
The cosine of the angle $\theta_0$ is then
\[ \cos \theta_0 = \mu_0 = \cos \theta \cos \theta' + \sin \theta \sin \theta' (\cos \phi \cos \phi' + \sin \phi \sin \phi'), \quad (5.1.9a) \]
or
\[ \mu_0 = f(\mu, \varphi; \mu', \varphi'). \quad (5.1.9b) \]
To proceed further, the Legendre polynomials $P_n(\mu_0)$ with argument $\mu_0$ must be expressed as functions of $\mu$ and $\mu'$. To this end, the so-called addition theorem for Legendre polynomials is useful (Eq. D.3, Appendix D).

The scattering integral in the Boltzmann equation may be reduced to a function of $x, \mu$ only. The expansions (5.1.2) and (5.1.4), and the addition theorem may be used in the integrand of the integral in Eq. (5.1.1). Only the term $\beta = 0$ in the sum over $\beta$, which arises from the
use of the addition theorem, contributes to the integral over \( \phi' \). Further, in the integration over \( \mu' \), only the combination \( m = n \) provides a nonvanishing contribution. By use of the expansions (5.1.4) and (5.1.6) in the remaining three terms of the Boltzmann equation, we find that

\[
\sum_n \frac{2n + 1}{2} \left[ \mu P_n(\mu) \frac{d}{dx} \phi_n(x) + \sigma t P_n(\mu) \phi_n(x) \right] = \sum_n \frac{2n + 1}{2} [\sigma s_n(x) P_n(\mu) \phi_n(x) + S_n(x) P_n(\mu)] .
\]

To derive the equation for each harmonic, we multiply (5.1.10) by \( P_N(\mu) \) and integrate over \( \mu \). The term in \( \mu P_n(\mu) \) is eliminated by use of a recurrence relation for the Legendre polynomials (Eq. D.8, Appendix D). After some elementary algebra, we have

\[
\frac{n + 1}{2n + 1} \frac{d}{dx} \phi_{n+1}(x) + \frac{n}{2n + 1} \frac{d}{dx} \phi_{n-1}(x) + \sigma \phi_n(x) = \sigma s_n \phi_n(x) + S_n(x), \quad n = 0, 1, \ldots .
\]

Equations (5.1.11) represent an infinite set of coupled differential equations for the harmonics of the flux. Various order approximations are obtained by truncating the series at some fixed \( N \). The truncation to order \( N \) consists of assuming all quantities with index \( N + 1 \) are zero. The first \( N + 1 \) equations are then used. The resulting set of equations are known as the \( P_N \) equations. The \( P_1 \) equations are

\[
\frac{d}{dx} \phi_1(x) + \sigma t \phi_0(x) = \sigma s_0 \phi_0(x) + S_0(x) ,
\]

and

\[
\frac{1}{3} \frac{d}{dx} \phi_0(x) + \sigma t \phi_1(x) = \sigma s_1 \phi_1(x) + S_1(x) .
\]

The \( P_3 \) equations are

\[
\frac{d}{dx} \phi_1(x) + \sigma t \phi_0(x) = \sigma s_0 \phi_0(x) + S_0(x) ,
\]

\[
\frac{2}{3} \frac{d}{dx} \phi_2(x) + \frac{1}{3} \frac{d}{dx} \phi_0(x) + \sigma t \phi_1(x) = \sigma s_1 \phi_1(x) + S_1(x) ,
\]

\[
\frac{3}{5} \frac{d}{dx} \phi_3(x) + \frac{2}{5} \frac{d}{dx} \phi_1(x) + \sigma t \phi_2(x) = \sigma s_2 \phi_2(x) + S_2(x) .
\]
and
\[
\frac{3}{7} \frac{d}{dx} \phi_3(x) + \sigma_t \phi_3(x) = \sigma_{s,3} \phi_3(x) + S_3(x) .
\] (5.1.13d)

For illustrative purposes we shall use the \( P_3 \) equations. Higher order approximations are readily derived, and the results to be obtained subsequently are easily generalized.

Because more terms are used in the \( P_3 \) approximation than in the \( P_1 \) approximation, the angular distribution can be more accurately represented, and the answers will be more precise. The existence of more terms in the \( P_3 \) approximation than in the \( P_1 \) also implies that the boundary conditions can be more accurately approximated. Consistent with the increased accuracy with which the interior of a medium is treated, more accurate boundary conditions are required. Neutron conservation requires that the directional flux be continuous at an interface between two materials. If the directional fluxes in the adjoining media are denoted \( \phi'(x, \mu) \) and \( \phi''(x, \mu) \), then the continuity condition is
\[
\phi'(x, \mu) = \phi''(x, \mu), \quad -1 \leq \mu \leq 1 .
\] (5.1.14)

In the \( P_N \) approximation, it is easily shown that condition (5.1.14) implies equality of each harmonic of the expansion (see problem 6). Thus, the boundary condition is
\[
\phi'_{N}(x) = \phi''_{N}(x), \quad \text{all } N .
\] (5.1.15)

At a vacuum-matter interface (or black absorber), the proper boundary condition is
\[
\phi(a, \mu) = 0, \quad -1 \leq \mu \leq 0 ,
\] (5.1.16)
where \( a \) is the boundary coordinate. Condition (5.1.16) cannot be satisfied in the \( P_N \) approximation for finite \( N \). The \( x \) directional flux cannot be represented by a finite polynomial expansion. A frequently used boundary condition, which approximates condition (5.1.16), is the Marshak condition
\[
\int_{-1}^{0} d\mu \, \phi(a, \mu) P_N(\mu) = 0, \quad N \text{ odd} .
\] (5.1.17)

At the opposite boundary for finite slabs, the Marshak condition is
\[
\int_{0}^{1} d\mu \, \phi(-a, \mu) P_N(\mu) = 0, \quad N \text{ odd} .
\] (5.1.18)
We shall use the Marshak conditions in our discussion of the $P_N$ method. It should be noted that other approximations have been suggested and applied. In the next section we consider the double spherical harmonics method which was designed to permit better approximations to discontinuities in the angular distribution.

The application of Marshak's boundary conditions are facilitated by the following relations:

$$
\int_0^1 d\mu P_m(\mu) P_n(\mu)
= \begin{cases} 
\frac{1}{2m+1}, & \text{if } m = n \\
0, & \text{if } m - n \text{ is even, } (m - n \neq 0) \\
\frac{(-)^{i+k} m! n!}{2^{m+n-1}(n-m)(n+m+1)(i!)^2(k!)^2}, & \text{if } m = 2k, n = 2i + 1
\end{cases}
$$

The Marshak conditions in the $P_3$ approximation are derived in a straightforward manner. From the condition (5.1.17), we find that

$$
\phi_0(a) - 2\phi_1(a) + \frac{5}{4} \phi_2(a) = 0 , \quad (5.1.19a)
$$

and

$$
\phi_0(a) - 5\phi_2(a) + 8\phi_3(a) = 0 . \quad (5.1.19b)
$$

In like manner, at $x = -a$, we obtain

$$
\phi_0(-a) + 2\phi_1(-a) + \frac{5}{4} \phi_2(-a) = 0 , \quad (5.1.20a)
$$

and

$$
\phi_0(-a) - 5\phi_2(-a) - 8\phi_3(-a) = 0 . \quad (5.1.20b)
$$

The four conditions at the exterior boundaries, plus the continuity conditions at interfaces, complete the specification for the $P_3$ approximation. Four boundary conditions suffice, since Eqs. (5.1.13) represent a single fourth order equation. This point may be seen by solving each equation for one unknown (or derivatives of it) in terms of all the others. The result may be used to eliminate this unknown from all other equations, whereupon the process may be repeated again to eliminate another unknown.
unknown. The boundary conditions (5.1.19) and (5.1.20) play an important role in designing numerical methods for treating the $P_N$ equations. Before turning to the numerical methods, we first illustrate the reduction of the $P_3$ equations to a generalized eigenvalue problem for criticality studies. Once we have obtained the statement of the problem, it is evident that one can define an adjoint function and use the method of successive approximations as detailed in Chapter IV to solve for the flux.

For simplicity we define the coefficients

$$\sigma_i = \sigma_t - \sigma_{s,i}, \quad i = 0, 1, 2, 3.$$  \hfill (5.1.21)

We also define the vectors $\psi(x)$ and $S(x)$ as

$$\psi(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \phi_2(x) \\ \phi_3(x) \end{bmatrix},$$  \hfill (5.1.22)

and

$$S(x) = \begin{bmatrix} S_0(x) \\ S_1(x) \\ S_2(x) \\ S_3(x) \end{bmatrix}. $$  \hfill (5.1.23)

The $P_3$ equations are then written in matrix form

$$A\psi(x) = S(x),$$ \hfill (5.1.24)

with

$$A = \begin{bmatrix} \sigma_0 & \frac{d}{dx} & 0 & 0 \\ \frac{1}{3} \frac{d}{dx} & \sigma_1 & \frac{2}{3} \frac{d}{dx} & 0 \\ 0 & \frac{2}{5} \frac{d}{dx} & \sigma_2 & \frac{3}{5} \frac{d}{dx} \\ 0 & 0 & \frac{3}{7} \frac{d}{dx} & \sigma_3 \end{bmatrix}. $$ \hfill (5.1.25)

The boundary conditions (5.1.19) and (5.1.20) are readily written in matrix form.

For criticality studies there is no external source, only fission. To an excellent approximation the fission neutron angular distribution is isotropic in laboratory coordinates and further, the fission cross section
is independent of the initial neutron direction. The source is therefore

\[ S(x, \mu) = \nu \int_{-1}^{1} d\mu' \sigma_f(x) \phi(x, \mu') = \nu \sigma_f(x) \phi_0(x). \quad (5.1.26) \]

The expansion coefficients for the source are then

\[ S_0(x) = \nu \sigma_f(x) \phi_0(x), \quad (5.1.27a) \]

and

\[ S_1(x) = S_2(x) - S_3(x) = 0. \quad (5.1.27b) \]

The \( P_3 \) equations are then

\[ A \psi(x) = \nu B \psi(x), \quad (5.1.28) \]

with

\[ B = \begin{bmatrix}
\sigma_f(x) & 0 & \cdots & 0 \\
0 & 0 & \cdots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{bmatrix}. \quad (5.1.29) \]

Equation (5.1.28) is the general eigenvalue equation we set out to find. For higher order \( P_N \) approximations, the formulation is exactly parallel to the above.

We now consider numerical procedures for solving the equations (5.1.28). The continuous space \( x, \mu \) has been replaced by the \( x, N \) space where \( N \) is a discrete variable. In order to derive appropriate difference equations for the harmonics, we again divide the interval \(-a \leq x \leq a\) into discrete points \( x_j \) such that \( x_0 = -a, x_J = a \). We again assume the mesh chosen so that all interfaces lie on an interpolation point. The discrete mesh appears as shown in Fig. 5.1.2.

To derive appropriate difference equations, we must consider the boundary conditions applicable to the problem. We note from Eqs. (5.1.19) that if any two functions \( \phi_n(a) \) are fixed, then the remaining two

---

**Fig. 5.1.2.** Discrete mesh for the numerical approximation to the \( P_3 \) equations.
\[ \phi_\alpha(a) \text{ are determined. Likewise for Eqs. (5.1.20). As an example, let us fix } \phi_2(a) \text{ and } \phi_3(a); \text{ then } \phi_0(a) \text{ and } \phi_1(a) \text{ are determined. We now integrate in the direction } a \to -a \text{ to compute } \phi_0(-a) \text{ and } \phi_1(-a). \text{ But then } \phi_2(-a) \text{ and } \phi_3(-a) \text{ are determined, and hence we should integrate in the direction } -a \to a \text{ to find new values of } \phi_2(a) \text{ and } \phi_3(a). \text{ Thus a circular path through the mesh is implied, and our difference equations will be derived on this basis. Note that the implied direction of integration says nothing whatsoever about the neutron direction.}

We now derive a set of difference equations based upon the above discussion. For the harmonics \( \phi_0(x) \) and \( \phi_1(x) \), we integrate over the interval \( x_j \) to \( x_{j-1} \). For the equation in \( \phi_0(x) \) we have

\[
\int_{x_j}^{x_{j-1}} dx \frac{d}{dx} \phi_1(x) + \int_{x_j}^{x_{j-1}} dx \sigma_0(x) \phi_0(x) = \int_{x_j}^{x_{j-1}} dx S_0(x). \tag{5.1.30}
\]

We shall use the double subscript notation

\[ f_n(x_j) = f_{n,j}. \tag{5.1.31} \]

The coefficient \( \sigma_0(x) \) is constant over the interval \( x_j \) to \( x_{j-1} \) and is denoted \( \sigma_{0,j} \). The spacing interval \( x_j \) to \( x_{j-1} \) is denoted \( \Delta_j \). To terms accurate to \( O(\Delta_j^2) \) we have

\[
\phi_{1, j-1} - \phi_{1,j} + \sigma_{0,j} \frac{\Delta_j}{2} (\phi_{0,j-1} + \phi_{0,j}) = \frac{\Delta_j}{2} (S_{0,j-1} + S_{0,j}). \tag{5.1.32}
\]

The equation for \( \phi_1(x) \) is treated in the same manner; we have

\[
\frac{1}{3} (\phi_{0,j-1} - \phi_{0,j}) + \frac{2}{3} (\phi_{2,j-1} - \phi_{2,j}) + \sigma_{1,j} \frac{\Delta_j}{2} (\phi_{1,j-1} + \phi_{1,j}) = 0. \tag{5.1.33}
\]

The above difference relations are used for \( 1 \leq j \leq J \).

For the harmonics \( \phi_2(x) \) and \( \phi_3(x) \), we integrate from \( x_j \) to \( x_{j+1} \). The difference equations are

\[
\frac{2}{5} (\phi_{1,j+1} - \phi_{1,j}) + \frac{3}{5} (\phi_{3,j+1} - \phi_{3,j}) + \sigma_{2,j+1} \frac{\Delta_{j+1}}{2} (\phi_{2,j+1} + \phi_{2,j}) = 0, \tag{5.1.34}
\]

and

\[
\frac{3}{7} (\phi_{2,j+1} - \phi_{2,j}) + \sigma_{3,j+1} \frac{\Delta_{j+1}}{2} (\phi_{3,j+1} + \phi_{3,j}) = 0. \tag{5.1.35}
\]

Equations (5.1.34) and (5.1.35) are used for \( 0 \leq j \leq J - 1 \).
The direction of integration is shown in Fig. 5.1.3.

![Fig. 5.1.3. Directions of integration through a mesh for the integration of the $P_3$ equations.](image)

There are numerous iteration procedures that can be used with the set of difference equations just derived. We outline one possible procedure below which is analogous to the method of successive displacements. First we assume an initial distribution for the $\phi_{n,j}$ consistent with the boundary conditions. The source is computed at each space point. Starting at $j = J$, we solve Eq. (5.1.32) in the form

$$\phi_{0,j-1}^1 = \frac{S_{0,j-1}^0 + S_{0,j}^0 + (2/\Delta_j) (\phi_{1,j}^0 - \phi_{1,j-1}^0)}{\sigma_{0,j}} - \phi_{0,j}^1,$$  \hspace{1cm} (5.1.36)

where the superscript is the iteration index. Equation (5.1.33) is written as

$$\phi_{1,j-1}^1 = -\frac{2}{3\Delta_j \sigma_{1,j}} (\phi_{1,j}^1 - \phi_{0,j-1}^0) + \frac{4}{3\Delta_j \sigma_{1,j}} (\phi_{2,j}^0 - \phi_{2,j-1}^0) - \phi_{1,j}^1,$$  \hspace{1cm} (5.1.37)

Equations (5.1.36) and (5.1.37) are used for $1 \leq j \leq J$. The analogous equations for the second and third harmonic are

$$\phi_{2,j+1}^1 = \frac{4}{5\Delta_j \sigma_{2,j+1}} (\phi_{1,j}^1 - \phi_{1,j+1}^1) + \frac{6}{5\Delta_j \sigma_{2,j+1}} (\phi_{3,j}^1 - \phi_{3,j+1}^1) - \phi_{2,j}^1,$$  \hspace{1cm} (5.1.38)

and

$$\phi_{3,j+1}^1 = \frac{6}{7\Delta_j \sigma_{3,j-1}} (\phi_{2,j}^1 - \phi_{2,j+1}^1) - \phi_{3,j}^1.$$  \hspace{1cm} (5.1.39)

The iteration may be repeated for the previously calculated source $S^0$, i.e., multiple inner iterations, or the source may be recomputed from
V. TRANSPORT METHODS

the newly found fluxes before continuing. The source is rescaled so that

<math>
\alpha^2(S_{0,j}^1, S_{0,j}^1) = (S_{0,j}^0, S_{0,j}^0).
</math> (5.1.40)

The scale factor \( \alpha^2 \) will approach an asymptote after a sufficient number of outer iterations to permit modifications of the assembly properties to achieve criticality. The process described above is merely indicative of the types of procedures that are possible.

