

# ENERGY AND TIME DISCRETIZATION

## Chapter 2

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### 2-1 INTRODUCTION

The forms of the transport equation derived in Chapter 1 establish a basis for proceeding to the following two classes of computational methods: deterministic and Monte Carlo. The stochastic techniques that constitute Monte Carlo methods are treated in Chapter 7. In this and the following four chapters we treat the variety of methods by which the transport equation is discretized and solved deterministically.

In the following sections, we first apply the energy discretization procedure that is common to virtually all deterministic computational methods: the multi-energy-group approximation.<sup>1,2</sup> We then consider the multigroup equations for time-independent fixed source problems, for criticality or eigenvalue problems, and for problems in which time dependence appears explicitly. The remainder of the chapter is devoted to the discussion of solution algorithms for each of these classes of equations. In each case the algorithms involve the repeated solution of fixed source within-energy-group equations from which explicit time and energy dependence have been removed. Treatment of space and angle, the independent variables of the within-group equations, is the subject of Chapters 3 through 6.

### 2-2 THE MULTIGROUP EQUATIONS

The discretization of the energy variable with the multigroup approximation may proceed from one of several starting points. The time-independent fixed source equation (Eq. 1-106), the  $\alpha$  or the  $k$  eigenvalue equations (Eqs. 1-109 and 1-110), or the kinetics equations (Eqs. 1-101 and 1-102) are all suitable points of departure depending on the application under consideration. We choose, for our examples, the time-independent fixed source equation, since it is applicable to both nonmultiplying and subcritical

systems, while at the same time it can be simply modified by setting  $q_{ex} = 0$  and replacing  $\nu$  by  $\nu/k$  to obtain the multiplication eigenvalue form. These two forms of the equations account for the vast majority of transport calculations. Hence we merely state the multigroup forms of the time absorption and kinetic equations with the parallel derivations left as an exercise for the reader.

For our starting point, then, we choose Eq. 1-106:

$$\begin{aligned} & [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r}, E)] \psi(\vec{r}, \hat{\Omega}, E) \\ &= q_{ex}(\vec{r}, \hat{\Omega}, E) + \int_0^{\infty} dE' \int d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') \psi(\vec{r}, \hat{\Omega}', E') \\ &+ \chi(E) \int_0^{\infty} dE' \nu \sigma_f(\vec{r}, E') \phi(\vec{r}, E'), \end{aligned} \quad (2-1)$$

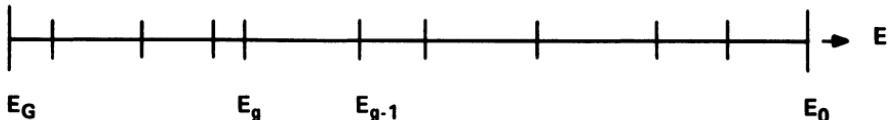
where  $\phi(\vec{r}, E)$  is the scalar flux.

To derive multigroup equations we first divide the energy ranges into  $G$  intervals as shown in Fig. 2-1, where  $E_G = 0$  and  $E_0$  is sufficiently large that the number of particles at higher energies is negligible. The particles in group  $g$  are taken to be just those with energies between  $E_g$  and  $E_{g-1}$ ; hence the group number increases as the energy decreases. Our objective now is to obtain an approximation to the transport equation in terms of the group angular flux

$$\psi_g(\vec{r}, \hat{\Omega}) = \int_g dE \psi(\vec{r}, \hat{\Omega}, E), \quad (2-2)$$

where for brevity we employ the shorthand notation

$$\int_g dE = \int_{E_g}^{E_{g-1}} dE. \quad (2-3)$$



**Figure 2-1** Division of the energy range into  $G$  energy groups.

We proceed by dividing the energy integrals in Eq. 2-1 into the contributions for each energy group

$$\int_0^\infty dE' = \sum_{g'=1}^G \int_{g'} dE', \quad (2-4)$$

and integrating between  $E_g$  and  $E_{g-1}$  to obtain

$$\begin{aligned} & \hat{\Omega} \cdot \vec{\nabla} \int_g dE \psi(\vec{r}, \hat{\Omega}, E) + \int_g dE \sigma(\vec{r}, E) \psi(\vec{r}, \hat{\Omega}, E) \\ &= \int_g dE q_{ex}(\vec{r}, \hat{\Omega}, E) \\ &+ \sum_{g'=1}^G \int_g dE \int_{g'} dE' \int d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}', E') \\ &+ \int_g dE \chi(E) \sum_{g'=1}^G \int_{g'} dE' \nu \sigma_f(\vec{r}, E') \phi(\vec{r}, E'). \end{aligned} \quad (2-5)$$

To express this equation in terms of the group fluxes we may proceed in one of two ways. We may either assume that the angular flux is separable in energy, or we may use the more elegant treatment of Bell, Hansen, and Sandmeier.<sup>3</sup> We discuss the flux separability approximation first.

## Energy Separability

Suppose that within each energy group the angular flux can be approximated as the product of a known function of energy  $f(E)$  and the group flux  $\psi_g(\vec{r}, \hat{\Omega})$ :

$$\psi(\vec{r}, \hat{\Omega}, E) \approx f(E) \psi_g(\vec{r}, \hat{\Omega}), \quad E_g < E \leq E_{g-1}, \quad (2-6)$$

where the energy-dependent spectral weighting function  $f(E)$  is normalized by the definition of the group flux (Eq. 2-2) to

$$\int_g dE f(E) = 1. \quad (2-7)$$

We discuss the determination of  $f(E)$  in the following subsection. To

proceed, we substitute Eqs. 2-6 and 2-7 into Eq. 2-5 and obtain

$$\begin{aligned}
 & \hat{\Omega} \cdot \vec{\nabla} \psi_g(\vec{r}, \hat{\Omega}) + \int_g dE f(E) \sigma(\vec{r}, E) \psi_g(\vec{r}, \hat{\Omega}) \\
 &= \int_g dE q_{ex}(\vec{r}, \hat{\Omega}, E) \\
 &+ \sum_{g'=1}^G \int_g dE \int_{g'} dE' \int d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) f(E') \psi_{g'}(\vec{r}, \hat{\Omega}') \\
 &+ \int_g dE \chi(E) \sum_{g'=1}^G \int_{g'} dE' \nu \sigma_f(\vec{r}, E') f(E') \phi_{g'}(\vec{r}). \tag{2-8}
 \end{aligned}$$

If we define the multigroup cross sections as

$$\sigma_g(\vec{r}) = \int_g dE \sigma(\vec{r}, E) f(E), \tag{2-9}$$

$$\nu \sigma_{fg}(\vec{r}) = \int_g dE \nu \sigma_f(\vec{r}, E) f(E), \tag{2-10}$$

$$\sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \int_g dE \int_{g'} dE' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) f(E'), \tag{2-11}$$

and let

$$\chi_g = \int_g dE \chi(E), \tag{2-12}$$

and

$$q_g^e(\vec{r}, \hat{\Omega}) = \int_g dE q_{ex}(\vec{r}, \hat{\Omega}, E), \tag{2-13}$$

then we may write Eq. 2-5 in the conventional multigroup form

$$\begin{aligned}
 [\hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r})] \psi_g(\vec{r}, \hat{\Omega}) &= \sum_{g'=1}^G \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}') \\
 &+ \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}) + q_g^e(\vec{r}, \hat{\Omega}). \tag{2-14}
 \end{aligned}$$

The boundary conditions to be used in conjunction with the foregoing multigroup equations are the same as those described in Chapter 1, with the exception that  $\psi(\vec{r}, \hat{\Omega}, E)$  is replaced by  $\psi_g(\vec{r}, \hat{\Omega})$ .

Before proceeding to other forms of the transport equation we note that we may obtain a multigroup balance equation, analogous to the continuous energy form of Chapter 1. To obtain this balance condition we integrate Eq. 2-14 over angle to yield

$$\begin{aligned} \vec{\nabla} \cdot \int d\Omega \hat{\Omega} \psi_g(\vec{r}, \hat{\Omega}) + \sigma_g(\vec{r}) \int d\Omega \psi_g(\vec{r}, \hat{\Omega}) \\ = \sum_{g'} \int d\Omega' \left[ \int d\Omega \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \right] \psi_{g'}(\vec{r}, \hat{\Omega}') \\ + \chi_g \sum_{g'=1}^G v \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}) + \int d\Omega q_g^e(\vec{r}, \hat{\Omega}). \end{aligned} \quad (2-15)$$

We define the group current as

$$\vec{J}_g(\vec{r}) = \int d\Omega \hat{\Omega} \psi_g(\vec{r}, \hat{\Omega}) \quad (2-16)$$

and the group external source as

$$q_g^e(\vec{r}) = \int d\Omega q_g^e(\vec{r}, \hat{\Omega}). \quad (2-17)$$

The bracketed integral on the right of Eq. 2-15 is just equal to the group-to-group scattering cross sections

$$\sigma_{gg'}(\vec{r}) = \int d\Omega \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}'). \quad (2-18)$$

Hence we may express the balance equation as

$$\vec{\nabla} \cdot \vec{J}_g(\vec{r}) + \sigma_g(\vec{r}) \phi_g(\vec{r}) = \sum_{g'} \sigma_{gg'}(\vec{r}) \phi_{g'}(\vec{r}) + \chi_g \sum_{g'} v \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}) + q_g^e(\vec{r}). \quad (2-19)$$

If we assume that Fick's law is a reasonable approximation,

$$\vec{J}_g(\vec{r}) = -D_g(\vec{r}) \vec{\nabla} \phi_g(\vec{r}), \quad (2-20)$$

where  $D_g(\vec{r})$  are group diffusion coefficients, then the balance condition leads to the multigroup diffusion equations<sup>2</sup>

$$\begin{aligned} [-\vec{\nabla} D_g(\vec{r}) \cdot \vec{\nabla} + \sigma_g(\vec{r})] \phi_g(\vec{r}) &= \sum_{g'} \sigma_{gg'}(\vec{r}) \phi_{g'}(\vec{r}) + \chi_g \sum_{g'} \nu \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}) \\ &\quad + q_g^e(\vec{r}). \end{aligned} \quad (2-21)$$

Just as this is an approximation to the multigroup transport equations, we must derive approximations to the boundary conditions on  $\psi_g(\vec{r}, \hat{\Omega})$ . It is left as an exercise to show that Fick's law implies that on a reflective boundary  $\hat{n} \cdot \vec{\nabla} \phi = 0$ , where  $\hat{n}$  is normal to the boundary, and on a vacuum boundary  $\hat{n} \cdot \vec{\nabla} \phi + 2D_g(\vec{r})\phi(\vec{r}) = 0$ .