An alternative approach to the numerical solution of the \( P_N \) equations of great merit has been considered by Marchuk (Reference 5, Chapter 13) and Gelbard et al. (Reference 6). We shall adopt Marchuk’s formulation. It turns out that the \( P_N \) equations can be reduced to a form identical to that of the multigroup equations. We shall illustrate this reduction for one case. The reduction then enables us to extend the use of any one of the many already existing multigroup diffusion codes to higher order spherical harmonic approximations.

Consider the \( P_N \) approximation to any order with \( N \) odd. The sources are assumed isotropic. The equations are of the form

<math>
\frac{d}{dx} \phi_1(x) + \sigma_0 \phi_0(x) = S_0(x),
</math>

<math>
\alpha_1 \frac{d}{dx} \phi_2(x) + \beta_1 \frac{d}{dx} \phi_0(x) + \sigma_1 \phi_1(x) = 0,
</math>

<math>
\vdots
</math>

<math>
\alpha_{N-1} \frac{d}{dx} \phi_N(x) + \beta_{N-1} \frac{d}{dx} \phi_{N-2}(x) + \sigma_{N-1} \phi_{N-1}(x) = 0,
</math>

and

<math>
\beta_N \frac{d}{dx} \phi_{N-1} + \sigma_N \phi_N(x) = 0. \quad (5.1.41)
</math>

We define the vectors \( \Psi_e(x) \) and \( \Psi_o(x) \) as

<math>
\Psi_e(x) = \begin{bmatrix} \phi_0(x) \\ \phi_2(x) \\ \vdots \\ \phi_{N-1}(x) \end{bmatrix}, \quad (5.1.42)
</math>

and

<math>
\Psi_o(x) = \begin{bmatrix} \phi_1(x) \\ \phi_3(x) \\ \vdots \\ \phi_N(x) \end{bmatrix}. \quad (5.1.43)
</math>
The vector \( \Phi_n(x) \) contains only even harmonics of the flux, whereas \( \Phi_0(x) \) contains only odd harmonics. The set of equations (5.1.41) may be written

\[
A_1 \frac{d}{dx} \Phi_n(x) + B_1 \Phi_n(x) = S(x), \tag{5.1.44a}
\]

and

\[
A_2 \frac{d}{dx} \Phi_n(x) + B_2 \Phi_n(x) = 0, \tag{5.1.44b}
\]

where the definitions of the matrices are evident upon comparison of Eqs. (5.1.41) and (5.1.44). It is easily seen that the matrices \( B_1 \) and \( B_2 \) are diagonal and nonsingular, whereas \( A_1 \) and \( A_2 \) are tridiagonal with all diagonal elements zero. Note also that \( A_1 \) and \( A_2 \) are not functions of \( x \), whereas \( B_1 \) and \( B_2 \) are functions of \( x \) in general. The matrix \( B_2 \) possesses an inverse and hence, from Eq. (5.1.44b),

\[
\Phi_n(x) = -B_2^{-1}A_2 \frac{d}{dx} \Phi_n(x). \tag{5.1.45}
\]

Using the above expression for \( \Phi_n(x) \) in (5.1.44a), we have

\[
- \frac{d}{dx} \left(A_1B_2^{-1}A_2\right) \frac{d}{dx} \Phi_n(x) + B_1 \Phi_n(x) = S(x). \tag{5.1.46}
\]

The set of equations (5.1.46) are in the same form as the multigroup diffusion equations. In the above case, the harmonic index plays the role of a group index. For the \( P_3 \) equations, analogous to a two-group diffusion problem, we have

\[
- \frac{d}{dx} \left[\frac{1}{3\sigma_1} \frac{d}{dx} \phi_0(x) + \frac{2}{3\sigma_1} \frac{d}{dx} \phi_1(x)\right] + \sigma_0 \phi_0(x) = S_0(x), \tag{5.1.47}
\]

In detail the equations are

\[
- \frac{d}{dx} \left[\frac{1}{3\sigma_1} \frac{d}{dx} (\phi_0 + 2\phi_2)\right] + \sigma_0 \phi_0(x) = S_0(x), \tag{5.1.48}
\]

and

\[
- \frac{d}{dx} \left[\frac{2}{15\sigma_1} \frac{d}{dx} \phi_0(x) + \left(\frac{4}{15\sigma_1} + \frac{9}{35\sigma_3}\right) \frac{d}{dx} \phi_2(x)\right] + \sigma_2 \phi_2(x) = 0. \tag{5.1.49}
\]

The numerical integration of Eqs. (5.1.48) and (5.1.49) may be done as outlined in Chapter IV.
A practical advantage of the formulation of the $P_N$ equations as multigroup type equations is that a standard multigroup diffusion program is readily used for $P_N$ calculations.

5.2 Double $P_N$ Approximation

The $P_N$ equations yield quite accurate approximations to the total flux in the interior of a reactor. They should, because the angular distribution deep inside a homogeneous medium is nearly isotropic and because the spherical harmonics method corresponds to an expansion in increasingly higher orders of anisotropy [see Eq. (5.1.4)]. The angular distribution deep within a reactor is nearly isotropic essentially because leakage processes, which are anisotropic by nature, do not enter importantly into the neutron balance and because nuclear processes, such as fission, tend to be isotropic. Elastic scattering by heavy elements, a predominant process, is isotropic; for the light elements scattering is somewhat anisotropic. However, after a few anisotropic scatterings the angular distribution is nearly isotropic. Consequently, in many cases the angular distribution predicted is therefore good in the interior. However, near strong discontinuities in material properties, such as the region near a strong absorber or vacuum boundaries, the angular distribution is usually much more anisotropic. The discontinuities impose step function changes upon the angular flux. The approximation of a step function by polynomials requires many harmonics, in particular the $P_3$ approximations would hardly be adequate to represent a discontinuity.

The essential idea of the method developed by Yvon (Reference 7) is to use a separate expansion over each region within which the angular distribution is smoothly and slowly varying, instead of one expansion for all angles. Thus, a discontinuity in the angular distribution can be accurately approximated by using a separate expansion on each side of the discontinuity, the discontinuity being represented by a corresponding discontinuity in the expansion coefficients. In particular, the directional flux is expanded into two series of Legendre polynomials for problems involving an interface between two media. As might be expected, the method of Yvon is very good for such problems. We shall discuss the method briefly and reduce the equations to a group diffusion form from which the numerical procedures remaining are evident. Our notation is that of Ziering and Schiff (see Reference 8). We assume slab geometry and isotropic sources and scattering.

We begin with the one group transport equation for slabs

$$\mu \frac{d\phi(x, \mu)}{dx} + \sigma \phi(x, \mu) = \frac{1}{2} \int_{-1}^{1} d\mu' \sigma_0(x) \phi(x, \mu') + \frac{S(x)}{2}. \quad (5.2.1)$$
We expand the directional flux in terms of the half-range polynomials

\[ P^+(\mu) = P_n(2\mu - 1), \quad 0 \leq \mu \leq 1, \]
\[ = 0, \quad \mu < 0, \quad (5.2.2a) \]
\[ P^-_n(\mu) = P_n(2\mu + 1), \quad -1 \leq \mu \leq 0, \]
\[ = 0, \quad \mu > 0, \quad (5.2.2b) \]

where \( P_n(2\mu \pm 1) \) is the Legendre polynomial of order \( n \). The orthogonality relations are

\[ \int_0^1 d\mu P^+_n(\mu) P^+_m(\mu) = \int_{-1}^0 d\mu P^-_n(\mu) P^-_m(\mu) = \frac{1}{2n + 1} \delta_{nm}. \quad (5.2.3) \]

The half-range polynomials obey the recurrence relation

\[ 2(2n + 1) \mu P^\pm_n(\mu) = (n + 1) P^\pm_{n+1}(\mu) \pm (2n + 1) P^\pm_n(\mu) + nP^\pm_{n-1}(\mu), \quad (5.2.4) \]

a relation that follows from the full range Legendre polynomial recurrence relations. The flux expansion is of the form

\[ \phi(x, \mu) = \sum_n (2n + 1) \left[ P^+_n(\mu) \phi^+_n(x) + P^-_n(\mu) \phi^-_n(x) \right], \quad (5.2.5) \]

where

\[ \phi^+_n(x) = \int_{-1}^0 d\mu \phi(x, \mu) P^-_n(\mu), \quad (5.2.6a) \]
\[ \phi^-_n(x) = \int_0^1 d\mu \phi(x, \mu) P^+_n(\mu). \quad (5.2.6b) \]

In view of Eqs. (5.2.2) and (5.2.5), \( \phi^+_n(x) \) may be regarded as describing the directional flux for \( \mu > 0 \), and \( \phi^-_n(x) \), for \( \mu < 0 \). If we insert the expansion (5.2.5) into (5.2.1) we have

\[ \sum_n (2n + 1) \mu \left[ P^+_n(\mu) \frac{d}{dx} \phi^+_n(x) + P^-_n(\mu) \frac{d}{dx} \phi^-_n(x) \right] \]
\[ + \sigma_t \sum_n (2n + 1) \left[ P^+_n(\mu) \phi^+_n(x) + P^-_n(\mu) \phi^-_n(x) \right] \]
\[ = \frac{1}{2} \sigma_s(x) \left[ \phi^+_0(x) + \phi^-_0(x) \right] + S_0(x). \quad (5.2.7) \]

We multiply by \( P^+_n(\mu) \) and integrate over the interval \( 0 \leq \mu \leq 1 \).
Again, we multiply Eq. (5.2.7) by $P_N^\pm(\mu)$ and integrate with respect to $\mu$ over the interval from $\pm 1$ to 0. After some algebra we find

$$\begin{align*} 
(N + 1) \frac{d}{dx} \phi_{N+1}^\pm(x) + N \frac{d}{dx} \phi_{N-1}^\pm(x) &\pm (2N + 1) \frac{d}{dx} \phi_N^\pm(x) \\
+ 2(2N + 1) \sigma_t \phi_N^\pm(x) &= \left[ \sigma_s(x)(\phi_0^+(x) + \phi_0^-(x)) + 2S_0(x) \right] \delta_{N0}. 
\end{align*}$$

(5.2.8)

The equations for the double $P_1$ expansion which we denote by $P_1^\pm$ are

$$\begin{align*} 
\frac{d}{dx} \phi_1^+(x) + \frac{d}{dx} \phi_0^+(x) + 2\sigma_t \phi_0^+(x) &= \sigma_s(x)(\phi_0^+(x) + \phi_0^-(x)) + 2S_0(x), \\
3 \frac{d}{dx} \phi_1^+(x) + \frac{d}{dx} \phi_0^+(x) + 6\sigma_t \phi_1^+(x) &= 0, \\
\frac{d}{dx} \phi_1^-(x) - \frac{d}{dx} \phi_0^-(x) + 2\sigma_t \phi_0^-(x) &= \sigma_s(x)(\phi_0^+(x) + \phi_0^-(x)) + 2S_0(x), \\
-3 \frac{d}{dx} \phi_1^-(x) + \frac{d}{dx} \phi_0^-(x) + 6\sigma_t \phi_1^-(x) &= 0.
\end{align*}$$

(5.2.9a-d)

Note that the expansions in $\phi_N^\pm(x)$ are coupled only through the zeroth harmonic. For anisotropic scattering the coupling occurs in the higher order terms also.

The method of Yvon makes it possible to satisfy certain types of boundary conditions exactly. As an example, consider a plane slab in the region $-a \leq x \leq a$. At $x = -a$, $\phi(-a, \mu) = 0$, $0 \leq \mu \leq 1$; at $x = +a$, $\phi(a, \mu) = 0$, $-1 \leq \mu \leq 0$. Thus, from Eq. (5.2.6) we learn that the proper boundary conditions are $\phi_n^+(-a) = 0 = \phi_n^-(a)$ all $n$. Since $\phi_n^\pm(x) = 0$ for $n \geq N + 1$, and since we can both require and satisfy $\phi_n^+(-a) = 0 = \phi_n^-(a)$, the boundary conditions can be precisely satisfied. Because the only approximation is the truncation, Yvon's method might be expected to give quite accurate results for this type of problem, as is in fact the case. However, the $P_N^\pm$ equations are usually as accurate as the $P_{2N+1}$ equations, particularly with regard to the angular distribution.

The set of equations (5.2.9) are readily reduced to a formal multigroup
5.2 DOUBLE $P_N$ APPROXIMATION

To this end, we add and subtract the Eqs. (5.2.9a, c) and (5.2.9b, d) to obtain the set of equations

\[
\frac{d}{dx}(\phi_1^+ + \phi_1^-) + \frac{d}{dx}(\phi_0^+ - \phi_0^-) + 2\sigma_0(\phi_0^+ + \phi_0^-) = 4S_0, \\
\frac{d}{dx}(\phi_1^+ - \phi_1^-) + \frac{d}{dx}(\phi_0^+ + \phi_0^-) + 2\sigma_1(\phi_0^+ - \phi_0^-) = 0, \\
3 \frac{d}{dx}(\phi_1^+ - \phi_1^-) + \frac{d}{dx}(\phi_0^+ + \phi_0^-) + 6\sigma_1(\phi_0^+ + \phi_0^-) = 0, \\
3 \frac{d}{dx}(\phi_1^+ + \phi_1^-) + \frac{d}{dx}(\phi_0^+ - \phi_0^-) + 6\sigma_1(\phi_0^+ - \phi_0^-) = 0,
\]

(5.2.10)

with $\sigma_0 = \sigma_1 - \sigma_s$. We define the vectors

\[
\Psi_s(x) = \begin{bmatrix} (\phi_0^+ + \phi_0^-) \\ (\phi_1^+ - \phi_1^-) \end{bmatrix},
\]

(5.2.11a)

and

\[
\Psi_s(x) = \begin{bmatrix} (\phi_0^+ - \phi_0^-) \\ (\phi_1^+ + \phi_1^-) \end{bmatrix}.
\]

(5.2.11b)

The set of equations (5.2.10) is then

\[
A_1 \frac{d}{dx} \Psi_s(x) + B_1 \Psi_s(x) = 0,
\]

(5.2.12a)

and

\[
A_2 \frac{d}{dx} \Psi_s(x) + B_2 \Psi_s(x) = S(x).
\]

(5.2.12b)

The matrix elements are evident. From the first of Eqs. (5.2.12) we have

\[
\Psi_s(x) = -B_1^{-1}A_1 \frac{d}{dx} \Psi_s(x),
\]

(5.2.13)

and hence

\[
-A_2 \frac{d}{dx} \left[ B_1^{-1}A_1 \frac{d}{dx} \Psi_s(x) \right] + B_2 \Psi_s(x) = S(x),
\]

(5.2.14)

which is the desired form of the equations. The difference equations for the set (5.2.14) are readily formed by methods considered earlier.
While Yvon's method has not had extensive application, because of its rapid convergence it is useful for treating problems involving sharp changes in material properties for plane boundaries or problems involving the interaction of two plane boundaries.