Analogous to the continuous energy forms of the transport equation, the differential scattering cross section appearing in the scattering term of the multigroup equation is frequently expressed as a Legendre expansion. Thus inserting Eq. 1-23 into Eq. 2-11 we obtain

$$\sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) = \sum_{l=0}^{\infty} (2l+1) \sigma_{lgg'}(\vec{r}) P_l(\hat{\Omega}' \cdot \hat{\Omega}), \quad (2-22)$$

where the orthogonality properties of the Legendre polynomials (Eq. A-17) allow us to write

$$\sigma_{lgg'}(\vec{r}) = \int_g dE \int_{g'} dE' \sigma_{sl}(\vec{r}, E' \rightarrow E) f(E'). \quad (2-23)$$

With this expansion the scattering term in Eq. 2-14,

$$q_g^s(\vec{r}, \hat{\Omega}) \equiv \sum_{g'=1}^G \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}'), \quad (2-24)$$

may be expressed in terms of the group-to-group scattering moments,  $\sigma_{lgg'}$ . Combining Eqs. 2-22 and 2-24, and using the Legendre addition theorem in a manner completely analogous to that in Eqs. 1-80 through 1-85, we obtain

$$q_g^s(\vec{r}, \hat{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}^*(\hat{\Omega}) \sum_{g'=1}^G \sigma_{lgg'}(\vec{r}) \phi_{lg'}^m(\vec{r}), \quad (2-25)$$

where the moments of the group flux are

$$\phi_g^m(\vec{r}) = \int d\Omega Y_{lm}(\hat{\Omega}) \psi_g(\vec{r}, \hat{\Omega}). \quad (2-26)$$

Equation 2-14 is the multigroup analog to the continuous energy form, Eq. 1-106. In one- and two-dimensional problems, where symmetries are imposed on the angular flux distribution, the form of Eq. 2-25 can be simplified. For one-dimensional cylindrical,  $x-y$ ,  $\rho-z$ , and spherical  $\rho-\theta$ , geometry where  $\psi_g(\vec{r}, \theta, \omega) = \psi_g(\vec{r}, \theta, -\omega)$ , we have, analogous to Eq. 1-92,

$$q_g^s(\vec{r}, \hat{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=0}^l (2 - \delta_{m0}) Y_{lm}^e(\hat{\Omega}) \sum_{g'=1}^G \sigma_{lgg'}(\vec{r}) \phi_{lg'}^m(\vec{r}), \quad (2-27)$$

where

$$\phi_{lg}^m(\vec{r}) = \int d\Omega Y_{lm}^e(\hat{\Omega}) \psi_g(\vec{r}, \hat{\Omega}). \quad (2-28)$$

For one-dimensional slab or spherical geometry in which the angular dependence of  $\psi_g$  is a function of only a single direction cosine  $\mu$ , we have, analogous to Eq. 1-88,

$$q_g^s(x, \mu) = \sum_{l=0}^{\infty} (2l + 1) P_l(\mu) \sum_{g'=1}^G \sigma_{lgg'}(x) \phi_{lg'}(x), \quad (2-29)$$

where

$$\phi_{lg}(x) = \int_{-1}^1 \frac{d\mu}{2} P_l(\mu) \psi_g(x, \mu). \quad (2-30)$$

Other forms of the transport equation may likewise be reduced to multi-group form. The multiplication eigenvalue form of Eq. 2-14, obtained by setting the external source to zero and replacing  $\nu$  by  $\nu/k$ , for example, becomes

$$\begin{aligned} [\hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r})] \psi_g(\vec{r}, \hat{\Omega}) &= \sum_{g'=1}^G \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}') \\ &\quad + \frac{1}{k} \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(\vec{r}) \phi_{g'}(\vec{r}). \end{aligned} \quad (2-31)$$

Similarly, the multigroup neutron kinetics equations may be shown to be

$$\begin{aligned}
 & \left[ \frac{1}{v_g} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r}) \right] \psi_g(\vec{r}, \hat{\Omega}, t) \\
 &= \sum_{g'=1}^G \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega}) \psi_{g'}(\vec{r}, \hat{\Omega}', t) \\
 &+ \chi_{pg} \sum_i (1 - \beta^i) \sum_{g'=1}^G \nu \sigma_{fg'}^i(\vec{r}) \phi_{g'}(\vec{r}, t) \\
 &+ \sum_l \chi_{lg} \lambda_l C_l(\vec{r}, t) + q_g^e(\vec{r}, \hat{\Omega}) \tag{2-32}
 \end{aligned}$$

and for six groups<sup>23</sup> of delayed neutrons

$$\frac{\partial}{\partial t} C_l(\vec{r}, t) = \sum_i \beta_l^i \sum_{g'=1}^G \nu \sigma_{fg'}^i(\vec{r}) \phi_{g'}(\vec{r}, t) - \lambda_l C_l(\vec{r}, t), \quad n = 1, 2, \dots, 6. \tag{2-33}$$

In Eq. 2-32, it is assumed that

$$\int_g dE \frac{1}{v} \frac{\partial \psi}{\partial t} = \frac{1}{v_g} \frac{\partial \psi_g}{\partial t}, \tag{2-34}$$

and thus

$$\frac{1}{v_g} = \int_g dE \frac{1}{v} f(E). \tag{2-35}$$

The adjoint operators described in Chapter 1 may be written in an analogous multigroup approximation. These reductions are left as exercises.

### Multigroup Cross Section Evaluation

Before multigroup transport calculations can be carried out, values of the multigroup cross sections  $\sigma_g$ ,  $\nu \sigma_{fg}$ ,  $\sigma_{gg'}$  must be available. As indicated by the definitions in Eqs. 2-9 through 2-11, however, the evaluation of group cross sections requires that both the detailed energy dependence of the cross section and the spectral weighting function  $f(E)$  be known. The energy

dependence of the microscopic cross sections is becoming available with ever increasing accuracy through evaluated data files, such as ENDF for neutrons. The evaluation of  $f(E)$  is a more subtle matter, for it depends a great deal on the characteristics of the system under analysis, and in particular on the analytical and/or computational models that are available for the description of that system.

The details of cross section evaluations are treated extensively in texts on shielding and reactor physics.<sup>1,2,3,4</sup> In many cases the techniques are similar whether the multigroup equations are employed in the transport equation or its diffusion approximation. While the evaluation of cross sections is considered to be outside the scope of the present text, the general remarks that follow may be instructive in indicating some of the considerations that typically arise in generating multigroup cross sections for transport calculations.

If an exceedingly fine-energy-group structure can be used, analytic or semianalytic approximations for  $f(E)$  may be adequate. The simplest of these is to take  $f(E)$  to be a constant,

$$f(E) = \frac{1}{\Delta E_g}, \quad E_g \leq E < E_{g-1}, \quad (2-36)$$

where  $\Delta E_g \equiv E_{g-1} - E_g$  assures that the normalization condition, Eq. 2-7, is met. Then

$$\sigma_g(\vec{r}) = \frac{1}{\Delta E_g} \int_g dE \sigma(\vec{r}, E), \quad (2-37)$$

and the group cross sections depend only on the energy-dependent cross sections. For cross sections with smooth energy dependence, weighting factors in which  $f(E) \propto 1/E$  or  $1/[E\sigma(E)]$  can be more easily justified on analytical grounds.<sup>1</sup> Where the cross section has the resonance structure of the neutron cross sections illustrated in Fig. 1-2, the foregoing recipes are most often inadequate even for very fine energy group discretization. In these cases the flux depression called energy self-shielding through the resonance energy must be taken into account through more sophisticated methods, such as the narrow and wide resonance models. More sophisticated modeling is also necessary to take into account the effects of thermalization in neutron transport,<sup>1</sup> of Compton edges in gamma ray calculations,<sup>4</sup> and of other phenomena.

**Infinite Medium Calculations.** The expense of solving multigroup transport problems often precludes the use of a number of energy groups that is large

enough for the semianalytic modeling of  $f(E)$  to be adequate. As a result it is common to first perform an infinite medium fine-energy-group calculation in which the spatial dependence is eliminated. From the results of such a calculation, an approximation for  $f(E)$  within each of the coarser energy groups can be obtained. The coarser energy group cross sections are then obtained by appropriately collapsing the fine-group results.

To illustrate, let us assume that the neutron flux is in an infinite medium and has no spatial or angular dependence. The streaming term in Eq. 2-31 then vanishes, and we can integrate over all angles to obtain infinite medium-multigroup equations in terms of the scalar flux:

$$\sigma_j^{\ddagger} \phi_j^{\ddagger} = \sum_{j'} \sigma_{jj'}^{\ddagger} \phi_{j'}^{\ddagger} + \frac{\chi_j^{\ddagger}}{k} F, \quad (2-38)$$

where

$$F \equiv \sum_{j'} \nu \sigma_{jj'}^{\ddagger} \phi_{j'}^{\ddagger}. \quad (2-39)$$

We hereafter use the subscript  $j, j'$  to denote the fine-group indices and the superscript  $\ddagger$  to denote the fine-group quantities of the problem. Since we will need only the relative magnitudes of the fine-group fluxes, we are not interested in the values of  $k$  or  $F$ . Thus we can take  $F/k = 1$  creating a fixed source problem, and allowing Eq. 2-38 to be solved for the  $\phi_j^{\ddagger}$ . Then within the broader energy group we can define  $f(E)$  as the normalized step function

$$f(E) = \frac{\phi_j^{\ddagger}}{\sum_{j' \in g} \phi_{j'}^{\ddagger}}, \quad E_j < E < E_{j-1}, \quad j \in g, \quad (2-40)$$

where  $j \in g$  includes only those fine groups lying within the broad group  $g$ ; i.e., for which  $E_g \leq E_j < E_{j-1} \leq E_{g-1}$ . With  $f(E)$  known, the fine-group cross sections can be collapsed to broader group cross sections. For example, Eq. 2-9 is approximated by

$$\sigma_g(\vec{r}) = \sum_{j \in g} \phi_j^{\ddagger} \sigma_j^{\ddagger}(\vec{r}) / \sum_{j \in g} \phi_j^{\ddagger}, \quad (2-41)$$

and similar expressions can be written from Eqs. 2-10 and 2-11.

**Lattice Cell Homogenization.** There are at least two important situations where the use of fine-group infinite medium calculations for the generation

of broader group cross sections is inadequate. The first of these arises frequently in reactor lattice calculations.<sup>1,2</sup> Such a calculation may have as its spatial domain many unit cells, each consisting of fuel and coolant in separated regions and arranged in a periodic array. Two simplified two-region unit cell configurations are depicted in Fig. 2-2. In most cases the computational cost of treating the heterogeneous structure of each cell explicitly within a larger many-cell problem would be prohibitive. Thus the cell cross sections are homogenized to cell-averaged values. In cases where the cell dimensions are small in mean free paths, simple volume averages may be acceptable. Often, however, the true flux may exhibit sufficiently large spatial variation between the regions of the cell that it must be accounted for in the homogenization procedures.

The most common procedure for accounting for cell flux variation in group cross sections may be illustrated in terms of the simple two-region cells shown in Fig. 2-2. Calculations are based on an infinite lattice problem in which reflective conditions are imposed at all of the cell boundaries. These provide fine energy mesh values of  $\phi_j^\pm$  and  $\phi_{j1}^\pm$ , the volume-averaged flux values in each of the cell regions. A wide variety of methods have been applied for such purposes ranging from semianalytic approximations for the flux ratios<sup>2</sup> to the use of numerical transport methods such as those discussed in Chapter 5. Knowing the flux value and the fine-group region cross sections,  $\sigma_{j1}^\pm$  and  $\sigma_{j2}^\pm$ , homogenized cross sections, averaged over fine groups, may be obtained. For example, the group total cross section is

$$\sigma_g = \frac{\sum_{j \in g} (V_1 \sigma_{j1}^\pm \phi_{j1}^\pm + V_2 \sigma_{j2}^\pm \phi_{j2}^\pm)}{\sum_{j \in g} (V_1 \phi_{j1}^\pm + V_2 \phi_{j2}^\pm)}, \quad (2-42)$$

while similar expressions may be written for the fission and scattering cross sections.

**Buckling Corrections.** A second situation where the use of fine-group infinite medium calculations for the evaluation of multigroup cross sections may arise is when the overall dimensions of the system are not large, for the

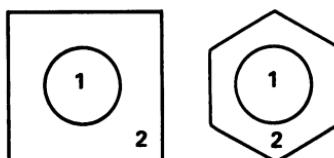


Figure 2-2 Two-region reactor lattice cells.

large net leakage of neutrons may then cause a significant distortion of the infinite medium fine-group energy distribution. For homogeneous media this leakage may be roughly accounted for by assuming the approximation<sup>2,5</sup>

$$\psi_j^\ddagger(\vec{r}, \hat{\Omega}) = \psi_j^\ddagger(\hat{\Omega}) e^{i\vec{B} \cdot \vec{r}}, \quad (2-43)$$

where  $B = |\vec{B}|$  is the buckling familiar from elementary reactor theory. It is chosen to be the lowest eigenvalue of the Helmholtz equation  $\nabla^2\phi + B^2\phi = 0$ , where  $\phi = 0$  on the extrapolated boundaries and  $\phi > 0$  within the reactor. Hence  $B$  increases and the leakage correction becomes larger as the size of the system decreases.