5.3 Multigroup Transport Methods

The derivation of the multigroup transport equations is very similar to the procedure adopted in Chapter IV for the multigroup diffusion equations. The basic purpose of this section is to reduce the lethargy dependent Boltzmann equation to a coupled set of transport equations which apply to each lethargy group separately. Once the coupled equations have been found, the remainder of the numerical treatment will be omitted. Instead, various procedures for finding the probabilities for neutron transfer from different groups and angles are considered.

The Boltzmann equation with lethargy dependence may be written 6

\[ \Omega \cdot \nabla \phi(r, u, \Omega) + \sigma_t \phi(r, u, \Omega) = \int_{u'} du' \int_{\Omega'} d\Omega' [\sigma_s(r'; u', \Omega'; u, \Omega) \phi(r, u', \Omega')] + S(r, u, \Omega), \]  \( (5.3.1) \)

where \( \phi(r, u, \Omega) \) is the number of neutrons of lethargy \( u \) per unit lethargy crossing a unit surface at \( r \) per unit time going in a unit solid angle centered in the direction \( \Omega \), and \( \sigma_s(r; u', \Omega'; u, \Omega) \) is the probability per unit path length that a neutron at \( r \) and going in a direction \( \Omega' \) with a lethargy \( u' \) is scattered into a unit solid angle centered at \( \Omega \) and a unit lethargy interval centered at \( u \). The remaining symbols are evident from Section 5.1.

The construction of the multigroup equations proceeds as in diffusion theory. We divide the lethargy range into \( G \) groups of arbitrary width and label the initial and final lethargies as \( 0 = w_0, w_{th} = w_G \). The thermal group is indexed by \( G + 1 \). Let \( \Delta u_g = u_g - u_{g-1} \). We then integrate Eq. (5.3.1) from \( u_{g-1} \) to \( u_g \) to obtain

\[ \Omega \cdot \nabla \bar{\phi}(r, \Omega) + \sigma_t \bar{\phi}(r, \Omega) = \bar{Q}(r, \Omega) + \bar{S}(r, \Omega), \quad g = 1, 2, ..., G. \]  \( (5.3.2) \)

We let

\[ Q(r, u, \Omega) = \int du' \int d\Omega' \sigma_s(r; u', \Omega'; u, \Omega) \phi(r, u', \Omega'). \]  \( (5.3.3) \)

6 The derivation of (5.3.1) is in Appendix A.
The averages are all weighted by the appropriate flux. Thus, for \( \sigma_i(r,u) \) we use
\[
\overline{\sigma}_i(r,\Omega) = \int_{u_{s-1}}^{u_s} du \sigma_i(r,u) \phi(r,u,\Omega) / \int_{u_{s-1}}^{u_s} du \phi(r,u,\Omega),
\]
(5.3.4)
whereas for \( Q(r,u,\Omega) \) we use
\[
\overline{Q}^g(r,\Omega) = \int_{u_{s-1}}^{u_s} du Q(r,u,\Omega) \phi(r,u,\Omega) / \int_{u_{s-1}}^{u_s} du \phi(r,u,\Omega).
\]
(5.3.5)

The thermal equation may be added to the set (5.3.2) in the form
\[
\Omega \cdot \nabla \phi^{G+1}(r,\Omega) + \sigma^{G+1}_i(r) \phi^{G+1}(r,\Omega) = Q^{G+1}(r,\Omega) + S^{G+1}(r,\Omega).
\]
(5.3.6)

The set (5.3.2) plus the thermal group equation and the boundary conditions furnish a multigroup transport formulation which is rigorous. The remaining steps are approximate, and each step is taken to reduce the complexity of the problem. The first problem is obtaining the appropriate group constants. Obviously weighting with the flux and even the directional flux is a time consuming process. Many alternative procedures have been suggested including: (1) use of infinite media spectra to eliminate iterative determination of group constants; (2) use of the fission spectrum as the weighting function; (3) use of diffusion theory spectra; (4) constant flux within groups and hence unweighted cross sections. We do not specify any procedure at the moment, but assume the group constants may be specified at the beginning of the computation.

The second problem is the relation of the average flux to the flux at the lethargy interfaces. A full range of possibilities exists as in diffusion theory. We shall use only one approximation, namely
\[
\overline{\phi}^g(r,\Omega) = \phi(r,u_g,\Omega) \equiv \phi^g(r,\Omega),
\]
(5.3.7)
which is accurate only to order \( \Delta u \). Likewise for the other variables.

The group equations are then
\[
\Omega \cdot \nabla \phi^g(r,\Omega) + \sigma^g_i(r) \phi^g(r,\Omega) = Q^g(r,\Omega) + S^g(r,\Omega), \quad g = 1, 2, ..., G + 1.
\]
(5.3.8)

Note that the angular dependence of \( \sigma^g_i \) has been dropped; \( \sigma^g_i \) must be only slightly dependent on \( \Omega \) as may be seen from Eq. (5.3.4), if the multigroup approximation (5.3.7) is a good one, since the total cross section itself is nearly independent of \( \Omega \).
The set of Eqs. (5.3.8) is the multigroup transport equations desired. The nature of the inhomogeneities will be considered in the remainder of this section. We shall describe a few ways of calculating them in detail. To this end, we observe that the set of equations (5.3.8) is equivalent to the assumption

$$\int_{u_{g-1}}^{u_g} du K(u) = \alpha^g K^g,$$  \hspace{1cm} (5.3.9)

where $\alpha^g$ is a constant which depends upon the weighting function assumed for the lethargy dependent constants, and $K(u)$ is a lethargy dependent variable. For instance,

$$\int_{u_{g-1}}^{u_g} du \sigma^g(r, u) \phi(r, u, \Omega) = \alpha^g \sigma^g(r) \phi(r, \Omega).$$  \hspace{1cm} (5.3.10)

The terms of particular interest are the inhomogeneous terms $Q^g(r, \Omega)$ and $S^g(r, \Omega)$. We consider first the scattering source $Q^g(r, \Omega)$. From Eq. (5.3.9) we have

$$\alpha^g Q^g(r, \Omega) = \int_{u_{g-1}}^{u_g} du Q(r, u, \Omega).$$  \hspace{1cm} (5.3.11)

The integration over $u'$ may be written as a sum

$$\int du' \sigma^g(r, u'; \Omega; u, \Omega) \phi(r, u', \Omega') = \sum_{g'=1}^{G+1} \alpha^{g'} \sigma^{g'}_{g'}(r, \Omega'; u, \Omega) \phi_{g'}(r, \Omega'),$$  \hspace{1cm} (5.3.12)

where $\sigma^{g'}_{g'}(r, \Omega'; u, \Omega)$ is the probability that a neutron at $r$ going in the direction $\Omega'$ in the group $g'$ will suffer a scattering in going a unit distance and be scattered into a unit solid angle centered at $\Omega$ and a unit lethargy centered at $u$. The integration of (5.3.12) over the interval $u_{g-1}$ to $u_g$ yields

$$\alpha^g \sum_{g'=1}^{G+1} \alpha^{g'} \sigma^{g'}_{g'}(r, \Omega'; \Omega) \phi^{g'}(r, \Omega'),$$  \hspace{1cm} (5.3.13)

and hence

$$Q^g(r, \Omega) = \sum_{g'=1}^{G+1} \alpha^{g'} \int d\Omega' \sigma^{g'}_{g'}(r, \Omega'; \Omega) \phi^{g'}(r, \Omega'),$$  \hspace{1cm} (5.3.14)

where $\sigma^{g', g}$ is the probability of transfer from group $g'$ with direction $\Omega'$.
to group \( g \) with direction \( \Omega \). The nature of the coefficient \( \sigma^{g',g}_g \) depends upon the materials within the assembly and the nature of the scattering law. For instance, if no upscattering is permitted, then

\[
\sigma^{g',g}_g = 0, \quad \text{if } g' > g.
\]  

(5.3.15)

For elastic scattering of heavy elements, then, only terms for \( g' \) near \( g \) enter.

We now consider the source term \( S_\Omega(r, \Omega) \). We again have

\[
\int_{u_{g-1}}^{u_g} du S(r, u, \Omega) = \omega S^\Omega(r, \Omega).
\]  

(5.3.16)

The source will consist of fission sources plus extraneous sources. The fission sources are

\[
S_f(r, u, \Omega) = \nu \chi(u) \int d\Omega' \sigma_f(r, u', \Omega'; u, \Omega) \phi(r, u', \Omega').
\]  

(5.3.17)

The integration over \( u' \) is replaced by a summation to yield

\[
S_f(r, u, \Omega) = \nu \chi(u) \sum_{g'=1}^{G+1} \sigma_f \phi^{g'}(r, \Omega'; u, \Omega') \phi(r, \Omega').
\]  

(5.3.18)

We then have

\[
S^\Omega(r, \Omega) = \nu \chi \sum_{g'=1}^{G+1} \sigma^{g',g}_g \phi^{g'}(r, \Omega'; \Omega') \phi^{g'}(r, \Omega').
\]  

(5.3.19)

The equations (5.3.14) and (5.3.19) imply that the right-hand side of Eq. (5.3.8) is

\[
Q^\Omega(r, \Omega) + S^\Omega(r, \Omega) = \sum_{g'=1}^{G+1} \int d\Omega' T^{g',g}(r; \Omega'; \Omega) \phi^{g'}(r, \Omega') + S^\Omega_e(r, \Omega),
\]

where \( S^\Omega_e \) is the external source and

\[
T^{g',g}(r; \Omega'; \Omega) = \omega \left[ \sigma^{g',g}_g + \nu \chi \sigma^{g',g}_g \right].
\]

\( T^{g',g}(r; \Omega'; \Omega) \) is called the transfer kernel for the multigroup equations. Physically \( T^{g',g}(r; \Omega'; \Omega) \) is the probability that a neutron appears in group \( g \) going in a unit solid angle centered at \( \Omega \) as a result of a neutron in group \( g' \) at \( r \) going a unit distance in a unit solid angle centered at \( \Omega' \).
laws and cross section weighting factors have been chosen. As an example, consider the case of isotropic scattering and fission in the laboratory coordinates. The scattering kernel is then of the form

\[ T^{a'}(r; \Omega'; \Omega) = \frac{1}{4\pi} T^{a}(r) . \]  

(5.3.20)

It is frequently useful to expand the transfer kernel in Legendre polynomials. If the cosine of the angle between \( \Omega' \) and \( \Omega \) is \( \mu_0 \), then we expand \( T^{a'}(r) \) in the form

\[ T^{a'}(r; \Omega'; \Omega) = \frac{1}{2\pi} \sum_n \frac{2n + 1}{2} T_n^{a'}(r) P_n(\mu_0) . \]  

(5.3.21)

The zeroth harmonic contains the isotropic components while the remaining harmonics include the anisotropic moments.

The angular and spatial variations are separable under certain conditions, e.g., for isotropic media. The transfer kernel may then be written

\[ T^{a'}(r; \Omega'; \Omega) = C^{a'}(r) f^{a'}(\Omega' \rightarrow \Omega) . \]  

(5.3.22)

\( C^{a'}(r) \) is the probability that a neutron appear in group \( g' \) as a result of a neutron in group \( g \) at \( r \) going a unit distance. For one group problems, the coefficient is merely \( C(r) \), the mean number of neutrons per collision. We shall make frequent use of Eq. (5.3.22) in the remainder of this chapter.

### 5.4 Discrete Ordinate Methods

In Section 5.1 we considered approximate solutions to the transport equation by use of an expansion in terms of Legendre polynomials. In particular the angle variable was eliminated from the equation in favor of harmonic coefficients. We now consider an alternative treatment of the angular dependence called the discrete ordinate method. We will merely outline the procedure for developing discrete ordinate approximations. In the next section we specialize to a particular method, the \( S_N \) method. The reason for the emphasis on the \( S_N \) method is due to its wide use in transport calculations.

For simplicity we consider the one group transport equation in slab geometry with isotropic scattering

\[ \mu \frac{d}{dx} \phi(x, \mu) + \sigma(x) \phi(x, \mu) = \frac{c(x)}{2} \int_{-1}^{1} d\mu' \phi(x, \mu') + S_e(x, \mu) . \]  

(5.4.1)
We have used the transfer kernel of the previous section, and hence the source \( S(x, \mu) \) is external.

Rather than expand the flux, we divide the \( \mu \) interval into a discrete number of intervals instead, hence the name discrete ordinate. Let the interpolation points be denoted as \( \mu_n \), \( n = 0, 1, \ldots, N \). The directional flux is to be evaluated at the points \( \mu_n \) and interpolated in between. We denote directional fluxes \( \phi(x, \mu_n) = \phi_n(x) \). Note the subscript \( n \) now refers to a given direction, not an index for an expansion.

The transfer integral is now approximated by a quadrature formula of the form

\[
\int_{-1}^{1} d\mu \phi(x, \mu') = \sum_{n'} w_n \phi_n(x),
\]

(5.4.2)

where the \( w_n \) are weighting factors. The Boltzmann equation is applied to each group separately in the form

\[
\mu_n \frac{d}{dx} \phi_n(x) + \sigma_1(x) \phi_n(x) = \frac{c(x)}{2} \sum_{n'} w_n \phi_n(x) + S(x, \mu_n), \quad n = 0, 1, \ldots, N.
\]

(5.4.3)

In order to avoid discontinuities the interpolation points are so chosen that \( \mu_n \neq 0 \), all \( n \).

A variety of quadrature formulas have been proposed and used. In particular, for interfaces where the directional flux may be discontinuous at \( \mu = 0 \), double expansions in \( \mu \) space are recommended. The most frequently suggested method for such problems is Gauss quadrature. This method has significant advantages regarding the accuracy of the approximation. The use of the Gaussian quadrature was suggested by Wick (Reference 9).

In the elementary integration formulas considered in Chapter III, it was indicated that \( N \) point integration formulas approximated the integrand as a polynomial of degree \( N - 1 \). The Gaussian integration formula has the property of being accurate to order \( 2N \), i.e., approximating the integrand as a polynomial of degree \( 2N - 1 \). The remarkable feature of this quadrature is that only \( N \) points are needed for the integrand. In order to derive the Gaussian quadrature, we consider the following problem. Suppose we have a polynomial \( f_{2N-1}(x) \) of degree \( 2N - 1 \). Is it possible to find another polynomial, of degree \( N - 1 \), \( g_{N-1}(x) \), which agrees with \( f_{2N-1}(x) \) at \( N \) points, say \( x_j, j = 1, 2, \ldots, N \), and such that

\[
\int_{-1}^{1} dx f_{2N-1}(x) = \int_{-1}^{1} dx g_{N-1}(x),
\]

(5.4.4)
for properly chosen \( x_j \)? If the above question can be answered in the affirmative, then the integration of \( g_{N-1}(x) \) can be replaced by a summation which gives exactly the value of the integral. In other words, it is then possible to approximate an integral with an \( N \)-point formula which has a truncation error of order \( 2N \).