To demonstrate the derivation of the fine-group fluxes, we take the simplest case where  $\vec{B}$  is in the  $x$  direction, and  $\mu = \hat{\Omega} \cdot \hat{e}_x$ . Our flux approximation is then

$$\psi_j^\ddagger(x, \mu) = \psi_j^\ddagger(\mu) e^{iBx}, \quad (2-44)$$

and the corresponding fine-group equation,

$$\begin{aligned} \left[ \mu \frac{\partial}{\partial x} + \sigma_j^\ddagger \right] \psi_j^\ddagger(x, \mu) &= \sum_{l=0}^L (2l+1) P_l(\mu) \sum_{j'} \sigma_{ljj'}^\ddagger \phi_{lj'}^\ddagger(x) \\ &\quad + \frac{\chi_j}{k} \sum_{j'} \nu \sigma_{jj'}^\ddagger \phi_{j'}^\ddagger(x), \end{aligned} \quad (2-45)$$

may be obtained by reducing Eq. 2-31 to slab geometry and using Eq. 2-29 to represent the scattering term. Inserting Eq. 2-44, we obtain

$$\sigma_j^\ddagger \left( 1 + \frac{i\mu B}{\sigma_j^\ddagger} \right) \psi_j^\ddagger(\mu) = \sum_{l=0}^L (2l+1) P_l(\mu) \sum_{j'} \sigma_{ljj'}^\ddagger \phi_{lj'}^\ddagger + \frac{\chi_j}{k} F, \quad (2-46)$$

and

$$F \equiv \sum_{j'} \nu \sigma_{jj'}^\ddagger \phi_{j'}^\ddagger, \quad (2-47)$$

where for simplicity we may normalize our results to  $F/k = 1$ . For isotropic scattering, we take  $L = 0$ . Then solving for  $\psi_j^\ddagger(\mu)$  on the left and integrating over angle we have, after some algebra, the scalar flux equations

$$\phi_j^\ddagger = \frac{1}{B} \tan^{-1} \left( \frac{B}{\sigma_j^\ddagger} \right) \left[ \sum_{j'} \sigma_{jj'} \phi_{j'}^\ddagger + \chi_j \right]. \quad (2-48)$$

These values then can be used to obtain multigroup cross sections, as in Eq. 2-41. When anisotropic scattering is present, somewhat more effort is required to solve Eq. 2-46; the result is the so-called  $B_N$  approximation. We again solve for  $\psi_j^\pm(\mu)$  on the left. Noting that

$$\phi_{lj}^\pm = \frac{1}{2} \int_{-1}^1 d\mu P_l(\mu) \psi_j^\pm(\mu), \quad (2-49)$$

we multiply Eq. 2-46 by  $\frac{1}{2}P_l(\mu)$  and integrate over  $\mu$  to obtain a set of equations for  $\phi_{lj}^\pm$ ,

$$\sigma_{lj}^\pm \phi_{nj}^\pm = \sum_{l=0}^L \alpha_{lnj} \sum_{j'} \sigma_{lj'j'} \phi_{lj'} + \alpha_{0nj} \chi_j, \quad (2-50)$$

where

$$\alpha_{lnj} \equiv \frac{1}{2} \int_{-1}^1 d\mu \left\{ 1 - \frac{i\mu B}{\sigma_j^\pm} \right\}^{-1} P_l(\mu) P_n(\mu). \quad (2-51)$$

With the  $B_N$  approximation we can obtain not only scalar flux weighted cross sections, but also the Legendre moments for anisotropic scattering.<sup>2</sup> From Eq. 2-50 we also have

$$\sigma_{lgg'} = \frac{\sum_j \sum_{j'} \sigma_{lj'j'}^\pm \phi_{lj'}^\pm}{\sum_{j'} \phi_{lj'}^\pm}; \quad (2-52)$$

in infinite media calculations, however, we can only approximate this expression by substituting  $\phi_{0j}^\pm$  for the  $\phi_{lj}^\pm$ .

### Alternative Derivation

The multigroup approximation can be formulated so that Eq. 2-14 is utilized without requiring the assumption of flux separability given by Eq. 2-6 in defining the cross sections. While the derivation is more lengthy, it has the advantage of allowing one to use the Legendre moments of the flux distribution, if they are available from space or buckling-dependent calculations, to obtain more realistic weighting of the multigroup cross sections.<sup>1,3</sup>

Since our objective is only to obtain improved definitions of the multi-group cross sections  $\sigma_g$ ,  $\nu\sigma_{fg}$ , and  $\sigma_{lgg'}$  appearing in Eqs. 2-14 through 2-34, it is adequate to consider the transport equation in the slab geometry form of Eq. 2-1 and expand the scattering term in a Legendre series as in Eq. 1-88:

$$\begin{aligned} \mu \frac{\partial}{\partial x} \psi(x, \mu, E) + \sigma(x, E) \psi(x, \mu, E) \\ = \sum_{l=0}^{\infty} (2l+1) P_l \int_0^{\infty} dE' \sigma_{sl}(x, E' \rightarrow E) \phi_l(x, E') \\ + \chi(E) \int_0^{\infty} dE' \nu\sigma_f(x, E') \phi(x, E') + q_{ex}(x, \mu, E). \quad (2-53) \end{aligned}$$

Dividing the integrals as in Eq. 2-4 and integrating this equation between  $E_g$  and  $E_{g-1}$  we have

$$\begin{aligned} \mu \frac{\partial}{\partial x} \int_g dE \psi(x, \mu, E) + \int_g dE \sigma(x, E) \psi(x, \mu, E) \\ = \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \sum_{g'=1}^G \int_g dE \int_{g'} dE' \sigma_{sl}(x, E' \rightarrow E) \phi_l(x, E') \\ + \int_g dE \chi(E) \sum_{g'=1}^G \int_{g'} dE' \nu\sigma_f(x, E') \phi(x, E') + \int_g dE q_{ex}(x, \mu, E), \quad (2-54) \end{aligned}$$

which may be rewritten as

$$\begin{aligned} \mu \frac{\partial}{\partial x} \psi_g(x, \mu) + \tilde{\sigma}_g(x, \mu) \psi_g(x, \mu) \\ = \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \sum_{g'=1}^G \sigma_{lgg'}(x) \phi_{lg'}(x) \\ + \chi_g \sum_{g'=1}^G \nu\sigma_{fg'}(x) \phi_{g'}(x) + q_g^e(x, \mu), \quad (2-55) \end{aligned}$$

where the multigroup cross sections are now defined as

$$\tilde{\sigma}_g(x, \mu) = \frac{\int_g dE \sigma(x, E) \psi(x, E, \mu)}{\psi_g(x, \mu)}, \quad (2-56)$$

$$\sigma_{lgg'}(x) = \frac{\int_g dE \int_{g'} dE' \sigma_{sl}(x, E' \rightarrow E) \phi_l(x, E')}{\phi_{lg'}(x)}, \quad (2-57)$$

$$\nu\sigma_{fg}(x) = \frac{\int_g dE \nu\sigma_f(x, E) \phi(x, E)}{\phi_g(x)}, \quad (2-58)$$

$$q_g^e(x, \mu) = \int_g dE q_{ex}(x, \mu, E), \quad (2-59)$$

and the angular group flux and its moments are again defined by Eqs. 2-2 and 2-30.

Equation 2-55 differs from the desired form in only one respect. The angular flux weighting leads to an angularly dependent group total cross section  $\tilde{\sigma}_g(x, \mu)$ . None of the widely used methods for solving multigroup transport problems are coded to treat angular dependence of the total cross sections. Hence it is advantageous to eliminate this angular dependence. This may be done by the following method.<sup>3</sup>

We begin by expanding the second term in Eq. 2-54 in a series of Legendre polynomials defined in Appendix A:

$$\psi(x, \mu, E) = \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \phi_l(x, E), \quad (2-60)$$

with the Legendre moments given by

$$\phi_l(x, E) = \frac{1}{2} \int_{-1}^1 d\mu P_l(\mu) \psi(x, \mu, E). \quad (2-61)$$

By using the Legendre flux expansion, the collision term may be written as

$$\int_g dE \sigma(x, E) \psi(x, \mu, E) = \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \sigma_{lg}(x) \phi_{lg}(x), \quad (2-62)$$

provided we define

$$\sigma_{lg}(x) = \frac{\int_g dE \sigma(x, E) \phi_l(x, E)}{\phi_{lg}(x)}, \quad (2-63)$$

where the group Legendre moments  $\phi_{lg}$  are just

$$\phi_{lg}(x) = \int_g dE \phi_l(x, E). \quad (2-64)$$

We next combine Eqs. 2-62 and 2-54 and move the Legendre expansion to the right of the equation:

$$\begin{aligned} \mu \frac{\partial}{\partial x} \psi_g(x, \mu) &= \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \sum_{g'=1}^G [\sigma_{lgg'}(x) - \sigma_{lg}(x) \delta_{gg'}] \phi_{lg'}(x) \\ &\quad + \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(x) \phi_{g'}(x) + q_g^e(x, \mu). \end{aligned} \quad (2-65)$$

We add  $\sigma_g(x) \psi_g(x, \mu)$  to both sides of the equation. In adding the term to the right side, we expand the angular flux in a Legendre series to yield

$$\sigma_g(x) \psi_g(x, \mu) = \sum_{l=0}^{\infty} \sigma_g(x) (2l+1) P_l(\mu) \phi_{lg}(x) \quad (2-66)$$

so that it also can be included in the scattering term:

$$\begin{aligned} \left[ \mu \frac{\partial}{\partial x} + \sigma_g(x) \right] \psi_g(x, \mu) &= \sum_{l=0}^{\infty} (2l+1) P_l(\mu) \sum_{g'=1}^G \tilde{\sigma}_{lgg'}(x) \phi_{lg'}(x) \\ &\quad + \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(x) \phi_{g'}(x) + q_g^e(x, \mu), \end{aligned} \quad (2-67)$$

where

$$\tilde{\sigma}_{lgg'}(x) \equiv \sigma_{lgg'}(x) + [\sigma_g(x) - \sigma_{lg}(x)] \delta_{gg'}. \quad (2-68)$$

Equation 2-67 now has the identical form to the multigroup equation derived from the separability assumption, the total cross section being

independent of angle. Moreover, the cross section definition allows one to use not only the scalar flux but also the Legendre moments from angularly dependent spectral calculations for purposes of determining the group cross sections. One problem remains. Thus far the group cross section  $\sigma_g(x)$  is arbitrary since it hasn't been specified. An obvious choice is to just use scalar flux weight,

$$\sigma_g(x) = \sigma_{0g}(x) = \int_g dE \frac{\sigma(x, E)\phi(x, E)}{\phi_g(x)}. \quad (2-69)$$

If this is done, the preceding equations are referred to as the consistent  $P_N$  approximation, since it may be shown that if the  $P_N$  approximation is applied to Eq. 2-67 (as in Appendix A), the first of the resulting equations is identical to that obtained if the energy-dependent angular flux is expanded in Legendre polynomials before the multigroup approximations are made.

A more elegant technique<sup>3</sup> is available for defining  $\sigma_g(x)$ . Normally the Legendre expansion in the scattering term is truncated after some finite number of terms, say  $l = L$ . We may choose  $\sigma_g(x)$  to cause the first neglected term,  $l = L + 1$ , to be small. That is, to cause

$$(2L + 1)P_{L+1}(\mu) \times \sum_{g'=1}^G \left\{ \sigma_{L+1, gg'}(x) + [\sigma_g(x) - \sigma_{L+1, g}(x)]\delta_{gg'} \right\} \phi_{L+1, g'}(x) \approx 0. \quad (2-70)$$

In reactor problems the scattering into a given energy group is often roughly equal to the scattering out for most energy groups. Hence to a first approximation we take

$$\sum_{g'=1}^G \sigma_{L+1, gg'}(x) \phi_{L+1, g'}(x) \approx \sum_{g'=1}^G \sigma_{L+1, g'g}(x) \phi_{L+1, g'}(x), \quad (2-71)$$

where scattering into and out of the group  $g$  are represented by the left and right sides of this equation respectively. Substituting this approximation into Eq. 2-70, and forcing the left-hand side to vanish, we obtain

$$\sigma_g(x) = \sigma_{L+1, g}(x) - \sum_{g'=1}^G \sigma_{L+1, g'g}(x). \quad (2-72)$$

This definition is called the "extended transport approximation."<sup>1</sup>

## 2-3 FIXED SOURCE PROBLEMS

In this section we first examine the reduction of fixed source transport calculations to a set of within-group calculations. The resulting within-group equations are the point of departure for the space and angle discretization procedures employed in Chapters 3 to 6. Moreover, these equations also provide a framework within which both the eigenvalue problems and the time-dependent calculations of the following sections can be discussed.

The remainder of this section is a preview to methods for solving the within-group equations, including methods for accelerating the convergence of iterative algorithms. Since most of the properties of the techniques discussed here are not dependent on the details of space-angle discretization procedures, their characteristics may be made more transparent by discussing them before specific angular approximations or spatial differencing schemes are introduced. Some readers, however, may prefer to examine first the techniques in Chapter 3 to 6 for reducing the within-group transport equation to sets of simultaneous algebraic equations.