The proof that such an integration formula is possible is simple. Since \( f_{2N-1}(x) \) is of order \( 2N - 1 \) and \( g_{N-1}(x) \) coincides with \( f_{2N-1}(x) \) at \( N \) points \( x_n \), we have

\[
f_{2N-1}(x) = g_{N-1}(x) + (x - x_1)(x - x_2) \ldots (x - x_N) G_{N-1}(x) ,
\]

where \( G_{N-1}(x) \) is a polynomial of degree \( N - 1 \). If we integrate Eq. (5.4.5) from \(-1 \leq x \leq 1\) and apply (5.4.4), then we must have

\[
\int_{-1}^{1} dx (x - x_1)(x - x_2) \ldots (x - x_N) G_{N-1} = 0 . \quad (5.4.6)
\]

If the integration formula is to be valid for all \( f_{2N-1}(x) \), then \( G_{N-1}(x) \) is arbitrary. Hence each power of \( x \) in \( G_{N-1}(x) \) which appears in (5.4.6) must vanish separately. That is,

\[
\int_{-1}^{1} dx (x - x_1)(x - x_2) \ldots (x - x_N) x^n = 0, \quad n = 0, 1, \ldots, N - 1 . \quad (5.4.7)
\]

The coefficient of \( x^n \) in the above integral is a polynomial of degree \( N \), and Eq. (5.4.7) states that this polynomial must be orthogonal to all polynomials of lower degree, over the interval \(-1 \leq x \leq 1\). It is well known that the Legendre polynomials satisfy this criterion. Therefore, if the interpolation points are the zeros of the Legendre polynomial of degree \( N \), then Eq. (5.4.7) and thus Eq. (5.4.4) are true. But then we have

\[
\int_{-1}^{1} dx f_{2N-1}(x) = \sum_{j=1}^{N} w_j f_{2N-1}(x_j) , \quad (5.4.8)
\]

which is exact. We now consider finding the \( w_j \). First consider \( f_{2N-1}(x) = \text{constant} \). Then

\[
\sum_{j=1}^{N} w_j = 2 . \quad (5.4.9)
\]
By continuing in this manner we arrive at a set of $N$ simultaneous equations of the form

\[
\begin{bmatrix}
    1 & 1 & \ldots & 1 \\
    x_1 & x_2 & \ldots & x_N \\
    x_1^2 & x_2^2 & \ldots & x_N^2 \\
    \vdots & \vdots & \ddots & \vdots \\
    x_1^N & x_2^N & \ldots & x_N^N
\end{bmatrix}
\begin{bmatrix}
    w_1 \\
    w_2 \\
    \vdots \\
    w_N
\end{bmatrix}
= \begin{bmatrix}
    c_1 \\
    c_2 \\
    \vdots \\
    c_N
\end{bmatrix},
\tag{5.4.10}
\]

where the $c_n$ are readily formed by inserting various powers of $x$ into Eq. (5.4.8). Since the rows of the square matrix in Eq. (5.4.10) are linearly independent, the inverse matrix always exists, and the $w_j$ may be found by solving Eq. (5.4.10). In fact it is readily shown that the weight factors are always positive (see problem 10). There are several other formulas that can be used to derive the weight coefficients $w_j$ (see, for instance, Reference 10, pp. 362-367).

The example we have used to derive the Gaussian integration formula was a particularly simple one. There exist many Gaussian formulas for different intervals of integration, and for more complicated integrands. We will not have occasion to use the more general formulas (for further details, see References 10 and 11).

To reiterate, the advantage of the Gaussian quadrature is the high order truncation error. A disadvantage is the location of the interpolation points. The intervals are not equally spaced in general, and for this reason the Gaussian type formula is rarely used for deriving difference approximations. Nevertheless for integration over the angular coordinate, the method is frequently used. It can be shown (see Reference 2, pp. 268-271) that for spherically symmetric scattering the discrete ordinate method using Gaussian quadrature is equivalent to the spherical harmonics method.

The discrete ordinate equations, Eqs. (5.4.3), are readily reduced to finite difference equations by standard techniques. In the next section a particular example of the formation of the spatial difference equations will be given in conjunction with the $S_N$ method. As a final word on the discrete ordinate method, we remark that anisotropic scattering can be incorporated into the equations, and multigroup problems considered. The discrete ordinate method is widely used for one dimensional problems; its use in multidimensional problems seems to have been limited.
5.5 The $S_N$ Method

The $S_N$ method is a special case of the discrete ordinate method and was originated by B. G. Carlson (see Reference 12). The characteristic feature of the $S_N$ method is the assumption of linear variation of the directional flux between interpolation points in both the angular and spatial variations. We shall derive the equations in a straightforward manner for spherical geometry in the multigroup model. Consideration is then given to a variant of the $S_N$ method, called the discrete $S_N$ method, also proposed by Carlson (Reference 13).

The transport equation for a given energy group $g$ in spherical geometry is

$$\mu \frac{\partial}{\partial r} \phi^g(r, \mu) + \frac{1}{r} (1 - \mu^2) \frac{\partial}{\partial \mu} \phi^g(r, \mu) + \sigma^a_t \phi^g(r, \mu) = S^g(r), \quad (5.5.1)$$

where $\mu$ is the cosine of the angle between the neutron direction and the radius vector where we have assumed all sources are isotropic. An isotropic source is not an essential feature of the $S_N$ method but it greatly simplifies the analysis. The extension to include anisotropies is direct but detailed, and we shall not consider such problems here. The interval $-1 \leq \mu \leq 1$ is divided into $N$ segments, usually of equal width, $\Delta \mu$.

The interpolation points are then defined as $\mu_n = -1 + 2n/N$ so that $\mu_0 = -1$ and $\mu_N = 1$. The directional flux is assumed to vary linearly between the interpolation points, and hence

$$\phi^g(r, \mu) = \frac{\mu - \mu_{n-1}}{\mu_n - \mu_{n-1}} \phi^g(r, \mu_n) + \frac{\mu_n - \mu}{\mu_n - \mu_{n-1}} \phi^g(r, \mu_{n-1}), \quad (5.5.2)$$

for $\mu_{n-1} \leq \mu \leq \mu_n$. A representative directional flux distribution is shown in Fig. 5.5.1 for an $S_4$ approximation.

Here

$$\phi_n(x) = \phi(r, \mu_n). \quad (5.5.2a)$$

The linear approximation in Eq. (5.5.2) may be substituted into Eq. (5.5.1) and the result integrated from $\mu_{n-1}$ to $\mu_n$. The integration yields

$$\left[ a_n \frac{d}{dr} + b_n \frac{1}{r} + \sigma_t^g \right] \phi_n^g(r) + \left[ a_n \frac{d}{dr} - b_n \frac{1}{r} + \sigma_t^g \right] \phi_{n-1}^g(r) = c_n S^g(r),$$

$$(n = 1, 2, ..., N) \quad (5.5.3)$$

7 For derivation see Appendix A.
5.5 THE $S_N$ METHOD

with

$$a_n = \frac{1}{3}(2\mu_n + \mu_{n-1}), \quad \tilde{a}_n = \frac{1}{3}(\mu_n + 2\mu_{n-1})$$

$$b_n = \frac{2}{3\Delta_n} (3 - \mu_n^2 - \mu_n\mu_{n-1} - \mu_{n-1}^2),$$

and

$$c_n = 2.$$ 

\[\text{FIG. 5.5.1.} \quad S_4 \text{ approximation to the directional flux distribution. The dashed line represents the directional flux; the solid line, the } S_N \text{ approximation.}\]

The set of equations (5.5.3) consists of $N$ equations in the $N + 1$ unknowns $\phi(r)$. The $N + 1$st equation is obtained by setting $\mu = -1$ and writing the transport equation, Eq. (5.5.1), directly. We have

$$-\frac{d}{dr} \phi_{0}(r) + \sigma_{i} \phi_{0}(r) = S_{0}(r). \quad (5.5.4)$$

The above equation may be included in the set (5.5.3) by choosing the constants

$$a_0 = -1,$$

$$b_0 = 0,$$

$$\phi_{-1}(r) = 0,$$

$$c_0 = 1.$$ 

It is evident that the approximations made are accurate to order $(\Delta \mu^2)$. The spatial dependence is obtained in the same manner. We divide the interval $0 \leq r \leq R$ into $j$ segments of width $\Delta_j = r_j - r_{j-1}$, which are not assumed equal. As usual the division is such that interfaces lie on
interpolation points. We order the points such that \( r_0 = 0, r_j = R \). The mesh in \( r - \mu \) space for any energy group is shown in Fig. 5.5.2.

\[
\begin{align*}
\text{Fig. 5.5.2. Mesh in } r - \mu \text{ space for an } S_4 \text{ calculation.}
\end{align*}
\]

In order to perform the spatial integrations, it is important to consider the direction of neutron motion. For the line \( \mu = -1 \), i.e., \( n = 0 \), the neutrons move from large \( r \) to small \( r \). For reduced truncation error, we should perform the spatial integration in the direction of neutron travel (see problem 11).

To derive the appropriate difference equations for \( n \) such that \( \mu_n \leq 0 \), we integrate from \( r_j \) to \( r_{j-1} \). Conversely, for \( \mu_n > 0 \), we integrate from \( r_{j-1} \) to \( r_j \). Let \( \Delta_j \) be defined as \( \Delta_j = r_j - r_{j-1} \). To terms of order \( \Delta_j^3 \), we approximate integrals as

\[
\int_{r_{j-1}}^{r_j} dr f(r) = \frac{f(r_{j-1}) + f(r_j)}{2} \Delta_j. \tag{5.5.5}
\]

The terms in \( 1/r \) are integrated by assuming an average value \( 1/\langle r_j \rangle \). The simplest choice is \( \langle r_j \rangle = (r_j + r_{j-1})/2 = \bar{r}_j \). Another choice is

\[
\langle r_j \rangle = \frac{r_j^3}{\bar{r}_j} = \frac{2 (r_j^3 - r_{j-1}^3)}{3 (r_j^2 - r_{j-1}^2)} \tag{5.5.6}
\]

The difference equations for \( n = 0, 1, \ldots, N/2 \) are found by integrating
from \( r_j \) to \( r_{j-1} \). Using Eq. (5.5.5) and any suitable approximation for \( \langle r_j \rangle \) in Eqs. (5.5.3) and (5.5.4), we have, after some algebra,

\[
\begin{align*}
&\left[-a_n + \frac{b_n}{\langle r_j \rangle} \frac{A_j}{2} + \sigma_i^q \frac{A_j}{2}\right] \phi_{n,j-1}^q + \left[a_n + \frac{b_n}{\langle r_j \rangle} \frac{A_j}{2} + \sigma_i^q \frac{A_j}{2}\right] \phi_{n,j}^q \\
&+ \left[-\bar{a}_n - \frac{b_n}{\langle r_j \rangle} \frac{A_j}{2} + \sigma_i^q \frac{A_j}{2}\right] \phi_{n-1,j-1}^p \\
&+ \left[\bar{a}_n - \frac{b_n}{\langle r_j \rangle} \frac{A_j}{2} + \sigma_i^q \frac{A_j}{2}\right] \phi_{n-1,j}^p = \frac{c_n A_j}{2} [S_{j-1}^q + S_j^p].
\end{align*}
\] (5.5.7)

Equation (5.5.7) may be used to compute successive iterates for the flux \( \phi_{n,j-1}^q \). The usual iteration algorithm is analogous to the method of successive displacements. We drop the group index \( g \) and use superscript \( p \) for the iteration index. Equation (5.5.7) is then used in the form

\[
\phi_{n,j-1}^{p+1} = a_{n,j}(S_{j-1}^p + S_j^p) - b_{n,j} \phi_{n,j}^{p+1} - c_{n,j} \phi_{n-1,j-1}^{p+1} - d_{n,j} \phi_{n-1,j}^{p+1},
\] (5.5.8)

where the coefficients are evident. Equation (5.5.8) applies for \( j = J, J - 1, \ldots, 1 \), and \( n = 0, 1, \ldots, N/2 \). For \( n = 0 \) the coefficients \( c_{n,j} \) and \( d_{n,j} \) are to be taken as zero.

An analogous equation is obtained for neutrons heading away from the reactor center; that is, for \( n > N/2 \). Without considering the details the basic difference equation is seen to be of the form

\[
\phi_{n,j}^{p+1} = a_{n,j}'(S_{j-1}^p + S_j^p) - b_{n,j}' \phi_{n,j}^{p+1} - c_{n,j}' \phi_{n-1,j-1}^{p+1} - d_{n,j}' \phi_{n-1,j}^{p+1}.
\] (5.5.9)

The iteration algorithm is similar to Eq. (5.5.8).

The boundary conditions to be used in conjunction with Eqs. (5.5.8) and (5.5.9) are simple. If there are any neutrons incident upon the external boundary, then the values \( \phi_{n,J} \) are determined for \( n \leq N/2 \). For a vacuum boundary the \( \phi_{n,J} \) are zero for \( n \leq N/2 \). At the center the directional fluxes are continuous and hence

\[
\phi_{n,0} = \phi_{N-n,0}, \quad 0 \leq n \leq \frac{N}{2}.
\] (5.5.10)

A mesh for a single group, with boundary conditions, and the difference equation point pattern is shown in Fig. 5.5.3.
The source function $S^\nu(r)$ consists of scattering, fission, and extraneous sources. Thus

$$S^\nu(r, u) = \int_0^{\mu_{\text{th}}} du' \sigma_s(r, u' \rightarrow u) \phi(r, u') + \nu_k(u) \int_0^{\mu_{\text{th}}} du' \sigma_f(r, u') \phi(r, u') + S^\nu_s(r, u), \quad (5.5.11)$$

where the isotropic assumption has been used. The integrals over lethargy are replaced by summations over the group index $g'$. Thus, Eq. (5.5.11) is written

$$S^\nu(r, u) = \sum_{g'=1}^{G+1} [\sigma_s^g \phi^g + \nu_k \sigma_f^g \phi^g] + S^\nu_s(r, u). \quad (5.5.12)$$

![Fig. 5.5.3. The $r - \mu$ mesh for an $S_4$ calculation in a sphere. The boundary conditions are shown as heavy dots. The 4-point difference equations are shown with directional arrows for the path of the computation. The points marked with a cross are to be computed using the points marked with a circle.](image)

The scalar flux $\phi^\nu(r)$ is determined from the angular components as

$$\phi^\nu(r) = \frac{1}{2} \int_{-1}^{1} d\mu \phi^\nu(r, \mu) = \sum_{n=0}^{N} w_n \phi^\nu_n(r) \quad (5.5.13)$$

where, for a uniform $\mu$ spacing,

$$w_0 = w_N = \frac{A}{4}, \quad (5.5.14a)$$

$$w_n = \frac{A}{2}, \quad n = 1, 2, ..., N - 1. \quad (5.5.14b)$$

The spatial integration of $S^\nu(r)$ is carried out as before; we omit the details.

The entire calculational procedure for the $S_N$ method is now evident. We again consider a criticality problem. The coefficients for the desired energy groups, angular segments, and spatial regions are computed in advance. To estimate the source an initial estimate of the scalar flux in each group is made. Note that only the scalar fluxes are needed, not the...
5.5 The \( S_N \) Method

Directional fluxes. After the source has been computed the directional fluxes in each group are computed, first for \( \mu_0 (= -1) \), then \( \mu_1 \), etc., up to \( \mu_{N/2} \) in the direction \( r = R \) to \( r = 0 \). The boundary conditions are invoked to yield starting values for \( \mu_{(N/2) + 1} \), etc., and the integration is from \( r = 0 \) to \( r = R \). After a group has been iterated once, we may go to the next group or recompute the source and recalculate the same group. Both procedures are used in practice. After every group has been iterated, the source may be recomputed and scaled appropriately. The entire procedure may be written in matrix form as a generalized eigenvalue problem (see problem 15).