### Nonmultiplying Systems

Since fixed source problems most frequently arise for nonmultiplying systems, we use as our starting point Eq. 2-14 with the fission source set equal to zero:

$$[\hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r})] \psi_g(\vec{r}, \hat{\Omega}) - \sum_{g'} \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi_{g'}(\vec{r}, \hat{\Omega}') = q_g^e(\vec{r}, \hat{\Omega}),$$

$$g = 1, 2, \dots, G. \quad (2-73)$$

The operator notation of Section 1-6 may be generalized to further condense these equations. The streaming collision operator for group  $g$  is defined as

$$H_{gg}^0 \psi_g = [\hat{\Omega} \cdot \vec{\nabla} + \sigma_g(\vec{r})] \psi_g(\vec{r}, \hat{\Omega}) \quad (2-74)$$

and the group-to-group scattering operator as

$$H_{gg'}^1 \psi_{g'} = \int d\Omega' \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi_{g'}(\vec{r}, \hat{\Omega}'). \quad (2-75)$$

We then define the multigroup transport operator as

$$H_{gg'} = \delta_{gg'} H_{gg}^0 - H_{gg'}^1. \quad (2-76)$$

Equation 2-73 may now be written as a coupled set of operator equations

$$\begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1g} & \cdots & H_{1G} \\ H_{21} & H_{22} & & & & \\ \vdots & & \ddots & & & \\ H_{g1} & & & H_{gg} & & \\ & & & & \ddots & \\ H_{G1} & & & & & H_{GG} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_g \\ \vdots \\ \psi_G \end{bmatrix} = \begin{bmatrix} q_1^e \\ q_2^e \\ \vdots \\ q_g^e \\ \vdots \\ q_G^e \end{bmatrix}, \quad (2-77)$$

or, using boldface type for matrices and vectors, simply

$$\mathbf{H}\boldsymbol{\psi} = \mathbf{q}^e. \quad (2-78)$$

For many problems, particularly photon transport and fast reactor neutronics calculations, there is no scattering of particles from lower to higher energy groups. Since  $g$  increases as energy decreases, this implies

$$H_{gg'} = 0, \quad g' > g. \quad (2-79)$$

Hence Eq. 2-77 can be solved,

$$\boldsymbol{\psi} = \mathbf{H}^{-1}\mathbf{q}^e, \quad (2-80)$$

by solving successively for energy groups of increasing index:

$$\begin{aligned} \psi_1 &= H_{11}^{-1}q_1^e, \\ \psi_2 &= H_{22}^{-1}(q_2^e - H_{21}\psi_1), \\ &\vdots \\ \psi_g &= H_{gg}^{-1}\left(q_g^e - \sum_{g' < g} H_{gg'}\psi_{g'}\right). \end{aligned} \quad (2-81)$$

In case upscatter is included, an iteration must be followed. The simplest of these is

$$\psi_g^{i+1} = H_{gg}^{-1}\left(q_g^e - \sum_{g' < g} H_{gg'}\psi_{g'}^{i+1} - \sum_{g' > g} H_{gg'}\psi_{g'}^i\right), \quad (2-82)$$

where  $i$  is the upscatter iteration index.

## Solution of Within-Group Equations

The foregoing procedures require that we be able to solve equations of the form  $H_{gg}\psi_g = s_g$ . Using Eqs. 2-74 through 2-76 we see that this is equivalent to solving the space-energy problem,

$$\hat{\Omega} \cdot \vec{\nabla}\psi(\vec{r}, \hat{\Omega}) + \sigma(\vec{r})\psi(\vec{r}, \hat{\Omega}) = \int d\hat{\Omega}' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}')\psi(\vec{r}, \hat{\Omega}') + s(\vec{r}, \hat{\Omega}), \quad (2-83)$$

where we have deleted the group index  $g$  since it appears only as a parameter. The  $g$ th group source for nonmultiplying problems is

$$s(\vec{r}, \hat{\Omega}) = s_g(\vec{r}, \hat{\Omega}) = \sum_{g' \neq g} \int d\hat{\Omega}' \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}')\psi_{g'}(\vec{r}, \hat{\Omega}') + q_g^e(\vec{r}, \hat{\Omega}), \quad (2-84)$$

and in Eq. 2-83

$$\sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \equiv \sigma_{gg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}'). \quad (2-85)$$

The group source consists of group-to-group scattering and external source terms. When fissionable isotopes are present it will also include fission neutron terms.

In the following chapters this equation is reduced to sets of simultaneous equations by a variety of approximations and differencing techniques. For the most part the resulting equations cannot be solved by straightforward Gauss elimination methods because of arithmetic and/or computer memory requirements that are too large. As a result, either iterative solution techniques are used, or the equation is transformed to a form more amenable to solution. Since such techniques may be understood without reference to specific angular approximations or differencing techniques we review them here.

**Iteration on the Scattering Source.** Probably the most widely used method for solving the discretized form of Eq. 2-83 is a form of Von Neumann's series solution<sup>6</sup> referred to as iteration on the scattering source. The method is used almost exclusively for the solution of the discrete ordinates equations<sup>7</sup> discussed in Chapters 3 and 4, and it may also be applied to integral and even-parity forms of the equations in Chapters 5 and 6. The method

derives its popularity from the fact that by knowing the right side of Eq. 2-83 one may often solve for  $\psi(\vec{r}, \hat{\Omega})$  on the left in a fairly efficient manner. Moreover, the iteration has a clear physical interpretation that allows one to predict the classes of problems for which convergence should be fast. The iteration procedure is given by

$$[\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \psi'^{l+1}(\vec{r}, \hat{\Omega}) = q^l(\vec{r}, \hat{\Omega}), \quad (2-86)$$

where the emission density—called the scattering source—is given by

$$q^l(\vec{r}, \hat{\Omega}) = \int d\Omega' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi'(\vec{r}, \hat{\Omega}') + s(\vec{r}, \hat{\Omega}), \quad (2-87)$$

and  $l$  is the iteration index.

We may give a physical interpretation to the iterates if we take

$$\psi^0 = 0 \quad (2-88)$$

and write the  $(l + 1)$ th iterate as a sum

$$\psi'^{l+1} = \sum_{m=0}^l \tilde{\psi}^m. \quad (2-89)$$

Combining Eqs. 2-86 and 2-87, and substituting this sum for  $\psi'^{l+1}$  and  $\psi'$ , we obtain

$$\begin{aligned} \sum_{m=0}^l [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \tilde{\psi}^m(\vec{r}, \hat{\Omega}) &= \sum_{m=0}^{l-1} \int d\Omega' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \tilde{\psi}^m(\vec{r}, \hat{\Omega}') \\ &\quad + s(\vec{r}, \hat{\Omega}). \end{aligned} \quad (2-90)$$

If this equation is required to hold for  $l = 0, 1, 2, \dots$ , then we know

$$[\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \tilde{\psi}^0(\vec{r}, \hat{\Omega}) = s(\vec{r}, \hat{\Omega}) \quad (2-91)$$

and

$$\begin{aligned} [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \tilde{\psi}^m(\vec{r}, \hat{\Omega}) &= \int d\Omega' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \tilde{\psi}^{m-1}(\vec{r}, \hat{\Omega}'), \\ m &= 1, 2, 3, \dots \end{aligned} \quad (2-92)$$

The first equation is the transport equation with the scattering term set

equal to zero. Thus  $\tilde{\psi}^0$  includes only those neutrons emitted directly from the group source; it is therefore the flux of uncollided neutrons. Following Eq. 2-92 for successive values of  $m$  we see that the only contribution to the emission density for  $\tilde{\psi}^1$  is the scattering term generated by  $\tilde{\psi}^0$ . Thus since only  $\tilde{\psi}^0$  contributes to  $\tilde{\psi}^1$ ,  $\tilde{\psi}^1$  is the flux of once-collided neutrons; since only  $\tilde{\psi}^1$  contributes to  $\tilde{\psi}^2$ ,  $\tilde{\psi}^2$  is the flux of twice-collided neutrons, and so on *ad infinitum*.

Since  $\tilde{\psi}^m$  consists of those neutrons that have made  $m$  collisions, the  $l + 1$  iteration  $\psi^{l+1}$  consists of all neutrons that have made fewer than  $l + 1$  collisions since being emitted by the source  $s(\vec{r}, \hat{\Omega})$ . This physical interpretation leads immediately to the qualitative physical argument that if the particles make few collisions on the average before escaping from the boundaries or being removed by absorption or scattering into other group, convergence will be rapid; otherwise it will be slow. This convergence behavior of iteration on the scattering source is found to be present regardless of which of the combinations of angular approximations and spatial differencing schemes discussed in Chapters 3 and 4 are employed.

**Integral Transport.** In some situations it may be desirable to eliminate explicit consideration of the angular neutron distribution by formulating the transport equation in terms of the scalar flux  $\phi(\vec{r})$ . If the group source and scattering are isotropic,  $s(\vec{r}, \hat{\Omega}) \rightarrow S(\vec{r})$  and  $\sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \rightarrow \sigma_s(\vec{r})$ , we may simplify Eq. 2-83 to

$$[\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \psi(\vec{r}, \hat{\Omega}) = \sigma_s(\vec{r}) \phi(\vec{r}) + S(\vec{r}). \quad (2-93)$$

The procedure for determining angular flux by iteration on the scattering source may be written formally as

$$\psi(\vec{r}, \hat{\Omega}) = [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})]^{-1} [\sigma_s(\vec{r}) \phi(\vec{r}) + S(\vec{r})]. \quad (2-94)$$

If we integrate over  $\hat{\Omega}$ , we obtain the scalar flux on the left of this equation. Regrouping terms then yields

$$\begin{aligned} & \left[ 1 - \int d\Omega [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})]^{-1} \sigma_s(\vec{r}) \right] \phi(\vec{r}) \\ &= \int d\Omega [\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})]^{-1} S(\vec{r}). \end{aligned} \quad (2-95)$$

Thus for isotropic scattering and sources we can formulate the within-group transport equation solely in terms of the scalar flux.

In Chapter 5 we discuss in detail numerical methods based on this integral form of the transport equation. A second transformation, to the even-parity form of the transport equation, may be used as the starting point for other numerical methods. Such even-parity methods are discussed in Chapter 6.

### Acceleration of Within-Group Calculations

Under many circumstances the iteration on the scattering source is not only computationally efficient in terms of arithmetical operations concerning iteration and memory requirements, but it also leads to convergence of the solution in a reasonable number of iterations.<sup>7</sup> For instance, it converges in one iteration for purely absorbing media. In problems with optically thick regions and a great deal of within-group scattering, however, the convergence becomes very slow, since in these circumstances neutrons that have already made many collisions within a given energy group are likely to make a substantial contribution to the scalar flux distribution.

This slow convergence is particularly notorious for transport computations involving one or a few groups describing the thermal neutron energy range from about 0 to 1 eV, for once the neutrons have completed the slowing-down processes they may make many scattering collisions unless strong thermal neutron absorbers are present. Even in higher energy ranges, the slow convergence may be a problem, particularly if only the heavier nuclides are present, because the neutrons must make a large number of collisions before losing enough energy on the average to be removed from the energy group. While using narrower groups will lead to increased rates of convergence of scattering source iteration, it also means that the transport equation must be solved for more energy groups. Hence the improvements in overall computational efficiency from this strategy are likely to be minimal.

Numerous techniques have been used for the acceleration of iteration on the scattering source. Some of these, such as Chebychev acceleration and two-cyclic overrelaxation,<sup>8, 9</sup> are particular adaptations of more general matrix iteration techniques.<sup>10</sup> Some of the most widely used methods have come originally from physical arguments about properties of the solution, with the mathematical rigor added after the fact. Into this category would fall coarse mesh rebalance and some synthetic methods.

Since the acceleration methods to be discussed may be applied in conjunction with a number of different angular approximations and spatial differencing techniques, we treat them in terms of accelerating the iteration on the scattering source of a transport equation that has yet to be dis-

cretized. Our starting point is the within-group transport equation, written as

$$[\hat{\Omega} \cdot \vec{\nabla} + \sigma(\vec{r})] \tilde{\psi}'(\vec{r}, \hat{\Omega}) = \int d\Omega' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi'(\vec{r}, \hat{\Omega}') + s(\vec{r}, \hat{\Omega}). \quad (2-96)$$

Here  $\psi'$  is the  $l$ th iterate, and  $\tilde{\psi}'$  results from applying iteration on the scattering source. If the iteration is unaccelerated,

$$\psi'^{+1}(\vec{r}, \hat{\Omega}) = \tilde{\psi}'(\vec{r}, \hat{\Omega}). \quad (2-97)$$

Our objective is to formulate a modification to Eq. 2-97 that allows  $\psi'^{+1}$  to represent more closely the true solution  $\psi(\vec{r}, \hat{\Omega})$  than  $\tilde{\psi}'$ .

**Coarse Mesh Rebalance.** Coarse mesh rebalance<sup>11-14</sup> makes use of the fact that the converged solution must obey the neutron conservation (or balance) equation. By imposing this balance condition on the unconverged solution over coarse regions of the problem domain it is possible to obtain an accelerated iteration procedure that usually converges more rapidly to the correct solution.

We begin by deriving the balance equation. Integrating Eq. 2-83 over angle we have

$$\begin{aligned} \vec{\nabla} \cdot \int d\Omega \hat{\Omega} \psi(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \int d\Omega \psi(\vec{r}, \hat{\Omega}) \\ = \int d\Omega' \left[ \int \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') d\Omega \right] \psi(\vec{r}, \hat{\Omega}') \\ + \int d\Omega s(\vec{r}, \hat{\Omega}), \end{aligned} \quad (2-98)$$

where we have used the fact that  $\hat{\Omega} \cdot \vec{\nabla} \psi = \vec{\nabla} \cdot \hat{\Omega} \psi$ . The first integral on the left is just the definition of the current vector  $\vec{J}$ ; likewise the second integral is the scalar flux  $\phi$ . On the right the bracketed integral is just the group scattering cross section  $\sigma_s(\vec{r})$ . Thus we have

$$\vec{\nabla} \cdot \vec{J}(\vec{r}) + \sigma_r(\vec{r}) \phi(\vec{r}) = S(\vec{r}), \quad (2-99)$$

where  $\sigma_r \equiv \sigma - \sigma_s$ , and  $S(\vec{r})$  is the isotropic component of the group source.

We now divide the problem domain into a number of subdomains  $\tilde{V}_m$ . Integration of Eq. 2-99 over each of these subdomains then yields

$$\int_{\tilde{V}_m} dV \vec{\nabla} \cdot \vec{J} + \int_{\tilde{V}_m} dV \sigma_r \phi = \int_{\tilde{V}_m} dVS, \quad (2-100)$$

or, applying the divergence theorem,

$$\sum_{m'} \int_{\Gamma_{mm'}} d\Gamma \hat{n} \cdot \vec{J} + \int_{\tilde{V}_m} dV \sigma_r \phi = \int_{\tilde{V}_m} dVS, \quad (2-101)$$

where  $\Gamma_{mm'}$  is the surface between  $\tilde{V}_m$  and  $\tilde{V}_{m'}$ . Dividing  $\hat{n} \cdot \vec{J}$ , the component of the current normal to the surface, into outward and inward partial currents,

$$J_{\pm} \equiv \int_{\hat{n} \cdot \hat{\Omega} \gtrless 0} d\Omega |\hat{n} \cdot \hat{\Omega}| \psi(\vec{r}, \hat{\Omega}), \quad (2-102)$$

allows us to write Eq. 2-101 as

$$\sum_{m'} \int_{\Gamma_{mm'}} d\Gamma J_+ - \sum_{m'} \int_{\Gamma_{mm'}} d\Gamma J_- + \int_{\tilde{V}_m} dV \sigma_r \phi = \int_{\tilde{V}_m} dVS. \quad (2-103)$$

Coarse mesh rebalance requires that the new iteration  $\psi'^{+1}(\vec{r}, \hat{\Omega})$  obey this balance equation for each subdomain  $\tilde{V}_m$ . This is accomplished by multiplying the unaccelerated iteration  $\tilde{\psi}'$  by a different constant  $f_m$  for each  $\tilde{V}_m$ . Thus

$$\psi'^{+1}(\vec{r}, \hat{\Omega}) = f_m \tilde{\psi}'(\vec{r}, \hat{\Omega}), \quad \vec{r} \in V_m. \quad (2-104)$$

Since our rebalance function  $f_m$  is discontinuous at the boundaries between coarse mesh regions some care must be taken with the current terms. Since neutrons contributing to  $J^+$  are leaving  $V_m$  we use  $f_m$ ; those contributing to  $J^-$  on  $\Gamma_{mm'}$  are coming from  $\tilde{V}_{m'}$ , however, and therefore they are weighed by  $f_{m'}$ :

$$\psi'^{+1}(\vec{r}, \hat{\Omega}) = f_m \tilde{\psi}'(\vec{r}, \hat{\Omega}), \quad \vec{r} \in \Gamma_{mm'}, \hat{n} \cdot \hat{\Omega} > 0, \quad (2-105)$$

$$\psi'^{+1}(\vec{r}, \hat{\Omega}) = f_{m'} \tilde{\psi}'(\vec{r}, \hat{\Omega}), \quad \vec{r} \in \Gamma_{mm'}, \hat{n} \cdot \hat{\Omega} < 0. \quad (2-106)$$

Hence, requiring Eq. 2-103 to be satisfied by  $\psi'^{+1}$  and using Eqs. 2-104

through 2-106 we may write

$$\left[ \int_{\tilde{V}_m} dV \sigma_t \tilde{\phi}' + \sum_{m'} \int_{\Gamma_{mm'}} d\Gamma \tilde{J}'_+ \right] f_m - \sum_{m'} \int_{\Gamma_{mm'}} d\Gamma \tilde{J}'_- f_{m'} = \int_{\tilde{V}_m} dVS. \quad (2-107)$$

Here

$$\tilde{\phi}' = \int d\Omega \tilde{\psi}'(\vec{r}, \hat{\Omega}), \quad (2-108)$$

$$\tilde{J}'_+ = \int_{\hat{\Omega} \cdot \hat{n} > 0} d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}'(\vec{r}, \hat{\Omega}) \quad (2-109)$$

and

$$\tilde{J}'_- = \int_{\hat{\Omega} \cdot \hat{n} < 0} d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}'(\vec{r}, \hat{\Omega}). \quad (2-110)$$

Equation 2-107 represents a sparse matrix equation since the  $m'$  sum is only over the 2, 4, or 6 neighboring values that occur in one-, two-, or three-dimensional orthogonal systems. For the volumes adjoining external boundaries of the problem domain,  $\tilde{J}'_- = 0$  on vacuum boundaries, while on reflective boundaries  $\tilde{J}'_- = \tilde{J}'_+$  and  $f_i = f_{i'}$ . Once these equations are solved, the necessary  $\phi_{im}$  to recompute the source are obtained by taking the appropriate integrals of Eq. 2-104.

The effect of coarse mesh rebalancing is to adjust the average amplitude of the flux over each volume  $\tilde{V}_m$  while leaving the detailed space angle distribution of the flux within the coarse mesh untouched. This complements nicely the iteration on the scattering source, which corrects details in the space-angle distribution rapidly but is poor in eliminating components of the error that extend over large spatial domains. Of course, as the solution converges,  $f_m \rightarrow 1$ , and detailed balance is satisfied.

In the implementation of coarse mesh rebalance a good deal of care must be exercised both in properly applying the foregoing equations to discretized approximations to the transport equation and in making a judicious choice of coarse mesh size.<sup>12, 13</sup> We have here only treated the simplest rebalance schemes. More sophisticated rebalance functions  $f(\vec{r})$  such as piecewise polynomials may also be used if the added expense in forming the rebalance equations can be justified by improved accelerations. Discussion of other trial functions as well as discussions of the theoretical basis for the method may be found elsewhere.<sup>11, 15</sup>

**Synthetic Acceleration.** In synthetic acceleration<sup>14, 16-18</sup> a low-order approximation—inevitably diffusion theory—is used as a mechanism for accelerating the numerical solution of the transport equation. For brevity we consider only the case of isotropic scattering and group source.

We first simplify the operator notation developed earlier by deleting the group subscripts from Eqs. 2-74 and 2-75. It follows that  $H_{gg} = H$ ,  $H_{gg}^0 = H^0$ , and  $H_{gg}^1 = H^1$ . Hence the within-group equation may be written as

$$H\psi = S, \quad (2-111)$$

where

$$H\psi = \left[ \hat{\Omega} \cdot \vec{\nabla} + \sigma - \sigma_s \int d\Omega \right] \psi, \quad (2-112)$$

and iteration on the scattering source becomes

$$H^0 \tilde{\psi}^l = H^1 \phi^l + S, \quad (2-113)$$

where  $l$  is the iteration index, and for unaccelerated iteration  $\psi^{l+1} = \tilde{\psi}^l$ . The streaming-collision operator is defined as

$$H^0 \psi = (\hat{\Omega} \cdot \vec{\nabla} + \sigma) \psi \quad (2-114)$$

and the within-group isotropic scattering operator by

$$H^1 \psi = \sigma_s \int d\Omega \psi = H^1 \phi, \quad (2-115)$$

when the normalization  $\int d\Omega = 1$  is used.

To derive the synthetic method we first integrate Eq. 2-111 over  $\hat{\Omega}$ :

$$\int d\Omega H\psi = S. \quad (2-116)$$

We now write the operator on the left as the sum of the low-order diffusion operator

$$H_L = -\vec{\nabla} D \vec{\nabla} + \sigma_r \quad (2-117)$$

and a correction ( $H - H_L$ ):

$$\int d\Omega [H_L + (H - H_L)] \psi = S. \quad (2-118)$$

Since  $H_L$  is independent of  $\hat{\Omega}$  we may write

$$\int d\Omega H_L \psi = H_L \phi. \quad (2-119)$$

Then rearranging terms yields

$$H_L \phi = S - \int d\Omega (H - H_L) \psi. \quad (2-120)$$

This expression suggests the acceleration scheme

$$H_L \phi'^{+1} = S - \int d\Omega (H - H_L) \tilde{\psi}', \quad (2-121)$$

where  $\tilde{\psi}'$  is determined from Eq. 2-113. Noting that  $H = H^0 - H^1$  and combining Eqs. 2-113 and 2-121, we may write this expression in the more convenient form

$$H_L (\phi'^{+1} - \tilde{\phi}') = H^1 (\tilde{\phi}' - \phi'). \quad (2-122)$$

Thus knowing  $\phi'$  and  $\tilde{\phi}'$  we need only solve the diffusion equation, by obtaining  $H_L^{-1}$ , to obtain  $\phi'^{+1}$ ; for isotropic scattering it follows from Eq. 2-75 that  $H^1 \phi = \sigma_s \phi$ . Thus we have

$$\phi'^{+1} = \tilde{\phi}' + H_L^{-1} \sigma_s (\tilde{\phi}' - \phi'). \quad (2-123)$$

Clearly as  $\tilde{\phi}' \rightarrow \phi'$ , the system converges.

**Two-Cyclic Acceleration.** The theory of two-cyclic matrices has played a prominent role in matrix iterative analysis.<sup>10</sup> For if a matrix equation can be written in the form

$$\begin{vmatrix} I & -A \\ -A^T & I \end{vmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix}, \quad (2-124)$$

a large body of mathematical analysis becomes applicable to the convergence of iteration processes that take the form

$$\psi_1'^{+1} = A \psi_2' + S_1, \quad (2-125)$$

$$\psi_2'^{+1} = A^T \psi_1'^{+1} + S_2. \quad (2-126)$$

In particular, estimates can be made of overrelaxation factors that optimize rates of convergence. The theory of two-cyclic Chebychev polynomials also is applicable to derive acceleration methods. Such two-cyclic methods are used extensively to accelerate solution of multidimensional neutron diffusion problems.<sup>10</sup> It is then not surprising that the within-group transport equation has been written in two-cyclic form in order to apply Chebychev and optimized overrelaxation acceleration.