The discrete \( S_N \) is a simplification of the original \( S_N \). For the discrete \( S_N \) the \( r - \mu \) space is again divided into segments \( r_j \) and \( \mu_n \). The spacing in \( \mu \) will again be assumed uniform. We define

\[
\Delta_j = r_j - r_{j-1}, \quad j = 1, 2, \ldots, J, \tag{5.5.15a}
\]

and

\[
\Delta_n = \mu_n - \mu_{n-1}, \quad n = 1, 2, \ldots, N. \tag{5.5.15b}
\]

Next we consider the cell \( \Delta_j \Delta_n \) and the average directional flux in the cell, say \( \bar{\phi}_{n,j} \).\(^8\) As before, the flux is assumed linear in both \( r \) and \( \mu \) directions. The average flux is then given as

\[
\bar{\phi}_{n,j} = \frac{\phi_{n,j} + \phi_{n,j-1} + \phi_{n-1,j} + \phi_{n-1,j-1}}{4}. \tag{5.5.16}
\]

The objective of the discrete \( S_N \) method is to re-express \( \bar{\phi}_{n,j} \) in terms of average values of the directional flux at the midpoints \( \bar{r}_j = (r_j + r_{j-1})/2 \) and \( \bar{\mu}_n = (\mu_n + \mu_{n-1})/2 \). The resulting equations are simpler in detail than the original \( S_N \) equations and are also somewhat easier to derive. We define

\[
\phi_n = \frac{\phi_{n,j} + \phi_{n,j-1}}{2}, \tag{5.5.17a}
\]

and

\[
\phi_j = \frac{\phi_{n,j} + \phi_{n-1,j}}{2}. \tag{5.5.17b}
\]

The average flux over the cell is then

\[
\bar{\phi}_{n,j} = \frac{\phi_n + \phi_{n-1}}{2} = \frac{\phi_j + \phi_{j-1}}{2}. \tag{5.5.18}
\]

\(^8\) The group index is omitted in the following since the results apply to each group.
Equation (5.5.18) is intuitively obvious since \( \phi_n \) and \( \phi_j \) represent midpoint values on the cell boundaries.

The difference equations are now found in terms of \( \phi_n \) and \( \phi_j \) by averaging the Boltzmann equation over the cell \( \Delta_n \Delta_j \). Each term of Eq. (5.5.1) may be treated separately. The first term is then

\[
\frac{1}{\Delta_n \Delta_j} \int_{\mu_{n-1}}^{\mu_n} d\mu \int_{r_{j-1}}^{r_j} dr \mu \frac{d}{dr} \phi(r, \mu) = \frac{1}{\Delta_j} \bar{\mu}_n [\phi_j - \phi_{j-1}],
\]

(5.5.19a)

where we have assumed \( \phi(r_j, \mu) \approx \phi(r_j, \bar{\mu}_n) \). This approximation is valid to order \( \Delta \mu \).

The second term is

\[
\frac{1}{\Delta_n \Delta_j} \int_{r_{j-1}}^{r_j} dr \int_{\mu_{n-1}}^{\mu_n} d\mu \left[ \frac{1 - \mu^2}{r} \frac{d}{d\mu} \phi(r, \mu) \right] = b_n \frac{1}{\Delta_j} \langle r_j \rangle [\phi_n - \phi_{n-1}],
\]

(5.5.19b)

where \( b_n \) is the average of the quantity \( (1 - \mu^2) \), \( \langle r_j \rangle \) is the average radius, usually taken as Eq. (5.5.6). The removal term is readily written as

\[
\frac{1}{\Delta_n \Delta_j} \int_{\mu_{n-1}}^{\mu_n} d\mu \int_{r_{j-1}}^{r_j} dr \sigma(r) \phi(r, \mu) = \sigma_j \left[ \frac{\phi_j + \phi_{j-1}}{2} \right],
\]

(5.5.19c)

with \( \sigma_j \) the midpoint value of \( \sigma(r) \). For the source, assumed isotropic, we have

\[
\frac{1}{\Delta_n \Delta_j} \int_{\mu_{n-1}}^{\mu_n} d\mu \int_{r_{j-1}}^{r_j} dr S(r) = S_j,
\]

(5.5.19d)

with \( S_j \) the midpoint value of \( S(r) \).

Collecting terms the difference equation is then

\[
\bar{\mu}_n [\phi_j - \phi_{j-1}] + b_n \Delta_j \langle r_j \rangle [\phi_n - \phi_{n-1}] + \Delta_j \sigma_j \left[ \frac{\phi_j + \phi_{j-1}}{2} \right] = \Delta_j S_j.
\]

(5.5.20)

The term in \( \phi_n \) may be eliminated by use of Eq. (5.5.18). Substituting and collecting terms we have

\[
\left( \bar{\mu}_n + \frac{b_n \Delta_j}{\Delta_n \langle r_j \rangle} + \frac{\sigma_j \Delta_j}{2} \right) \phi_j + \left( -\bar{\mu}_n + \frac{b_n \Delta_j}{\Delta_n \langle r_j \rangle} + \frac{\sigma_j \Delta_j}{2} \right) \phi_{j-1} = \Delta_j S_j + \frac{2b_n \Delta_j}{\Delta_n \langle r_j \rangle} \phi_{n-1}.
\]

(5.5.21)

Equation (5.5.21) is the desired difference relation. Note that, in contrast to the original \( S_N \) method, this equation is only 3-point in terms.
of the unknowns. As before an additional equation is obtained for 
\( \mu = -1 \). The mesh pattern is actually triangular shaped for the discrete 
\( S_N \) as shown in Fig. 5.5.4.

![Fig. 5.5.4. Mesh point pattern for the discrete \( S_N \) method. The arrows indicate the direction of integration.](image)

The procedure for solving the discrete \( S_N \) equations is very similar
to the original \( S_N \) method. For a criticality problem the scalar flux must
be estimated, which gives the source term. The integration is started
along the line \( \bar{\mu}_0 = -1 \). The \( \phi_{j+1} \) are evaluated from \( j = J \) to \( j = 1 \). At
\( j = J \) the boundary condition of zero incident flux is used. Once the
line \( \bar{\mu}_0 \) is computed, the lines \( \bar{\mu}_1, \bar{\mu}_2, \ldots, \bar{\mu}_{(N/2)} \) are computed in turn. Note
that the values of \( \phi_n \) are readily found by linear interpolation. For
\( \bar{\mu}_n, \ n > N/2 \), the direction of integration reverses. As before, the
boundary conditions at \( j = 0 \) are

\[
\phi_0(\bar{\mu}_n) = \phi_0(\bar{\mu}_{N-n}) . \tag{5.5.22}
\]

The source is computed as

\[
S_j = \frac{1}{N} \sum_n A_{n,j} \phi_n , \tag{5.5.23}
\]

where the matrix \( A_{n,j} \) represents the scattering plus fission processes,
averaged over the interval \( j - 1 \) to \( j \).

The proper value of \( b_n \) to be used is determined by the condition that
the net outflow of neutrons from the element \( \Delta_j \) be equal to the source
strength in that element. The neutron current, \( J(r) \), is defined as

\[
J_j = \int_{-1}^{1} d\mu \mu \phi(r, \mu) = \frac{1}{N} \sum_{n=1}^{N} \bar{\mu}_n \phi_j . \tag{5.5.24}
\]

Integration of the Boltzmann equation over \( \mu \) yields

\[
\frac{d}{dr} J(r) + \frac{2}{r} J(r) + \sigma \phi(r) = S(r) . \tag{5.5.25}
\]
Integrating over the interval $\Delta_j$ then yields

$$J_i - J_{i-1} + \frac{\Delta_j}{\langle r_j \rangle} \left[ J_i + J_{i-1} \right] + \sigma_i \Delta_j \bar{\phi}_i = \Delta_j S_j.$$  \hspace{1cm} (5.5.26)

Equation (5.5.26) is the difference equation for the integral over the element. The difference equation (5.5.21) is the equation in the interval $\Delta_n$. Therefore, if we sum Eq. (5.5.21) over all $n$, the resulting sum must equal Eq. (5.5.26). It suffices to define $b_n$ to obey the relation (see problem 17),

$$b_n - b_{n-1} = -\Delta_n (\bar{\mu}_m + \bar{\mu}_{m-1}).$$ \hspace{1cm} (5.5.27)

Note that $b_0 = 0$, and hence the $b_n$ are readily evaluated by recursion.

Further modifications of the discrete $S_N$ have been suggested by Carlson and are discussed in Reference 13.

5.6 Time Dependent Transport Methods

All of the numerical procedures for the transport equation considered thus far may be generalized to include transient effects. We consider examples in one-group slab geometry. The time dependent transport equation is (see Appendix A)

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \mu \frac{\partial \phi}{\partial x} + \sigma_t \phi = S.$$ \hspace{1cm} (5.6.1)

The time dependent equation is readily transformed into the time dependent $P_N$ equations. By the methods considered in Section 5.1, we obtain, for the $P_3$ equations,

$$\frac{1}{v} \frac{\partial \phi_0}{\partial t} + \frac{\partial \phi_1}{\partial x} + \sigma_t \phi_0 = \sigma_{s,0} \phi_0 + S_0,$$ \hspace{1cm} (5.6.2a)

$$\frac{1}{v} \frac{\partial \phi_1}{\partial t} + \frac{2}{3} \frac{\partial}{\partial x} \phi_2 + \frac{1}{3} \frac{\partial}{\partial x} \phi_0 + \sigma_t \phi_1 = \sigma_{s,1} \phi_1 + S_1,$$ \hspace{1cm} (5.6.2b)

$$\frac{1}{v} \frac{\partial \phi_2}{\partial t} + \frac{3}{5} \frac{\partial}{\partial x} \phi_3 + \frac{2}{5} \frac{\partial}{\partial x} \phi_1 + \sigma_t \phi_2 = \sigma_{s,2} \phi_2 + S_2.$$ \hspace{1cm} (5.6.2c)

$$\frac{1}{v} \frac{\partial \phi_3}{\partial t} + \frac{3}{7} \frac{\partial}{\partial x} \phi_2 + \sigma_t \phi_3 = \sigma_{s,3} \phi_3 + S_3.$$ \hspace{1cm} (5.6.2d)
We define the vectors
\[
\Psi = \begin{bmatrix}
\phi_0 \\
\phi_1 \\
\phi_2 \\
\phi_3
\end{bmatrix}, \quad (5.6.3a)
\]
\[
S = \begin{bmatrix}
S_0 \\
S_1 \\
S_2 \\
S_3
\end{bmatrix}. \quad (5.6.3b)
\]

The \( P_3 \) equations may then be written
\[
\frac{1}{v} \frac{\partial}{\partial t} \Psi + A \frac{\partial}{\partial x} \Psi + \sigma \Psi = B \Psi + S, \quad (5.6.4)
\]
with
\[
A = \begin{bmatrix}
0 & 1 & 0 & 0 \\
1/3 & 0 & 2/3 & 0 \\
0 & 2/5 & 0 & 3/5 \\
0 & 0 & 3/7 & 0
\end{bmatrix}, \quad (5.6.5a)
\]
\[
B = \begin{bmatrix}
\sigma_{s,0} & 0 & 0 & 0 \\
0 & \sigma_{s,1} & 0 & 0 \\
0 & 0 & \sigma_{s,2} & 0 \\
0 & 0 & 0 & \sigma_{s,3}
\end{bmatrix}. \quad (5.6.5b)
\]

In the absence of external sources, Eq. (5.6.4) becomes
\[
\frac{1}{v} \frac{\partial}{\partial t} \Psi + A \frac{\partial}{\partial x} \Psi + \sigma \Psi = \nu B' \Psi, \quad (5.6.6)
\]
where \( B' \) includes the fission sources, and \( \sigma \) the cross sections.

One simple difference approximation for Eq. (5.6.6) is
\[
\frac{\Psi_{j+1}^l - \Psi_j^l}{v \Delta t} + A \frac{(\Psi_{j+1}^l - \Psi_{j-1}^l)}{2 \Delta x} + \sigma \Psi_j^l = \nu B' \Psi_j^l, \quad (5.6.7)
\]
with \( j \) the space index, \( l \) the time index, and
\[
\Psi_j^l = \begin{bmatrix}
\phi_0(x_j, t_l) \\
\phi_1(x_j, t_l) \\
\phi_2(x_j, t_l) \\
\phi_3(x_j, t_l)
\end{bmatrix}. \quad (5.6.8)
\]
V. TRANSPORT METHODS

The difference equation (5.6.7) is explicit in time and has truncation error $O(\Delta t) + O(\Delta x^2)$.

To study the stability of the procedure, we consider a generalization of the Von Neumann method. We recall that the Von Neumann method was based upon a Fourier expansion of the form

$$\phi(x_j, t) = \sum_n (\xi_i)^m e^{i\xi x}.$$  \hspace{1cm} (5.6.9)

The difference equation for the function $\phi(x_j, t)$ was used to find the behavior of the amplification factor $\xi_i$. In the case of equation (5.6.7), the difference equation relates to vectors and hence a generalization of the expansion (5.6.9) is needed. Obviously an expansion of the form

$$\psi_j^l = \sum_n u_j^l e^{i\xi x}.$$  \hspace{1cm} (5.6.10)

is necessary. In the particular problem considered here, each vector $u_j^l$ consists of four components. To study stability the difference relation is used to relate the vectors $u_j^{l+1}$ and $u_j^l$. In general, a relation of the form

$$u_j^{l+1} = C(\Delta x, \Delta t) u_j^l$$  \hspace{1cm} (5.6.11)

is found. The quantity $C(\Delta x, \Delta t)$ is a matrix called the amplification matrix. Stability depends upon the eigenvalues of the amplification matrix.

Equation (5.6.7) will serve as a useful example of the generalization of the Von Neumann method. Inserting the expansion (5.6.10) into the difference equation, we find, for a particular index $n$,

$$\frac{(u_j^{l+1} - u_j^l)}{v\Delta t} e^{i\beta_n x} + \frac{A(e^{i\beta_n x} - e^{-i\beta_n x})}{2\Delta x} u_j^l e^{i\beta_n x} + \sigma u_j^l e^{i\beta_n x} = vB' u_j^{l+1} e^{i\beta_n x}.$$  \hspace{1cm} (5.6.12)

Collecting terms and transposing, we have

$$u_j^{l+1} = \left[ I + v\Delta t(vB' - \sigma) - \frac{v\Delta t}{\Delta x} \sin \beta_n \Delta x A \right] u_j^l.$$  \hspace{1cm} (5.6.13)

The quantity in brackets is the amplification matrix, $C(\Delta x, \Delta t)$.

To find the eigenvalues of the amplification matrix, we consider the following simplification. Let the ratio $\Delta t/\Delta x$ be a fixed quantity, say $\alpha$. In the limit of very small $\Delta t$, the amplification matrix is then

$$C(\Delta x, 0) = \left[ I - i\alpha \sin \beta_n \Delta x A \right].$$  \hspace{1cm} (5.6.14)
The matrix $A$ has at least one nonzero eigenvalue, say $\lambda_0$. Hence $C(\Delta x, 0)$ has an eigenvalue with magnitude given by

$$|\gamma_0| = \sqrt{1 + \alpha^2 \sin^2 \beta_n \Delta x \lambda_0^2} \geq 1,$$  \hspace{1cm} (5.6.15)

and hence the difference relation (5.6.7) is unstable.

Richtmyer (Reference 14, pp. 132-134) has shown that Eq. (5.6.7) is stable for a fixed ratio $\Delta t/(\Delta x)^2$. The stability criterion is then eventually found to be of the form

$$\Delta t \leq K(\Delta x)^2,$$  \hspace{1cm} (5.6.16)

with $K$ some constant. The increment in $t$ is too small for practical use.