Two-cyclic solution of the transport equation has been implemented for  $x-y$  and  $\rho-z$  calculations through the so-called up-down iteration scheme.<sup>8</sup> Although it has been implemented with linear anisotropic scattering, for purposes of illustration we confine our attention to isotropic scattering. In analytical form the scheme is derived as follows. In  $x-y$  geometry we divide the angular flux into two contributions:

$$\psi(\vec{r}, \hat{\Omega}) = \begin{cases} \psi_+(\vec{r}, \hat{\Omega}), & \hat{\Omega} \cdot \hat{j} > 0, \\ \psi_-(\vec{r}, \hat{\Omega}), & \hat{\Omega} \cdot \hat{j} < 0, \end{cases} \quad (2-127)$$

where  $\hat{j}$  is the unit vector in the  $y$  direction. The within-group equation may then be written as

$$(\hat{\Omega} \cdot \vec{\nabla} + \sigma) \psi_+ = \sigma_s \int_{\hat{\Omega} \cdot \hat{j} > 0} d\Omega \psi_+ + \sigma_s \int_{\hat{\Omega} \cdot \hat{j} < 0} d\Omega \psi_- + S, \quad \hat{\Omega} \cdot \hat{j} > 0, \quad (2-128)$$

and

$$(\hat{\Omega} \cdot \vec{\nabla} + \sigma) \psi_- = \sigma_s \int_{\hat{\Omega} \cdot \hat{j} > 0} d\Omega \psi_+ + \sigma_s \int_{\hat{\Omega} \cdot \hat{j} < 0} d\Omega \psi_- + S, \quad \hat{\Omega} \cdot \hat{j} < 0. \quad (2-129)$$

Solving formally for  $\psi^+$  and  $\psi^-$  and including the iteration index we obtain

$$\left( \hat{\Omega} \cdot \vec{\nabla} + \sigma - \sigma_s \int_{\hat{\Omega} \cdot \hat{j} > 0} d\Omega \right) \psi_+^{l+1} = \sigma_s \int_{\hat{\Omega} \cdot \hat{j} < 0} d\Omega \psi_-^l + S, \quad \hat{\Omega} \cdot \hat{j} > 0,$$

$$\left( \hat{\Omega} \cdot \vec{\nabla} + \sigma - \sigma_s \int_{\hat{\Omega} \cdot \hat{j} < 0} d\Omega \right) \psi_-^{l+1} = \sigma_s \int_{\hat{\Omega} \cdot \hat{j} > 0} d\Omega \psi_+^{l+1} + S, \quad \hat{\Omega} \cdot \hat{j} < 0. \quad (2-130)$$

In this form we have the Gauss–Seidel form of the iteration. To obtain overrelaxation we replace  $\psi_{\pm}^{l+1}$  by  $\tilde{\psi}_{\pm}^l$  in these expressions and then obtain the accelerated iterative from

$$\psi_{\pm}^{l+1} = \omega(\tilde{\psi}_{\pm}^l - \psi_{\pm}^l) + \psi_{\pm}^l, \quad (2-131)$$

where the overrelaxation factor,  $\omega$ , or the more general Chebychev polynomials are estimated by techniques discussed elsewhere.<sup>8</sup> Convergence of the accelerated methods has been proven except in the case of all reflective boundaries where one must revert to the Gauss–Seidel equations, obtained by taking  $\omega = 1$ .

In contrast to the coarse mesh and synthetic methods, no auxiliary set of simultaneous equations must be satisfied each time an up–down iteration is performed. On the other hand, the inversion of the operators indicated formally in Eqs. 2-130 is not carried out by direct methods for the differenced equations in two dimensions. Rather, an additional level of iteration must be introduced because of the inclusion of part of the scattering term in the iteration matrix. While these procedures tend to converge within a few iterations, they do add complexity when compared to unaccelerated iteration on the scattering source.

## 2-4 CRITICALITY CALCULATIONS

In the preceding section we examined the solution of the multigroup problem,  $\mathbf{H}\psi = \mathbf{q}^e$ , for a nonmultiplying medium. In this section we examine problems in multiplying media, most particularly the multiplication eigenvalue problem which requires the use of another iterative procedure.

To begin, we define the row vectors:

$$\mathbf{f}^T = \{ \nu\sigma_{f1}(\vec{r}), \nu\sigma_{f2}(\vec{r}), \dots, \nu\sigma_{fg}(\vec{r}), \dots, \nu\sigma_{fG}(\vec{r}) \}, \quad (2-132)$$

and

$$\mathbf{x}^T = \{ x_1, x_2, \dots, x_g, \dots, x_G \}. \quad (2-133)$$

The fission term in Eq. 2-14 can then be written in vector form:

$$\sum_{g'} \nu\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r}) = \mathbf{f}^T(\vec{r}) \int d\Omega \psi(\vec{r}, \hat{\Omega}), \quad (2-134)$$

$$\mathbf{q}_f = \mathbf{x} \mathbf{f}^T(\vec{r}) \int d\Omega \psi(\vec{r}, \hat{\Omega}). \quad (2-135)$$

The fission contribution to the group emission density can thus be incorporated into Eqs. 2-73 through 2-78 to yield the matrix form of the multigroup equation:

$$\mathbf{H}\psi = \chi \mathbf{f}^T \int d\Omega \psi + \mathbf{q}^e. \quad (2-136)$$

In this form a nonnegative solution for  $\psi$  can be found only if the system is subcritical.<sup>2</sup> We are more interested in the multiplication eigenvalue form of the multigroup equations given by Eq. 2-31. Using our matrix notation we obtain

$$\mathbf{H}\psi = \frac{1}{k} \chi \mathbf{f}^T \int d\Omega \psi. \quad (2-137)$$

For purposes of solution, it is useful to define the scalar quantity

$$F(\vec{r}) = \mathbf{f}(\vec{r})^T \int d\Omega \psi(\vec{r}, \hat{\Omega}), \quad (2-138)$$

which is the spatial distribution of fission neutrons produced in the reactor; we may reformulate our eigenvalue problem in terms of  $F(\vec{r})$  as follows. We first invert  $\mathbf{H}$  in Eq. 2-137 and operate on  $\psi$  with  $\mathbf{f}^T / d\Omega$  to obtain

$$\mathbf{f}^T \int d\Omega \psi = \frac{1}{k} \mathbf{f}^T \int d\Omega \mathbf{H}^{-1} \chi \mathbf{f}^T \int d\Omega \psi. \quad (2-139)$$

Therefore, using the definition of  $F(\vec{r})$ , we have

$$\mathbf{f}^T \int d\Omega \mathbf{H}^{-1} \chi F = kF. \quad (2-140)$$

Defining the scalar multigroup transport operator as

$$A \equiv \mathbf{f}^T \int d\Omega \mathbf{H}^{-1} \chi, \quad (2-141)$$

the eigenvalue equation becomes simply

$$AF = kF. \quad (2-142)$$

## Power Iteration Solution

Multiplication eigenvalue problems are invariably solved by the method of power iteration.<sup>10, 11, 19</sup> To formulate the method, we first assume that the eigenvalue problem has a largest positive eigenvalue,  $k > 0$ , that is real and unique and has a corresponding fission distribution  $F(\vec{r})$  that is nonnegative. We then take  $k_0 > 0$  and  $F_0(\vec{r}) > 0$  as initial guesses and iterate as follows so that given the  $i$ th iterates  $k_i$  and  $F_i(\vec{r})$  we calculate the  $i + 1$  iterates. Using Eq. 2-142 we obtain  $F_{i+1}$  from

$$F_{i+1} = \frac{1}{k_i} AF_i. \quad (2-143)$$

To obtain  $k_{i+1}$  we first weight Eq. 2-142 by a positive weight function  $w(\vec{r})$  and integrate over the reactor volume

$$\int dV wAF = k \int dV wF. \quad (2-144)$$

Solving for  $k$  we are able to estimate  $k_{i+1}$  from  $F_i$ :

$$k_{i+1} = \frac{\int dV wAF_i}{\int dV wF_i}. \quad (2-145)$$

In this, Eq. 2-143 can be used to eliminate the operator  $A$ , yielding

$$k_{i+1} = k_i \frac{\int dV wF_{i+1}}{\int dV wF_i}. \quad (2-146)$$

The weight function is open to choice, the simplest being  $w = 1$ ; faster convergence is often obtained, however, if  $w = F_{i+1}$  is used, because it weights the estimate toward those areas of the reactor that are most important to sustaining the chain reaction.

The foregoing method is referred to as the power method since it may be shown that the  $n$ th iteration on the fission distribution is obtained by applying the operator  $A$  a total of  $n$  times, yielding an estimate that is

proportional to the initial guess raised to the  $n$ th power:<sup>10</sup>

$$F_n = \left( \prod_{i=1}^{n-1} k_i^{-1} \right) A^n F_0. \quad (2-147)$$

That the method converges to the fission distribution for the largest eigenvalue may be illustrated heuristically as follows. Suppose that the distinct eigenvalue solutions of Eq. 2-142 are

$$AF^l = \kappa_l F^l, \quad l = 1, 2, \dots, \quad (2-148)$$

where

$$\kappa = \kappa_1 > \kappa_2 > \kappa_3 \dots. \quad (2-149)$$

Now suppose our initial guess is a linear combination of these solutions

$$F_0 = \sum_l \alpha_l F^l. \quad (2-150)$$

Applying the operator,  $A$ ,  $n$  times yields

$$A^n F_0 = \sum_l \alpha_l \kappa_l^n F^l = \alpha_1 \kappa_1^n F^1 + \sum_{l>1} \alpha_l \kappa_l^n F^l. \quad (2-151)$$

But it is clear from Eq. 2-149 that as  $n$  becomes large,  $(\kappa_l/\kappa_1)^n$  tends toward zero for  $l > 1$ . This causes the terms in the sum on the right to vanish as compared to the first term, yielding

$$A^n F_0 \rightarrow \alpha_1 \kappa_1^n F^1, \quad n \rightarrow \infty. \quad (2-152)$$

For the finite-differenced diffusion theory, these results have been proved mathematically.<sup>10</sup> For computational transport methods rigorous proof is often problematical. Nevertheless, in practice the power iteration is found to converge for all of the computational methods described in the following chapters.

The evaluation of  $\mathbf{H}^{-1}$  appearing in the preceding equations most often must be carried out iteratively. Thus power iteration often is referred to as the outer iteration, while the iterative processes used to obtain  $\mathbf{H}^{-1}$ , or more precisely the  $H_{gg}^{-1}$  of Eq. 2-81, are referred to as inner iterations. A difficult problem in the solution of transport criticality problems often arises in determining how tightly the inner iterations must be converged before one proceeds to the next outer iteration. If the inner iterations are converged

more tightly than necessary, a substantial amount of computer time may be wasted, but if they are not converged tightly enough the procedure may become unstable. Since there are few quantitative criteria, one frequently must rely on experience, folklore, and intuition.

Power iteration is the overwhelming choice for the solution of neutronics eigenvalue problems. The rate of convergence, however, may be quite slow in some situations. If  $\kappa_1 - \kappa_2 \ll 1$ , Eq. 2-151 indicates that the error terms in the successive estimate of the fission distribution, and therefore of the fundamental mode, will decay very slowly. Such situations tend to arise particularly in neutronically loosely coupled systems, in which the dimensions are large compared to the root-mean-squared distance traveled by neutrons between fission and absorption. Because of the importance of power iteration, a variety of acceleration methods have been developed to reduce the number of iterations required to obtain a given level of accuracy in  $k$  and the fission distribution. We briefly discuss three classes of these: extrapolation techniques,<sup>10, 11</sup> coarse mesh rebalance,<sup>11-13</sup> and synthetic acceleration.<sup>20, 21</sup>

While the power iterations may be formulated in terms of the fission neutron distribution,  $F(\vec{r})$ , acceleration techniques often require modifications to be made to the angular or scalar flux iterates. Thus before proceeding, we reformulate the power iteration in terms of the angular flux. We first write Eq. 2-137 in an iterative form equivalent to Eq. 2-143:

$$\tilde{\psi}_i = \frac{1}{k_i} \mathbf{H}^{-1} \chi \mathbf{f}^T \int d\Omega \psi_i, \quad (2-153)$$

where  $\tilde{\psi}_i$  is the unaccelerated iterate. The unaccelerated fission distribution

$$\tilde{F}_i = \mathbf{f}^T \int d\Omega \tilde{\psi}_i \quad (2-154)$$

is then given in terms of  $F_i$  by

$$\tilde{F}_i = \frac{1}{k_i} A F_i \quad (2-155)$$

with the operator  $A$  again defined by Eq. 2-141. With no acceleration we have simply

$$\psi_{i+1} = \tilde{\psi}_i, \quad (2-156)$$

and

$$F_{i+1} = \tilde{F}_i. \quad (2-157)$$

The unaccelerated eigenvalue is obtained from Eq. 2-146, which may be written in terms of the angular flux as

$$k_{i+1} = k_i \frac{\int dV w \mathbf{f}^T \int d\Omega \Psi_{i+1}}{\int dV w \mathbf{f}^T \int d\Omega \Psi_i}. \quad (2-158)$$