An alternative difference relation for the $P_N$ equations has been suggested by Friedrichs (Reference 14, pp. 135-136). In this method the vector $\psi^l_j$, in Eq. (5.6.7), is replaced by the spatial average, i.e.,

$$\psi^l_j = \frac{1}{2}(\psi^l_{j+1} + \psi^l_{j-1}).$$  \hspace{1cm} (5.6.17)

The resulting difference equation is then

$$\frac{2\psi^{l+1}_j - \psi^l_{j+1} - \psi^l_{j-1}}{2v\Delta t} + \frac{A(\psi^l_{j+1} - \psi^l_{j-1})}{2\Delta x} + \frac{\alpha}{2}(\psi^l_{j+1} + \psi^l_{j-1}) = \frac{vB'}{2} (\psi^l_{j+1} + \psi^l_{j-1}).$$  \hspace{1cm} (5.6.18)

The difference equation (5.6.18) is explicit and the amplification matrix is readily found. Inserting the Fourier expansion for $\psi^l_j$ we have, for the $n$th harmonic,

$$\frac{u^{l+1}_n - \cos \beta_n \Delta x u^l_n}{v\Delta t} + \frac{A}{\Delta x} \sin \beta_n \Delta x u^l_n + \alpha \cos \beta_n \Delta x u^l_n = vB' \cos \beta_n \Delta x u^l_n.$$  \hspace{1cm} (5.6.19)

The amplification matrix is then

$$C(\Delta x, \Delta t) = [(I + v\Delta t(vB' - \alpha)) \cos \beta_n \Delta x - \frac{v\Delta t}{\Delta x} A \cdot \sin \beta_n \Delta x].$$  \hspace{1cm} (5.6.20)

For small $v\Delta t$ and fixed $\Delta t/\Delta x$ we have

$$C(\Delta x, 0) = [I \cos \beta_n \Delta x - \alpha A \sin \beta_n \Delta x].$$  \hspace{1cm} (5.6.21)
Let $\lambda_0$ be the largest eigenvalue of $A$. The eigenvalues of $C(\Delta x, 0)$ are bounded by unity provided

$$\alpha \lambda_0 \leq 1,$$  \hspace{1cm} (5.6.22)

and therefore

$$\Delta t \leq \frac{\Delta x}{\lambda_0 \psi}$$  \hspace{1cm} (5.6.23)

is the stability condition.$^9$

Time dependent problems in the $S_N$ method are solved in a less straightforward manner than considered thus far. In particular, the time dependent difference equations are derived by consideration of the direction of particle flow. Recall from Eqs. (5.5.3) et seq. that the coefficient $a_n$ has the properties

$$a_n > 0, \quad \mu_n > 0;$$

$$a_n < 0, \quad \mu_n \leq 0.$$  

Furthermore, $|a_n|$ increases as $|\mu_n|$ increases. The distance that a particle travels radially in a time $\Delta t$ is dependent upon $|a_n|$. We define the quantity

$$A_t = t_{t+1} - t_t,$$  \hspace{1cm} (5.6.24)

and consider two cases of particle flow:

(a) $|a_n| < \frac{A_j}{v_g A_t}$,  \hspace{1cm} (5.6.25a)

(b) $|a_n| > \frac{A_j}{v_g A_t}$,  \hspace{1cm} (5.6.25b)

where $A_j$ is the space increment and $v_g$ the group speed. The two cases are illustrated in Fig. 5.6.1.

The directional flux at point $C$ must be determined from values at points $A, B, D$ which are assumed known. We consider the two cases separately.

**Case a:** In this case the coefficient $|a_n|$ is small, i.e., $|\mu_n|$ small and hence the neutron does not travel far along the radius vector in a time $A_t$. The direction line $EC$ intersects the line $AB$. We assume the variation of the directional flux is linear in time as well as space and angle. The interpolation points $AB$ should be used for the evaluation of the flux at $C$.

$^9$ We have neglected the effect of terms of $O(\Delta t)$ in the eigenvalue. Richtmyer, in Reference 14, shows that a more general condition of the form $1 + O(\Delta t)$ is sufficient and in some cases necessary.
Case b: In this case \(| a_n |\) is large and hence the neutron travels a large distance along the radius vector in a time \(\Delta l\). The direction line \(EC\) intersects the line \(DA\). The interpolation points \(DA\) should be used to evaluate the flux at \(C\).

Notice that the meaning of \(r_h\) depends upon the sign of \(a_n\). For \(a_n > 0\) neutrons move out along the radius vector and

\[ r_h = r_{j-1}. \]

For \(a_n < 0\) neutrons move inward and hence

\[ r_h = r_{j+1}. \]

In order to approximate the time and space derivatives, we consider the one group, time-dependent analog of Eq. (5.5.3). We have

\[
\left( \frac{1}{v} \frac{\partial}{\partial t} + a_n \frac{\partial}{\partial r} \right) \phi_n(r, t) + \left( \frac{1}{v} \frac{\partial}{\partial t} + \bar{a}_n \frac{\partial}{\partial r} \right) \phi_{n-1}(r, t) = R_n(r, t) \tag{5.6.26}
\]

with \(R_n(r, t)\) given as

\[
R_n(r, t) = c_n S(r, t) - \left( \frac{b_n}{r} + \sigma_t \right) \phi_n(r, t) + \left( \frac{b_n}{r} - \sigma_t \right) \phi_{n-1}(r, t). \tag{5.6.27}
\]

Consider the case \(a\); that is, the \(EC\) intersects the line \(AB\). The space derivative should be evaluated at points \(AB\) along time line \(t_l\). The
V. TRANSPORT METHODS

time derivative should be evaluated along the space line \( r_j \) from points \( BC \). From the approximation of linearity, we have then

\[
\frac{\partial}{\partial r} \phi_n(r, t) = \frac{\phi_n(r_j, t_i) - \phi_n(r_h, t_i)}{\Delta_j},
\]

(5.6.28a)

and

\[
\frac{\partial}{\partial t} \phi_n(r, t) = \frac{\phi_n(r_j, t_{i+1}) - \phi_n(r_j, t_i)}{\Delta_t}.
\]

(5.6.28b)

Conversely, for case b, where the line \( EC \) intersects \( AD \), we should use the following:

\[
\frac{\partial}{\partial r} \phi_n(r, t) = \frac{\phi_n(r_j, t_{i+1}) - \phi_n(r_h, t_{i+1})}{\Delta_j}
\]

(5.6.29)

and

\[
\frac{\partial}{\partial t} \phi_n(r, t) = \frac{\phi_n(r_h, t_{i+1}) - \phi_n(r_h, t_i)}{\Delta_t}.
\]

(5.6.30)

We shall indicate the details for case a. With the above derivatives, Eq. (5.6.26) becomes

\[
\frac{1}{v\Delta_t} [\phi_n(r_j, t_{i+1}) - \phi_n(r_j, t_i)] + \frac{a_n}{\Delta_j} [\phi_n(r_j, t_i) - \phi_n(r_h, t_i)]
\]

\[
+ \frac{1}{v\Delta_t} [\phi_{n-1}(r_j, t_{i+1}) - \phi_{n-1}(r_j, t_i)]
\]

\[
+ \frac{\bar{a}_n}{\Delta_j} [\phi_{n-1}(r_j, t_i) - \phi_{n-1}(r_h, t_i)] = R_n(r, t).
\]

(5.6.31)

One possible approach is to evaluate \( R_n(r, t) \) at \( r_j, t_i \) and solve Eq. (5.6.31) for \( \phi_n(r_j, t_{i+1}) \).

An alternative procedure is usually used however. In particular, the quantity \( R_n(r, t) \) is evaluated at the midpoint of the time-space interval. This makes the resulting equations implicit, but a simple iteration reduces the effort. The midpoint values are given as

\[
R_n(\bar{r}, \bar{t}) = c_n \left[ \frac{S(r_h, t_i) + S(r_j, t_{i+1})}{2} \right]
\]

\[
- \left( b_n - \sigma_t \right) \frac{[\phi_n(r_h, t_i) + \phi_n(r_j, t_{i+1})]}{2}
\]

\[
+ \left( b_n - \sigma_t \right) \frac{[\phi_{n-1}(r_h, t_i) + \phi_{n-1}(r_j, t_{i+1})]}{2}.
\]

(5.6.32)
Inserting Eq. (5.6.32) into (5.6.31) and solving for $\phi_n(r_j, t_{t+1})$ yields

$$
\phi_n(r_j, t_{t+1}) = \frac{1}{1 + (v\Delta_t/2)(b_n/r_j + \sigma_t)} \left\{ 1 - \frac{v\Delta_t a_n}{\Delta_j} \right\} \phi_n(r_j, t_i) \\
+ v\Delta_t \left[ \frac{a_n}{\Delta_j} - \frac{b_n}{2\langle r_j \rangle} - \frac{\sigma_t}{2} \right] \phi_n(r_h, t_i) \\
- \left[ 1 - \frac{v\Delta_t}{2} \left( \frac{b_n}{\langle r_j \rangle} - \sigma_t \right) \right] \phi_{n-1}(r_j, t_{t+1}) + \left[ 1 - \frac{v\Delta_t \bar{a}_n}{\Delta_j} \right] \phi_{n-1}(r_j, t_i) \\
+ v\Delta_t \left[ \frac{\bar{a}_n}{\Delta_j} + \frac{b_n}{2\langle r_j \rangle} - \frac{\sigma_t}{2} \right] \phi_{n-1}(r_h, t_i) \\
+ \frac{v\Delta_t c_n}{2} \left[ S(r_j, t_{t+1}) + S(r_h, t_i) \right].
$$

(5.6.33)

Notice that the only implicit term in Eq. (5.6.33) is the source term. The usual procedure for using equation (5.6.33) is to assume $S(r_j, t_{t+1}) = S(r_j, t_i)$ and compute tentative values for $\phi_n(r_j, t_{t+1})$. The tentative values are then used to recompute $S(r_j, t_{t+1})$, and the final values of $\phi_n(r_j, t_{t+1})$ are computed. The difference expression for case b is readily found to be of the same form.

Although the equation (5.6.33) appears formidable, the coefficients are computed only once. The relation is actually a 5-point equation, save for the source terms, and is easy to use.

No proof of the stability of the $S_N$ difference method has been found thus far. Based upon many experiments at Los Alamos and elsewhere, the method is usually considered to be stable.

5.7 Moments Method

The last method we shall discuss for treating the Boltzmann equation is the moments method, also called the Spencer-Fano method. The moments method is an expansion technique for solving the transport equation in infinite media. The method has been devised to treat the difficult problem of neutron and gamma-ray deep penetration (see References 15–21). As will be noted in Chapter VI, the Monte Carlo treatment of the deep penetration problem is difficult since the expected penetration is small. Direct numerical integration is also difficult for the deep penetration problem since the number of spatial points required is usually very large. The moments method is semi-analytic in nature; the angle, space, and energy variations are treated by polynomial expansion. The series are truncated to obtain the solution. In general the numerical aspects of the
method are simple. The method illustrates the general principle that the analytic work should be carried as far as possible before resorting to the numerics.

We shall apply the method here to the gamma-ray problem and treat the algebraically much more complex neutron problem in Appendix C. Before entering the details, we first outline the motivations for each of the steps involved. Consider the case of a plane shield with an incident plane source of monoenergetic photons. The angular dependence of the flux is to be approximated by a polynomial. The particular expansion polynomials are the Legendre polynomials, $P_n(\mu)$, as used in the spherical harmonics method. By using the series expansion for the directional flux, an infinite series of equations for the expansion coefficients results. Note that the expansion coefficients will be functions of position and energy. In general, shielding calculations are performed in order to find the nondirectional flux at any point, and hence the zeroth moment of the expansion is of primary interest. The nondirectional flux is next expanded in a simple power series $x^n$, $n = 0, 1, ...$, to compute the coefficients of the spatial powers, which are in turn functions of energy. The resultant expression is then solved for the coefficients. With these preliminary remarks, we now move into the details.

The transport equation for photons is (see Appendix A)

$$\mathbf{\Omega} \cdot \nabla \phi(x, \Lambda, \mathbf{\Omega}) + \sigma(x, \Lambda) \phi(x, \Lambda, \mathbf{\Omega})$$

$$= \frac{1}{2\pi} \int_0^\Lambda d\Lambda' \int_4\pi d\mathbf{\Omega}' K(\Lambda', \Lambda) \delta[1 + (\Lambda' - \Lambda) - \mathbf{\Omega}' \cdot \mathbf{\Omega}] \phi(x, \Lambda', \mathbf{\Omega}')$$

$$+ S(x, \Lambda, \mathbf{\Omega}) , \quad (5.7.1)$$

where $K(\Lambda', \Lambda)$ is given by Eq. (A.40).

The first step in the analysis is to expand the directional flux in the Legendre polynomials. The details of method have been indicated in Section 5.1 so we shall merely state the result of the transformation. For plane geometry we have

$$\phi(x, \Lambda, \mu) = 2\pi \phi(x, \Lambda, \mathbf{\Omega}) , \quad (5.7.2)$$

and

$$\phi(x, \Lambda, \mu) = \sum_{n=0}^{\infty} \frac{2n + 1}{2} \phi_n(x, \Lambda) P_n(\mu) , \quad (5.7.3a)$$

with

$$\phi_n(x, \Lambda) = \int_{-1}^{1} d\mu \phi(x, \Lambda, \mu) P_n(\mu) . \quad (5.7.3b)$$
By inserting (5.7.3a) into the transport equation and following the steps outlined before, we obtain

\[
\frac{n + 1}{2n + 1} \frac{d}{dx} \phi_{n+1}(x, A) + \frac{n}{2n + 1} \frac{d}{dx} \phi_{n-1}(x, A) + \sigma(x, A) \phi_{n}(x, A) = S_n(x, A) + \int_{0}^{A} dA' P_{n}(1 + A' - A) K(A', A) \phi_{n}(x, A') \tag{5.7.4}
\]

Note that the argument of the Legendre polynomial is given in terms of \(A, A'\) by virtue of the Compton relation (A.36).