### Acceleration by Extrapolation Methods

A number of extrapolation methods may be used to improve the iterates of flux or fission sources. The simplest of these is overrelaxation. Applied to the fission neutron source, the  $(i + 1)$ th iterate of  $F(\vec{r})$  is obtained by first determining the unaccelerated iterate  $\tilde{F}_i$  from Eq. 2-155. For no acceleration we would then have  $F_{i+1} = \tilde{F}_i$ . Instead we take

$$F_{i+1} = \omega (\tilde{F}_i - F_i) + F_i, \quad (2-159)$$

where  $1 \leq \omega < 2$ , is the overrelaxation factor. More frequently used is Chebychev's polynomial acceleration,<sup>10, 11</sup> where the accelerated fission distribution is determined from

$$F_{i+1} = F_i + \alpha_{i+1} (\tilde{F}_i - F_i) + \beta_i (F_i - F_{i-1}). \quad (2-160)$$

Here the acceleration parameters  $\alpha_i$  and  $\beta_i$  are iteration dependent; they are chosen for optimal attenuation of the higher eigenmodes in Eq. 2-148 through the use of Chebychev polynomials. The theory is the same for transport as for diffusion calculations, and for the latter case it is developed in detail elsewhere.<sup>10</sup>

### Acceleration by the Rebalance Method

As discussed in Section 2-3, the idea of rebalance<sup>12</sup> consists of multiplying the unaccelerated flux by a spatial function  $g(\vec{r})$  such that the new flux iterate is given by

$$\Psi_{i+1} = \tilde{\Psi}_i g(\vec{r}). \quad (2-161)$$

To determine  $g(\vec{r})$  we require that  $\Psi_{i+1}$  satisfy the transport equation in the following weighted residual sense. First integrate Eq. 2-137 over all angle and then sum over energy group by premultiplying by the weight factor

$$\mathbf{1}^T \equiv \{1, 1, \dots, 1\} \quad (2-162)$$

to obtain

$$\mathbf{1}^T \int d\Omega \mathbf{H} \psi = \frac{1}{k} \mathbf{1}^T \chi \mathbf{f}^T \int d\Omega \psi, \quad (2-163)$$

where we have used the normalization condition  $\int d\Omega = 1$ .

Requiring this balance equation to be satisfied by  $\psi_{i+1}$  and  $k_{i+1}$  then yields

$$\left[ \mathbf{1}^T \int d\Omega \mathbf{H} \tilde{\psi}_i \right] g(\vec{r}) = \frac{1}{k_{i+1}} \left[ \mathbf{1}^T \chi \mathbf{f}^T \int d\Omega \tilde{\psi}_i \right] g(\vec{r}). \quad (2-164)$$

Note that we must solve an eigenvalue problem for  $g(\vec{r})$  and for  $k_{i+1}$  each time we apply rebalance. Unlike the calculation for  $\tilde{\psi}_i$ , however, the inverse operator  $\mathbf{H}^{-1}$  no longer appears. Thus to evaluate the bracketed coefficients we need only evaluate integrals of the known function  $\tilde{\psi}_i$ .

In this form, the differenced equation would be referred to as fine mesh rebalance since  $g(\vec{r})$ , in general, would have the same detail in spatial distribution as the flux iterates  $\tilde{\psi}_i$ . In coarse mesh rebalancing  $g(\vec{r})$  is expressed as a linear combination of known functions  $g_l(\vec{r})$ . Thus Eq. 2-161 is replaced by

$$\psi_{i+1} = \tilde{\psi}_i \sum_{l'} \gamma_{l'} g_{l'}(\vec{r}). \quad (2-165)$$

The coefficients are determined by the following weighted residual technique; Eq. 2-164 is multiplied by a series of known spatial weight functions  $h_l(\vec{r})$  and integrated over the problem volume. Then, upon substituting in Eq. 2-164 for  $\psi_{i+1}$  we obtain

$$\sum_{l'} \left[ \int dV h_l \mathbf{1}^T \int d\Omega \mathbf{H} \psi_i g_{l'} \right] \gamma_{l'} - \frac{1}{k_{i+1}} \mathbf{1}^T \chi \sum_{l'} \int dV h_l \mathbf{f}^T \int d\Omega \tilde{\psi}_i g_{l'} \right] \gamma_{l'} = 0. \quad (2-166)$$

Since the number of terms in the series may be relatively small compared to the spatial mesh upon which  $\tilde{\psi}_i$  is calculated, the solution of this equation is much less time consuming than that of the transport equation. Nevertheless, the method is not usually employed after each iteration, for the time required to evaluate the coefficients from Eq. 2-166 and to solve the coarse mesh eigenvalue problem may be equivalent to several power iterations.

The most common choice for coarse mesh rebalance is to make the function piecewise constant over sub or rebalance volumes of the problem

domain.<sup>12</sup> Thus we designate

$$V = \sum_l V_l \quad (2-167)$$

and  $\Gamma_l$  is the surface of  $V_l$  with outward normal  $\hat{n}_l$ . Then

$$g_l(\vec{r}) = \begin{cases} g_l, & \vec{r} \in V_l, \\ 0, & \vec{r} \notin V_l, \end{cases} \quad (2-168)$$

and  $h_l(\vec{r}) = g_l(\vec{r})$ , and the method is analogous to the rebalance scheme of Section 2-3.

Since the  $\hat{\Omega} \cdot \vec{\nabla}$  operator included in  $\mathbf{H}$  operates on  $g_l$ , care must be taken in specifying the discontinuous behavior of  $g_l(\vec{r})$  at the  $\Gamma_l$  surfaces. By taking

$$g_l(\vec{r}) = \begin{cases} g_l, & \vec{r} \in \Gamma_l, \hat{n}_l \cdot \hat{\Omega} > 0, \\ g_{l'}, & \vec{r} \in \Gamma_l, \hat{n}_l \cdot \hat{\Omega} < 0, \end{cases} \quad (2-169)$$

neutrons leaving  $V_l$  are weighted by  $g_l$ , while those entering  $V_l$  are weighted by the  $g_{l'}$  for the rebalance volume from which they are emerging. The significance of this condition is discussed in Section 2-3 with regard to the acceleration of inner iterations.

### Synthetic Acceleration Methods

Synthetic methods are characterized by the use of a low-order angular approximation—most often diffusion theory—to accelerate the iterative solution of a higher order representation of the transport equation,<sup>18, 20, 21</sup> The methods were first introduced for the acceleration of fixed-source problems, as discussed in Section 2-3. More recently they have been successfully applied in transport criticality calculations. Before discussing three variants of synthetic eigenvalue acceleration, we first set forth some necessary properties that are common to all of the methods.

We begin by writing

$$\mathbf{G} = \chi \mathbf{f}^T \quad (2-170)$$

and expressing the fission term of Eq. 2-137 in terms of the scalar flux:

$$\mathbf{H}\psi = \frac{1}{k} \mathbf{G}\phi. \quad (2-171)$$

For synthetic acceleration we require that the transport equation be integrated over angle. With the normalization,  $\int d\Omega = 1$ , we obtain

$$\int d\Omega \mathbf{H}\psi = \frac{1}{k} \mathbf{G}\phi, \quad (2-172)$$

since

$$\int d\Omega \mathbf{G}\phi = \mathbf{G}\phi. \quad (2-173)$$

For our low-order approximation we use diffusion theory. The diffusion approximation to Eq. 2-171 is

$$\mathbf{H}_L\phi_L = \frac{1}{k_L} \mathbf{G}\phi_L, \quad (2-174)$$

where the diffusion-scattering operator is

$$[\mathbf{H}_L]_{gg'} = \delta_{gg'} \left[ -\vec{\nabla} D_g(\vec{r}) \vec{\nabla} + \sigma_g(\vec{r}) \right] - \sigma_{gg'}(\vec{r}), \quad (2-175)$$

with the  $D_g$ ,  $\sigma_g$ , and  $\sigma_{gg'}$  being the diffusion coefficients, total cross sections, and group-to-group scattering cross sections, respectively. We hereafter take  $k_L$  as the largest positive eigenvalue and  $\phi_L$  as the corresponding nonnegative fundamental mode solution of Eq. 2-174.

We also shall have need of the adjoint multigroup diffusion equations. The adjoint operators for the multigroup approximation are defined in a manner similar to the continuous energy operators discussed in Chapter 1. Let  $\xi(\vec{r})$  and  $\xi_*(\vec{r})$  be any two vectors that are continuous in  $\vec{r}$  and go to zero on the surface  $\Gamma$  of the problem domain  $V$ . We require that the adjoint operators  $\mathbf{H}_L^+$  and  $\mathbf{G}^+$  satisfy

$$\int dV \xi_*^T \mathbf{H}_L \xi = \int dV \xi_*^T \mathbf{H}_L^+ \xi_* \quad (2-176)$$

and

$$\int dV \xi_*^T \mathbf{G} \xi = \int dV \xi_*^T \mathbf{G}^+ \xi. \quad (2-177)$$

The adjoint diffusion equation is

$$\mathbf{H}_L^+ \phi_* = \frac{1}{k_L} \mathbf{G}^+ \phi_*, \quad (2-178)$$

where  $\phi_*$  is the adjoint fundamental mode solution. It is easily shown that

$$\mathbf{G}^+ = \mathbf{f} \chi^T, \quad (2-179)$$

$$[\mathbf{H}_L^+]_{gg'} = [\mathbf{H}_L]_{g'g}, \quad (2-180)$$

and that the largest eigenvalue  $k_L$  appearing in Eq. 2-178 is identical to that appearing in Eq. 2-174. By using Eqs. 2-176 through 2-178 the following useful identity is easily proven:

$$\int dV \phi_*^T \mathbf{H}_L \phi = \frac{1}{k_L} \int dV \phi_*^T \mathbf{G} \phi. \quad (2-181)$$

We are now prepared to develop three variants of the synthetic method. In each case we assume that the adjoint diffusion problem has been solved, so that  $k_L$  and  $\phi_*$  are known.

**First Variant.** We begin by writing  $\mathbf{H}$  in Eq. 2-172 as the sum of  $\mathbf{H}_L$  and a correction ( $\mathbf{H} - \mathbf{H}_L$ ):

$$\int d\Omega [\mathbf{H}_L + (\mathbf{H} - \mathbf{H}_L)] \psi = \frac{1}{k} \mathbf{G} \phi. \quad (2-182)$$

Rearranging terms gives

$$\mathbf{H}_L \phi = \frac{1}{k} \mathbf{G} \phi - \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi, \quad (2-183)$$

where since  $\mathbf{H}_L$  is independent of  $\hat{\Omega}$ ,

$$\int d\Omega \mathbf{H}_L \psi = \mathbf{H}_L \phi. \quad (2-184)$$

If we multiply Eq. 2-183 by  $\phi_*^T$  and integrate over the volume  $V$ , then

$$\int dV \phi_*^T \mathbf{H}_L \phi = \frac{1}{k} \int dV \phi_*^T \mathbf{G} \phi - \int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi. \quad (2-185)$$

Using Eq. 2-181, we may immediately reduce this expression to

$$\frac{1}{k} = \frac{1}{k_L} + \frac{\int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi}{\int dV \phi_*^T \mathbf{G} \phi}. \quad (2-186)$$

Provided the difference between the operators  $\mathbf{H}$  and  $\mathbf{H}_L$  is not large, Eqs. 2-183 and 2-186 provide a basis for an acceleration method in which  $k$  is estimated in terms of  $k_L$  and a correction term. Our unaccelerated power iterate is defined from Eq. 2-171:

$$\mathbf{H}\tilde{\psi}_i = \frac{1}{k_i} \mathbf{G}\phi_i. \quad (2-187)$$

Then we use  $\tilde{\psi}_i$  in the numerator of Eq. 2-186 to estimate a new eigenvalue,

$$\frac{1}{k_{i+1}} = \frac{1}{k_L} + \frac{\int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \tilde{\psi}_i}{\int dV \phi_*^T \mathbf{G} \phi_i}. \quad (2-188)$$

With  $k_{i+1}$  calculated, we use Eq. 2-183 to estimate  $\phi_{i+1}$ :

$$\mathbf{H}_L \phi_{i+1} = \frac{1}{k_{i+1}} \mathbf{G} \phi_i - \int d\Omega (\mathbf{H} - \mathbf{H}_L) \tilde{\psi}_i. \quad (2-189)$$

These three equations constitute an acceleration method; Eq. 2-187 and the properties of the adjoint operators may be used to write the acceleration iteration procedure in a computationally more convenient form involving only the scalar flux:

$$\tilde{\phi}_i = \frac{1}{k_i} \int d\Omega \mathbf{H}^{-1} \mathbf{G} \phi_i, \quad (2-190)$$

$$\frac{1}{k_{i+1}} = \frac{1}{k_i} - \frac{1}{k_L} \frac{\int dV \phi_*^T \mathbf{G} (\tilde{\phi}_i - \phi_i)}{\int dV \phi_*^T \mathbf{G} \phi_i}, \quad (2-191)$$

$$\mathbf{H}_L (\phi_{i+1} - \tilde{\phi}_i) = \left( \frac{1}{k_{i+1}} - \frac{1}{k_i} \right) \mathbf{G} \phi_i. \quad (2-192)$$

Clearly as  $\tilde{\phi}_i \rightarrow \phi_i$  the accelerated iteration converges to the correct solution. Each time that the acceleration is applied one fixed-source multigroup diffusion problem must be solved to obtain  $\mathbf{H}_L^{-1}$ . It is expected, however, that most often the bulk of the computation time will be incurred in solving Eq. 2-190 for the unaccelerated flux, since the inverting of the transport

operation  $\mathbf{H}$  usually involves convergence of an inner iteration at each energy group. To eliminate such inner iterations a second variant of synthetic eigenvalue acceleration has been proposed.