We now desire to eliminate the spatial dependence to find an equation for coefficients as functions of energy only. To this end, we expand \(\phi_{n}(x, A)\) in a power series in \(x\). We define the expansion coefficients \(\phi_{jn}(A)\) as

\[
\phi_{jn}(A) = \alpha_{j} \int_{-\infty}^{\infty} dx \, x^{j} \phi_{n}(x, A),
\]

where the coefficient \(\alpha_{j}\) will be obtained subsequently. These coefficients are arbitrary to this point, but will be chosen to simplify the equation that determines the moments. To find an equation relating the \(\phi_{jn}(A)\), we multiply both sides of Eq. (5.7.4) by \(\alpha_{j} x^{j}\) and integrate. To treat the left-hand side, we consider the general expression

\[
\alpha_{j} \int_{-\infty}^{\infty} dx \, x^{j} \frac{d}{dx} \phi_{n}(x, A) = \alpha_{j} \left[ x^{j} \phi_{n}(x, A) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx \, \frac{d}{dx} \phi_{n}(x, A) j x^{j-1},
\]

where we have integrated by parts. In order to continue, we must require that \(x^{j} \phi_{n+1}(x, A)\) vanish at \(\pm \infty\). Therefore, we must assume we have an infinite medium. (This assumption of an infinite medium is one of the most serious limitations of the moments method.) Then we find that

\[
\alpha_{j} \int_{-\infty}^{\infty} dx \, x^{j} \frac{d}{dx} \phi_{n}(x, A) = - \frac{j \alpha_{j}}{\alpha_{j-1}} \phi_{j-1, n}(A). \tag{5.7.7}
\]

In order to integrate the term \(\sigma(x, A) \phi_{n}(x, A)\), we make the second major assumption of the moments method, i.e., the medium is homogeneous so that \(\sigma(x, A)\) is only a function of \(A\). We then have

\[
\alpha_{j} \int_{-\infty}^{\infty} dx \, x^{j} \sigma(A) \phi_{n}(x, A) = \sigma(A) \phi_{j, n}(A). \tag{5.7.8}
\]

To find the right-hand side, we recall that the source was assumed plane and monoenergetic, i.e., \(S_{n}(x, A) = S_{n}(A) \delta(x) = S_{n} \delta(A - A_{0}) \delta(x)\).
Finally, the last term of the right-hand side is
\[
\int_0^A d\Lambda' P_n(1 + \Lambda' - \Lambda) K(\Lambda', \Lambda) \alpha_j \int_{-\infty}^{\infty} dx x^i \phi_n(x, \Lambda')
\]
\[
= \int_0^A d\Lambda' P_n(1 + \Lambda' - \Lambda) K(\Lambda', \Lambda) \phi_{jn}(\Lambda').
\]

Collecting terms and transposing, we have
\[
\sigma(\Lambda) \phi_{jn}(\Lambda) = \alpha_j S_n \delta(\Lambda - \Lambda_0) \delta_{j0} + \int_0^A d\Lambda' P_n(1 + \Lambda' - \Lambda) K(\Lambda', \Lambda) \phi_{jn}(\Lambda')
\]
\[
+ \frac{1}{2n + 1} \frac{j \alpha_j}{\alpha_{j-1}} [(n + 1) \phi_{j-1, n+1}(\Lambda) + n \phi_{j-1, n-1}(\Lambda)].
\]

To find the coefficient \( \alpha_j \) from a dimensional analysis of each term of Eq. (5.7.11), we note that \( \alpha_j/\alpha_{j-1} \) must have the dimensions of \((\text{length})^{-1}\). We now choose the arbitrary coefficients \( \alpha_j \): the choice
\[
\frac{j \alpha_j}{\alpha_{j-1}} = \sigma(\Lambda_0) \equiv \sigma_0, \quad j \geq 1, \quad \alpha_0 = \sigma_0,
\]
leads to a simple result. We find that
\[
\alpha_j = \frac{(\sigma_0)^{j+1}}{j!}.
\]

Finally we have
\[
\sigma(\Lambda) \phi_{jn}(\Lambda) = \int_0^A d\Lambda' P_n(1 + \Lambda' - \Lambda) K(\Lambda', \Lambda) \phi_{jn}(\Lambda')
\]
\[
+ \frac{\sigma_0^{j+1}}{j!} S_n \delta(\Lambda - \Lambda_0) \delta_{j0} + \frac{\sigma_0}{2n + 1} [(n + 1) \phi_{j-1, n+1}(\Lambda) + n \phi_{j-1, n-1}(\Lambda)].
\]

To compute \( \phi_{jn}(\Lambda) \) requires some simple numerical steps; however, before considering the actual computation, we first discuss the properties of the Eq. (5.7.14).

Of primary importance is the nature of the coupling between various coefficients. Notice that \( \phi_{jn}(\Lambda) \) is a function only of the coefficients with indices \( j, n; j - 1, n - 1; \text{ and } j - 1, n + 1 \). Thus the coefficients for a given \( j, n \) can be computed without truncation of a series in contradiction to the usual \( P_n \) method. This result greatly simplifies application of
the moments method since computations with higher order approxima-
tions merely require calculation of the additional coefficients.

We can exploit a feature of the present problem to greatly simplify the
numerical analysis. The integral term involves integration from
\( \Lambda' = 0 \) to \( \Lambda \), i.e., the range of integration is limited due to the fact that
photons only down scatter in energy. The evaluation of the \( \phi_{jn}(\Lambda) \) can
consequently be accomplished without iteration.

We now consider the detailed steps in evaluating the coefficients
\( \phi_{jn}(\Lambda) \). For simplicity we assume the source is isotropic, and hence
\( S_n = 0, n \neq 0 \). The coefficients at \( \Lambda = \Lambda_0 \) are found as described
below.

Figure 5.7.1 displays the order in which the coefficients may be found.
From this figure it is seen that

\[
\begin{align*}
\phi_{jn}(\Lambda_0) &\neq 0 & \text{if } j \geq n \text{ and if } j + n = \text{even integer}, \\
\phi_{jn}(\Lambda_0) &= 0 & \text{if } j < n \text{ or } j + n = \text{odd integer}.
\end{align*}
\]

![Diagram](image)

**Fig. 5.7.1.** The \( j,n \) plane for \( \Lambda = \Lambda_0 \) showing the linkage between nodes
according to Eq. (5.7.14). Nonzero points for a plane, monoenergetic, isotropic
source are indicated by arrows pointing away from or towards points. The arrows
indicate the relationships between nodes. The value of \( \phi_{jn} \) at the node \((n,j)\)
may be found from the \( \phi_{j' n'} \) at the nodes at the heads of the arrows pointing away
from the node \((n,j)\).

In deriving these results, it is simplest to start with the case of \( j = 0 \)
and determine all \( \phi_{0,n} \) using Eq. (5.7.14). Next we examine \( \phi_{1,n} \), all \( n \),
with Eq. (5.7.14) and so on. Of course, one does not compute more
\( \phi_{jn}(\Lambda_0) \) than are needed. To this end, we remark that symmetries can
frequently be exploited to reduce the number of nonzero coefficients.

In order to find further values, we must approximate the integral
term in Eq. (5.7.14). The kernel \( P_n(1 + \Lambda' - \Lambda)K(\Lambda', \Lambda) \) is a simple
polynomial in $\lambda'$ which can be accurately approximated. If a series of values of $\lambda$, say $\lambda_g$, be picked, then the integral can be written

$$\int_{\lambda_0}^{\lambda} d\lambda' P_n(1 + \lambda' - \lambda) K(\lambda', \lambda) \phi_{jn}(\lambda') \approx \sum_{g' = 0}^{g} H_n(g', g) \phi_{jn}(g'),$$  \hspace{1cm} (5.7.15)$$

where the $H_n(g', g)$ are weighting coefficients and depend upon the quadrature formula used. As an example, for the first step we shall use the trapezoidal rule, and Simpson’s rule for each step thereafter. Thus, we have

$$\int_{\lambda_0}^{\lambda} d\lambda' P_n(1 + \lambda' - \lambda) K(\lambda', \lambda) \phi_{jn}(\lambda')$$

$$\approx [P_n(1 + \lambda_0 - \lambda_1) K(\lambda_0, \lambda_1) \phi_{jn}(\lambda_0) + P_n(1) K(\lambda_1, \lambda_1) \phi_{jn}(\lambda_1)] \frac{\Delta \lambda}{2},$$  \hspace{1cm} (5.7.16)$$

in which we note that $P_n(1) = 1$ and $K(\lambda_1, \lambda_1) = 2\pi(1)(e^2/mc^2)^2$ [see Eq. (A.40)]. Similarly, for an even number of intervals of integration, we can use Simpson’s rule and find

$$\int_{\lambda_0}^{\lambda} d\lambda' P_n(1 + \lambda' - \lambda) K(\lambda', \lambda) \phi_{jn}(\lambda')$$

$$\approx \frac{\Delta \lambda}{3} [P_n(1 + \lambda_0 - \lambda_g) K(\lambda_0, \lambda_g) \phi_{jn}(\lambda_0)$$

$$+ 4P_n(1 + \lambda_1 - \lambda_g) K(\lambda_1, \lambda_g) \phi_{jn}(\lambda_1) + ...$$

$$+ P_n(1) K(\lambda_g, \lambda_g) \phi_{jn}(\lambda_g)].$$  \hspace{1cm} (5.7.17)$$

We remark that for $\lambda' < \lambda - 1$, the kernel $K(\lambda', \lambda)$ is zero, and hence the integration is significantly simplified.

Regardless of the quadrature formula used, it is always possible to write the integral in Eq. (5.7.16) in the form

$$\int_{\lambda_0}^{\lambda} d\lambda' P_n(1 + \lambda' - \lambda) K(\lambda', \lambda) \phi_{jn}(\lambda')$$

$$\approx H_n(g, g) \phi_{jn}(\lambda_g) + \sum_{g' = 0}^{g-1} H_n(g', g) \phi_{jn}(\lambda_g),$$  \hspace{1cm} (5.7.18)$$

and hence solve Eq. (5.7.14) in the form

$$\phi_{jn}(\lambda_g) = \frac{1}{\sigma(\lambda)} - H_n(g, g) \left[ \sum_{g' = 0}^{g-1} H_n(g', g) \phi_{jn}(\lambda_{g'}) + \frac{\sigma_{g+1}}{j!} S_n \delta(\lambda_g - \lambda_0) \delta_{j0}$$

$$+ \frac{\sigma_g}{2n + 1} [(n + 1) \phi_{j-1,n+1}(\lambda) + n \phi_{j-1,n-1}(\lambda)] \right].$$  \hspace{1cm} (5.7.19)$$
The weighting coefficients are universal and may be computed once and for all, or else generated when needed. The computational process is straightforward; one first computes for \( g = 0 \). One then goes to \( g = 1 \) and computes the needed portion of the \( j, n \) plane. The details are as before.

To this point the analysis has been on obtaining the expansion coefficients \( \phi_{jn}(\Lambda_y) \). We now address ourselves to the problem of deriving expressions for the flux in terms of the \( \phi_{jn}(\Lambda_y) \). In particular, we consider the calculation of \( \phi_n(x, \Lambda_y) \). One possibility is a simple polynomial expansion of the form

\[
\phi_n(x, \Lambda_y) = \sum_{j=0}^{j} \alpha_{j,n}(\Lambda_y) x^j, \quad (5.7.20)
\]

where the \( \alpha_{j,n} \) are to be determined from the known moments \( \phi_{jn}(\Lambda_y) \). An expansion such as Eq. (5.7.20) is limited to a certain range of \( x \) since for very deep penetrations the number of terms necessary becomes prohibitive.

A better approach is to assume the spatial behavior of the flux is given predominantly by some function of \( f(x) \); then we may assume an expansion in the form

\[
\phi_n(x, \Lambda_y) = f(x) \sum_{j=0}^{j} \alpha_{j,n}(\Lambda_y) x^j, \quad (5.7.21)
\]

where the summation represents a modulation of the predominant behavior. The hope is that for a properly chosen \( f(x) \), we need only a few terms in the series expansion. In practice it is convenient to use an expansion in the form

\[
\phi_n(x, \Lambda_y) = f(x) \sum_{j=0}^{j} b_{j,n}(\Lambda_y) p_j(x), \quad (5.7.22)
\]

where the \( p_j(x) \) are polynomials of degree \( j \) in \( x \). The purpose is to select the \( p_j(x) \) as orthogonal polynomials with respect to the weighting function \( f(x) \), i.e.,

\[
\int dx p_j(x) f(x) p_k(x) = \delta_{jk} . \quad (5.7.23)
\]

Such a choice facilitates the calculation of the coefficients \( b_{n,j} \). (We remark that not all weight functions possess a set of orthogonal polynomials; however, an adjoint set of polynomials \( p_j^*(x) \) may be defined such that a relation similar to Eq. (5.7.23) exists.)
As an example of the utility of the above approach, we consider the following physically reasonable case: for deep penetrations the flux to first order is given by the unscattered contribution, and so we use the weighting function

\[
\begin{align*}
  f(x) &= e^{-\sigma_0 x}; \quad x > 0; \\
  f(x) &= 0; \quad x < 0; \\
\end{align*}
\]

(5.7.24)

where the quantity \( \sigma_0 \) is the total macroscopic cross section at the energy of the source, assumed monoenergetic, in the expansion (5.7.23). The orthogonal expansion polynomials are then the Laguerre polynomials \( L_j(\sigma_0 x) \). (See Appendix D.)

To determine the coefficients \( b_{j,n}(A_g) \), we proceed as follows: we rewrite Eq. (5.7.22) in the form

\[
\phi_n(x, A_g) = e^{-\sigma_0 x} \sum_{j=0}^j b_{j,n}(A_g) L_j(\sigma_0 x). 
\]

(5.7.25)

We multiply by \( L_k(\sigma_0 x) \) and integrate to obtain

\[
b_{j,n}(A_g) = \int_0^\infty dx \phi_n(x, A_g) L_j(\sigma_0 x). 
\]

(5.7.26)

We recall that the coefficients \( \phi_{j,n}(A_g) \) are defined as

\[
\phi_{j,n}(A_g) = \frac{\sigma_0^{j+1}}{j!} \int_0^\infty dx \phi_n(x, A_g) x^j.
\]

(5.7.27)

Obviously we can expand \( L_j(\sigma_0 x) \) in terms of \( x \) and find the relation between \( b_{j,n}(A_g) \) and the \( \phi_{j,n}(A_g) \). Without performing the details, it is evident that a relation of the form

\[
b_{j,n}(A_g) = \sum_{k=0}^j \gamma_k \phi_{k,n}(A_g),
\]

(5.7.28)

is obtained, where the \( \gamma_k \) are known. Equation (5.7.26) is then the desired result. Other expansions give rise to different series, but are computed the same way.

The procedures for testing the expansions are very interesting. The first crude test is to see if higher terms in \( j \) contribute significantly. After the magnitude of \( b_{j,n} \) is sufficiently small, the series is truncated. The amount of truncation error acceptable depends upon the nature of the problem under investigation.
A second procedure is to study the effect of the weighting function for a fixed number of terms. Let us assume the weight function $e^{-na^2}$ has been used and the number of terms $J$ determined by some truncation criterion. If $J$ is sufficiently large, then the results should be relatively independent of $a_0$. That is, for a large enough number of terms, the weight function may be varied and the computed results should still agree to within a small tolerance. In practice, the coefficient $a_0$ is modified to $a_0 \alpha$, and $\alpha$ is varied near $\alpha = 1$ (hence the test is called an $\alpha$ test). In the region of $\alpha$ where the results are the same to within a small error, one concludes the expansion is valid. Further variations and applications of the moments method are found in the references.

References

There are several excellent books that deal with the neutron transport equation, the spherical harmonics expansion, and other procedures. References 1, 2, and 3 are particularly recommended. The spherical harmonics and other orthogonal series are considered in 4. The remaining references relate to special items discussed in the text. An excellent collection of the coefficients for use in the $S_n$ method for various geometries may be found in reference 13. Reference 14 contains an excellent discussion of the solution of transient problems involving the transport equation. References 15–21 contain both the basic derivation of the moments method and many detailed examples of the use of the technique.


**Problems**

1. Show that

\[ \hat{\phi}_{+1}(r, t, v) = \sqrt{\frac{3}{8\pi}} \left[ \pm J_2(r, t, v) - i J_3(r, t, v) \right] , \]

\[ \hat{\phi}_{0}(r, t, v) = \sqrt{\frac{3}{4\pi}} J_1(r, t, v) , \]

\( J(r, t, v) \) being the current of neutrons at point \( r \), at time \( t \) of speed \( v \), as defined by Eq. (A.11). Express the directional flux in terms of the scalar flux and the current. This expression is accurate, of course, only to zeroth and first order.

2. Derive the diffusion equation from the \( P_1 \) approximation.

3. Derive the spherical harmonic expansion in three dimensions. To this end, expand the directional flux as follows:

\[ \phi(r, t, v, \Omega) = \sum_{\mu=\lambda=-\infty}^{\infty} \sum_{\nu} Y_{\nu}^{\lambda}(\mu, \varphi) \phi_{n}^{\nu}(r, t, v) . \]

Expand the source rate density similarly. Prove that

\[ \Omega \cdot \nabla = \sin \theta \cos \varphi \frac{\partial}{\partial x} + \sin \theta \sin \varphi \frac{\partial}{\partial y} + \cos \theta \frac{\partial}{\partial z} \]

Next, show that

\[ - \left[ \frac{1}{v} \frac{\partial}{\partial t} + \sigma(v) \right] \hat{\phi}_{1}^{\mu}(r, t, v) + S_{1}^{\mu}(r, t, v) \]

\[ + 2\pi \int_{0}^{\infty} dv' f_i(v', v) c(v') \sigma(v') \hat{\phi}_{1}^{\mu}(r, t, v') \]
where

\[ -l \leq m \leq l, \quad f(v', v) = \int_{-1}^{1} d(\cos \Theta_0) P_l(\cos \Theta_0) f(v', v, \Theta_0), \]

and \( f(v', v, \Theta_0) \) is the probability of a neutron of speed \( v' \) being scattered through the angle \( \Theta_0 \) in the laboratory system and emerging with a speed \( v \).

The following relations will be useful in the above derivation:

\[
N_n^k P_n^k(\mu) \frac{e^{ik(k+1)}}{2} \sin \theta
= \frac{1}{2} \left[ \sqrt{\frac{(n + k + 2)(n + l + 1)}{(2n + 3)(2n + 1)}} \ Y_{n+1}^{k+1}(\Omega) - \sqrt{\frac{(n - k)(n - k - 1)}{(2n + 1)(2n - 1)}} \ Y_{n-1}^{k+1}(\Omega) \right].
\]

\[
N_n^k P_n^k(\mu) \frac{e^{ik(k-1)}}{2} \sin \theta
= \frac{1}{2} \left[ \sqrt{\frac{(n - k + 2)(n - k + 1)}{(2n + 1)(2n + 3)}} \ Y_{n+1}^{k-1}(\Omega) + \sqrt{\frac{(n + k - 1)(n + k)}{(2n + 1)(2n - 1)}} \ Y_{n-1}^{k-1}(\Omega) \right].
\]

\[
N_n^k P_n^k e^{ik\varphi} \cos \theta
= \sqrt{\frac{(n + k)(n - k)}{(2n + 1)(2n - 1)}} \ Y_{n-1}^{k}(\Omega) + \sqrt{\frac{(n + k + 1)(n - k + 1)}{(2n + 3)(2n + 1)}} \ Y_{n+1}^{k}(\Omega).
\]

\[
N_n^k = \sqrt{\frac{(2n + 1)(n - k)!}{4\pi(n + k)!}}.
\]

\[ Y_n^k(\mu, \varphi) = N_n^k P_n^k(\mu) e^{ik\varphi}. \]

4. Find the propagation constants in the \( P_1 \) and \( P_3 \) approximations for one-dimensional problems. In other words, find \( \kappa \) in the solutions \( \phi_i = c_i e^{i\xi z} \) of the homogeneous parts of the \( P_1 \) or \( P_3 \) equations. Express the directional flux in terms of \( \phi_0 \) and \( \phi_1 \) in the \( P_1 \) approximation and in terms of \( \phi_0, \phi_1, \phi_2, \) and \( \phi_3 \) in the \( P_3 \) approximation.
5. Find the flux in the \( P_3 \) approximation for an infinite, isotropic plane source at \( z = 0 \) in an infinite medium.

6. Show that the condition (5.1.14) implies equality of each coefficient of the expansion (5.1.4).

7. Find the directional flux in the \( P_3 \) approximation and the extrapolation length for a nonabsorbing, isotropically scattering, homogeneous medium that fills the half space to the right of the origin. Vacuum occupies the space to the left of the origin. The extrapolation distance is the distance from the interface at which the asymptotic component of the nondirectional flux extrapolates linearly to zero. Assume a source of neutrons far to the right in the scattering medium. This source creates a current that travels towards the left.

8. Show that the second order double \( P_n \) approximation is as follows:

\[
D_{\pm}\phi_{\pm} + \frac{1}{2} \frac{d}{dx} \phi_{\pm} = \frac{1}{2} \sigma \left[ \phi_0^+ + \phi_0^- \right] + S_0,
\]

\[
\frac{1}{2} \frac{d\phi_0^\pm}{dx} + 3D_{\pm}\phi_1^\pm + \frac{d}{dx}\phi_2^\pm = 0,
\]

\[
\frac{d}{dx}\phi_1^\pm + 5D_{\pm}\phi_2^\pm = 0,
\]

where \( D_{\pm} = \pm \frac{1}{2} \frac{d}{dx} + \sigma \); and

\[
\left[ 3D_+^2 - \frac{9}{20} D_+ \frac{d^2}{dx^2} \right] \phi_0^\pm = \left[ 3D_+^2 - \frac{1}{5} \frac{d^2}{dx^2} \right] \sigma \left[ \frac{\phi_0^+ + \phi_0^-}{2} \right] + S_0,
\]

and

\[
\left[ \frac{d^4}{dx^4} + (24\sigma_0 - 84\sigma) \sigma \frac{d^4}{dx^4} + \left( 420\sigma_0 - \frac{860}{3} \sigma_0 \right) \sigma^3 \frac{d^2}{dx^2} + 400(\sigma_0 - \sigma) \sigma^2 \right] \left[ \frac{\phi_0^+ + \phi_0^-}{2} \right] = \left[ -24\sigma^2 \frac{d^4}{dx^4} + \frac{860}{3} \sigma^4 \frac{d^2}{dx^2} - 400\sigma \right] S_0.
\]

9. Solve Milne's problem in the \( P_4^+ \) approximation. The Milne problem consists of a pure scatterer filling half of all space and a vacuum in the other half of all space. Mono-energetic neutrons are incident upon the interface from the medium and leak out. The problem is to find the directional flux within the medium. Suppose that the medium fills the right half of all space. Note that the solution of an ordinary differential equation with constant coefficients consists of a linear combination of exponentials with arguments that must be determined plus a particular solution. This particular solution is a linear function of \( x \), because the coefficient of \( \phi_0^+ + \phi_0^- \) vanishes in our present case. Assume then the solution in the form

\[
\phi = c_1 + c_2 x + c_3 e^{-\kappa x}.
\]

(a) Show that the characteristic equation for the roots is \( \kappa = \sqrt{12} \sigma \).

(b) Why may one of the coefficients \( c_1, c_2, c_3 \) be arbitrarily chosen? Pick \( c_2 = 1 \).
PROBLEMS 235

(c) What boundary conditions must be satisfied? Express these conditions in terms of \( \phi^0(0), \phi^1(0) \), where \( x = 0 \) is the plane of the interface.

(d) Find the \( c_i \).

(e) Choose \( \phi^0(x) = B_{10}^+ + B_{20}^+ \alpha x + B_{20}^+ \epsilon^{-\alpha x}; \phi^1(x) = B_{10}^+ + B_{21}^+ \alpha x + B_{21}^+ \epsilon^{-\alpha x} \). Show that:

\[
B_{21}^+ = 0, \quad B_{20}^+ = 1
\]

\[
B_{10}^+ = c_1 + \frac{1}{2}
\]

\[
B_{11}^+ = -\frac{1}{6}
\]

\[
B_{30}^+ = \frac{(\mp \kappa/2 + \sigma) c_3 \sigma}{(\mp \kappa/2 + \sigma)^2 - \kappa^2/12}
\]

\[
B_{31}^+ = \frac{(\kappa/6) c_3 \sigma}{(\pm \kappa/2 + \sigma)^2 - \kappa^2/12}
\]

\[
\begin{cases}
B_{30}^+ + B_{10}^+ = 0 \\
B_{31}^+ + B_{11}^+ = 0
\end{cases}
\]

(f) Find \( c_1, c_3, B_{30}^-, B_{31}^- \) and show that

\[
n = 0.71132 + \alpha x - 0.13397 \exp(-3.464 \alpha x),
\]

\[
n^{-0, \mu} = \frac{1}{4\pi} \left[ c_1 + \frac{1}{2} + B_{30}^- + 3(2\mu + 1)(-\frac{1}{6} + B_{31}^-) \right].
\]

10. Show that the weight factors \( w_i \) in Eq. (5.4.10) are positive.

11. Show that the truncation error in the \( S_n \) method is reduced by spatially integrating in the direction in which the neutrons travel. Consider the problem of neutron penetration of a thick slab on which a current \( J_i \) is incident, in which \( S \) is the source density, and from which a current \( J_e \) emerges. Let \( E \) be the attenuation of neutrons through the slab. Relate \( J_e, J_i, E, \) and \( S \) to each other for the two directions and consider the errors resulting in the answer for small errors in the independent variables.

12. Show that in the \( S_2 \) approximation in which the intervals are equal

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \phi_n )</th>
<th>( \phi_{n-1} )</th>
<th>( \mu_n )</th>
<th>( a_n )</th>
<th>( \bar{a}_n )</th>
<th>( b_n )</th>
<th>( c_n )</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( \phi_0 )</td>
<td>0</td>
<td>(-1 )</td>
<td>(-1 )</td>
<td>0</td>
<td>1</td>
<td></td>
<td>(5.5.8)</td>
</tr>
<tr>
<td>1</td>
<td>( \phi_1 )</td>
<td>( \phi_0 )</td>
<td>0</td>
<td>(-\frac{1}{3} )</td>
<td>(-\frac{2}{3} )</td>
<td>\frac{4}{3}</td>
<td>2</td>
<td>(5.5.8)</td>
</tr>
<tr>
<td>2</td>
<td>( \phi_2 )</td>
<td>( \phi_1 )</td>
<td>(-1 )</td>
<td>\frac{2}{3}</td>
<td>\frac{1}{3}</td>
<td>\frac{4}{3}</td>
<td>2</td>
<td>(5.5.9)</td>
</tr>
</tbody>
</table>
and in the $S_1$ approximation in which all intervals are equal

\[
\begin{array}{cccccc}
n & \phi_n & \phi_{n-1} & \mu_n & a_n & b_n & c_n & \text{Equation} \\
0 & \phi_0 & 0 & -1 & -1 & 0 & 1 & (5.5.8) \\
1 & \phi_1 & \phi_0 & -1 & -2 & -5 & 5 & 2 (5.5.8) \\
2 & \phi_2 & \phi_1 & 0 & -1 & -11 & 3 & 2 (5.5.8) \\
3 & \phi_3 & \phi_2 & +1 & +1 & 1 & 11 & 2 (5.5.9) \\
4 & \phi_4 & \phi_3 & +1 & +5 & 2 & 5 & 2 (5.5.9)
\end{array}
\]

13. Find the coefficients $a_{ni}$, $b_{ni}$, $c_{ni}$, $d_{ni}$, $a'_{ni}$, $b'_{ni}$, $c'_{ni}$, $d'_{ni}$ in Eqs. (5.5.8) and (5.5.9).

14. The modifications due to anisotropic scattering are to be explored in this problem. Let us assume one dimensional geometry and let this one spatial dimension be specified by $r$. The source $S$ will be a function $S(r, \mu)$ of both $r$ and the cosine $\mu$ between the radius vector $r$ and the velocity $v$ of the neutron, and we assume there are no external sources not proportional to the flux. Define

\[
P_{n,\alpha} = \int_{\mu_{n-1}}^{\mu_n} d\mu' P_{\alpha}(\mu')
\]

\[
s'_{\gamma'\gamma} = \int_{-1}^{1} d\bar{\mu} s'_{\gamma'\gamma}(\bar{\mu}) P_{\alpha}(\bar{\mu}).
\]

Let $a_{\alpha n'}$ be a coefficient such that

\[
\phi^i(r) = \sum_{\alpha, n'} a_{\alpha n'} \phi^i_{n'}(r),
\]

where $\phi^i_{n'}(r)$ is a spherical harmonic component of the directional flux as given by Eq. (5.1.4) and $\phi^i(r)$ is an $S_n$ component of the directional flux as given by Eqs. (5.5.2) and (5.5.2a). In other words, $[a_{\alpha n}]$ is the matrix transforming the $S_n$ components of the directional flux into the spherical harmonic components. Show that

\[
S_n^\epsilon(r) = \frac{1}{4\pi} \sum_{\xi'} \int_{\mu_{n-1}}^{\mu_n} d\mu \int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\phi' a_{\epsilon\xi'}(\hat{\mu}) \phi^{\epsilon'}(r, \mu')
\]

\[
= \sum_{\gamma'} \sum_{\alpha=0}^{\infty} \sum_{n'=0}^{\infty} P_{n\alpha} s'_{\gamma'\gamma} 2\alpha + \frac{1}{4} a_{\alpha n} \phi^{\epsilon'}_{n'}(r), \quad n = 0, 1, 2, ..., N.
\]
Show for the $S_2$ approximation that

$$
\begin{align*}
S^{s''}_2(r) &= \begin{bmatrix}
1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
\sigma^{s''}_{s0} & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\frac{1}{8} & 1 & \frac{1}{8}
\end{bmatrix}
\begin{bmatrix}
\phi^{s''}_0(r)
\end{bmatrix},
\end{align*}
$$

$S^{s''}_1(r) = \begin{bmatrix}
1 & -\frac{1}{2} & 0
\end{bmatrix}
\begin{bmatrix}
0 & \sigma^{s''}_{s1} & 0
\end{bmatrix}
\begin{bmatrix}
-\frac{1}{4} & 0 & \frac{1}{4}
\end{bmatrix}
\begin{bmatrix}
\phi^{s''}_1(r)
\end{bmatrix},
$$

$S^{s''}_2(r) = \begin{bmatrix}
1 & -\frac{1}{2} & 0
\end{bmatrix}
\begin{bmatrix}
0 & 0 & \sigma^{s''}_{s2}
\end{bmatrix}
\begin{bmatrix}
\frac{5}{32} & -\frac{5}{16} & \frac{5}{32}
\end{bmatrix}
\begin{bmatrix}
\phi^{s''}_2(r)
\end{bmatrix}
$$

where $S^{s''}_n(r)$ is such that

$$
S_n^{s''}(r) = \sum_{s'} S^{s''}_n(r).
$$

Note that $S^{s''}_n(r) = S^{s''}(r, -1)$. This source is now used in the $S_n$ approximation as the source term.

15. Formulate the $S_n$ method in matrix form as a generalized eigenvalue problem.

16. Construct a flow diagram of the $S_2$ method of calculating the critical size of a sphere consisting of two different material regions, a multiplicative core and a nonmultiplicative reflector. Use 15 zones in the core and 10 in the reflector, and 3 speed groups. Test for convergence by use of a source at the center. Assume all data needed are in fast memory. In each box where a calculation is to be made, indicate the symbol for the quantity to be calculated and write the formula number in the box used to calculate the symbol. The logic, control, tests used, transfers, and the like are to be indicated on the flow diagram. Do not diagram the calculation of the formulas themselves.

17. Show that Eq. (5.5.26) is satisfied upon summing Eq. (5.5.21) over all $n$ if the $b_n$ satisfy Eq. (5.5.27).

18. Work out the time independent $S_n$ method for plane geometry. Develop the time dependent $S_n$ method for spherical geometry.

19. Find a dual between the time dependent $S_n$ method for the transport equation for infinitely long cylindrical geometry and the time dependent, multispeed transport equation for spherical geometry. Establish a duality between the time independent transport equation for an infinite cylinder and the time independent multispeed transport equation for spherical geometry.

20. The purpose of this problem is the development of the $S_n$ method for cylindrical geometry. Note the expression for $\Omega \cdot \nabla \phi$ from problem 3 of Appendix A. Assume an isotropic source density $S(r, z, t, v)$. Show that

$$
S(r, z, t, v) = \frac{1}{2n} \sum_{s'} \sigma^{s''} \int_{-1}^{1} d\mu' \int_{-1}^{1} \frac{d\gamma' \phi(r, z, \eta', t, \nu', \mu')}{\sqrt{1 - \eta'^2}}.
$$

Write down the appropriate time independent transport equation for cylindrical geometry and establish a dual between it, suitably quantized, and the time dependent, multispeed, transport equation for spherical geometry by
putting related variables into correspondence. Use the Gauss quadrature formula for the angle variable not treated by the $S_n$ approximation. Determine the order of the Gauss quadrature, i.e., the number of roots required and the order of the corresponding Legendre polynomial, to be consistent with the $S_n$ approximation.