**Second Variant<sup>20</sup>** To eliminate the inner iterations we replace Eq. 2-187 by a different unaccelerated iteration:

$$\mathbf{H}^0 \tilde{\psi}_i = \frac{1}{k_i} \mathbf{G} \phi_i + \mathbf{H}^1 \phi_i. \quad (2-193)$$

Here  $\mathbf{H}^0$  and  $\mathbf{H}^1$  are respectively the multigroup streaming-collision and scattering operators as defined in Eqs. 2-114 and 2-115. For brevity we assume isotropic scattering, and hence  $\mathbf{H}^1 \psi = \mathbf{H}^1 \phi$ . We choose the form of Eq. 2-193 because we may often invert the streaming collision operator  $\mathbf{H}^0$  conveniently, without recourse to iterative techniques.

For acceleration, we derive identities similar to Eqs. 2-183 and 2-186. First we write Eq. 2-172 in terms of  $H_L$ ,  $k_L$  and corrections:

$$\int d\Omega [\mathbf{H}_L + (\mathbf{H} - \mathbf{H}_L)] \psi = \left[ \frac{1}{k_L} + \left( \frac{1}{k} - \frac{1}{k_L} \right) \right] \mathbf{G} \phi. \quad (2-194)$$

Using Eq. 2-184 and rearranging terms, we obtain

$$\left( \mathbf{H}_L - \frac{1}{k_L} \mathbf{G} \right) \phi = \left( \frac{1}{k} - \frac{1}{k_L} \right) \mathbf{G} \phi - \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi. \quad (2-195)$$

Once again we multiply by  $\phi_*^T$  and integrate over the reactor volume to obtain

$$\begin{aligned} \int dV \phi_*^T \left( \mathbf{H}_L - \frac{1}{k_L} \mathbf{G} \right) \phi &= \left( \frac{1}{k} - \frac{1}{k_L} \right) \int dV \phi_*^T \mathbf{G} \phi \\ &\quad - \int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi. \end{aligned} \quad (2-196)$$

From Eq. 2-181, the left-hand side is seen to vanish. Hence we obtain, once again,

$$\frac{1}{k} = \frac{1}{k_L} + \frac{\int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \psi}{\int dV \phi_*^T \mathbf{G} \phi}. \quad (2-197)$$

Used in conjunction with Eq. 2-193, the following iterative acceleration is suggested:

$$\frac{1}{k_{i+1}} = \frac{1}{k_L} + \frac{\int dV \phi_*^T \int d\Omega (\mathbf{H} - \mathbf{H}_L) \tilde{\psi}_i}{\int dV \phi_*^T \mathbf{G} \phi_i} \quad (2-198)$$

and

$$\left[ \mathbf{H}_L - \frac{1}{k_L} \mathbf{G} \right] \phi_{i+1} = \left( \frac{1}{k_{i+1}} - \frac{1}{k_L} \right) \mathbf{G} \phi_i - \int d\Omega (\mathbf{H} - \mathbf{H}_L) \tilde{\psi}_i. \quad (2-199)$$

As in the case of the first variant we may use the structure of Eq. 2-193 and the adjoint operator properties to write the iteration in the more convenient form

$$\tilde{\phi}_i = \int d\Omega (\mathbf{H}^0)^{-1} \left[ \frac{1}{k_i} \mathbf{G} + \mathbf{H}^1 \right] \phi_i, \quad (2-200)$$

$$\frac{1}{k_{i+1}} = \frac{1}{k_i} - \frac{\int dV \phi_*^T \left( \frac{1}{k_L} \mathbf{G} + \mathbf{H}^1 \right) (\tilde{\phi}_i - \phi_i)}{\int dV \phi_*^T \mathbf{G} \phi_i}, \quad (2-201)$$

and

$$\left( \mathbf{H}_L - \frac{1}{k_L} \mathbf{G} \right) (\phi_{i+1} - \tilde{\phi}_i) = \left( \frac{1}{k_{i+1}} - \frac{1}{k_i} \right) \mathbf{G} \phi_i + \left( \frac{1}{k_L} \mathbf{G} + \mathbf{H}^1 \right) (\tilde{\phi}_i - \phi_i), \quad (2-202)$$

which converges as  $\tilde{\phi}_i \rightarrow \phi_i$ . We have now eliminated the need for inner iterations in obtaining  $\tilde{\phi}_i$ , but at the expense of requiring a more extensive diffusion calculation. For inverting  $[\mathbf{H}_L - (1/k_L)\mathbf{G}]$  entails a comparable effort to solving a subcriticality problem; a power iteration solution of the diffusion problem is required at each iteration step  $i$ , and this in turn may require acceleration.

**Third Variant<sup>21</sup>** A third variant of the synthetic methods was developed earlier and independently of the foregoing formulations. For brevity, how-

ever, we treat it as a variant of the preceding method. Suppose we let the low-order operator become iteration dependent,  $\mathbf{H}_L \rightarrow \mathbf{H}_L^i$ , and hence the low-order eigenvalue also becomes iteration dependent,  $k_L \rightarrow k_L^i$ . In particular at each iteration we choose  $\mathbf{H}_L^i$  such that

$$\int d\Omega (\mathbf{H} - \mathbf{H}_L^i) \tilde{\psi}_i = 0. \quad (2-203)$$

If this can be accomplished, then instead of Eqs. 2-198 and 2-199, we have for our iteration scheme simply

$$k_{i+1} = k_L^i \quad (2-204)$$

and

$$\left[ H_L^i - \frac{1}{k_L^i} G \right] \phi_{i+1} = 0. \quad (2-205)$$

To impose Eq. 2-203, the diffusion coefficients and removal cross sections of  $\mathbf{H}_L^i$  are allowed to become functions of  $\tilde{\psi}_i$ .

Synthetic methods have led to spectacular accelerations in many cases.<sup>22</sup> Such techniques, however, must be used with care. For if  $\mathbf{H}_L$  is differenced by a technique that is incompatible with that applied to the transport operator, instabilities may arise. The nonlinear third variant also may lead to another difficulty. If in satisfying Eq. 2-203 negative or infinite diffusion coefficients or other anomalies are introduced, the technique may become unstable. We return to the subject of differencing acceleration equations at the end of Chapter 3.

## 2-5 TIME-DEPENDENT PROBLEMS

In most situations numerical solutions are sought to the time-independent transport equation in either the fixed source or eigenvalue forms discussed in the preceding sections. In the analysis of pulsed neutron experiments, in the photon transport problems encountered in the dynamics of stellar atmospheres, and in the kinetics of nuclear reactors it is necessary to follow the time-dependent behavior of particle transport problems. The characteristic times at which such systems evolve frequently are very short, being determined by the mean particle life between birth and death. For photons it is the speed of light multiplied by the total track length of the particle to the point of absorption. For neutrons it is much longer because of the

slower velocities. But even then neutrons lifetimes typically range from about  $10^{-4}$  to  $10^{-8}$  seconds depending on the systems under consideration.

As a result of these characteristics, very short time steps usually are required in the discretization of transport problems, and even very long running problems may cover only a fraction of a second. Reactor kinetics present a particularly difficult computational problem, for the time-dependent behavior is governed by the  $10^{-4}$  to  $10^{-8}$  second life of neutrons produced promptly at the time of fission on the one hand, and the delayed neutrons produced by the decay of fission products on the other.<sup>23</sup> The characteristic half lives of delayed neutrons range from times of a second up to nearly a minute, and therefore in the many situations where delayed neutron behavior is the governing factor, transients may run over many minutes, even while the time differencing is governed by the prompt neutron lifetime.

As a result of the wide disparity in characteristic times encountered in reactor kinetics equations, a great deal of effort has been required to develop approximation methods that allow longer time steps to provide adequate representation of slower transients. Such methods invariably take the few energy group diffusion approximations as a starting point. Additional adiabatic or quasi-static approximations to the space-time coupling are most often employed in order to make the methods tractable for slower transients. Such methods are covered in advanced reactor theory texts<sup>1,2</sup> but fall outside the scope of transport computational methods.

In superprompt critical excursions, where the multiplication exceeds the delayed neutron fraction, the time dependence is determined by prompt neutron behavior and hence the transient is rapid compared to the delayed neutron half lives.<sup>23</sup> In such cases the prompt neutron approximation, in which delayed neutrons are ignored, often is used in conjunction with the transport equation. In the following subsection we first write the multigroup kinetics equation in a convenient operator form and then reduce it to the prompt neutron transport equation. This form of the transport equation, which is also applicable to problems in nonmultiplying media and for photon transport, is then used as a basis for examining a number of techniques for discretizing the time variable. We conclude the section by demonstrating a method for carrying out time discretization when the effects of delayed neutrons must also be taken into account. As in the preceding sections, no discretization is applied in space or angle, that being the topic of the following chapters.

### Forms of the Kinetics Equations

As a point of departure we take the multigroup kinetics equations given by Eqs. 2-32 and 2-33. We may extend the operator notation of the preceding

section to write these equations in more compact form. Let

$$\tilde{\mathbf{f}}_i^T = \{ \nu \sigma_{f1}^i, \nu \sigma_{f2}^i, \dots, \nu \sigma_{fg}^i \} \quad (2-206)$$

be the fission neutron operator for the  $i$ th fissionable isotope. Also,

$$\chi_p^T = \{ \chi_{p1}, \chi_{p2}, \dots, \chi_{pg}, \dots, \chi_{pG} \} \quad (2-207)$$

and

$$\chi_l^T = \{ \chi_{l1}, \chi_{l2}, \dots, \chi_{lg}, \dots, \chi_{lG} \} \quad (2-208)$$

are the multigroup fission spectra for prompt neutrons and for neutrons of delayed group  $l$  respectively. If we define the diagonal matrix

$$[\mathbf{V}]_{gg'} = \delta_{gg'} v_g \quad (2-209)$$

of group neutron speeds, then Eqs. 2-32 and 2-33 may be written as

$$\mathbf{V}^{-1} \frac{\partial \psi}{\partial t} + \mathbf{H}\psi = \chi_p \sum_i (1 - \beta^i) \tilde{\mathbf{f}}_i^T \int d\Omega \psi + \sum_l \chi_l \lambda_l C_l + \mathbf{q}^e, \quad (2-210)$$

and

$$\frac{\partial C_l}{\partial t} = \sum_i \beta_l^i \tilde{\mathbf{f}}_i^T \int d\Omega \psi - \lambda_l C_l, \quad (2-211)$$

where  $\mathbf{H}$  is the nonmultiplying transport operator defined by Eqs. 2-74 through 2-78.

We next divide the fission operator into prompt and delayed components

$$\mathbf{f} = \mathbf{f}_p + \mathbf{f}_d, \quad (2-212)$$

where

$$\mathbf{f}_p = \sum_i (1 - \beta^i) \tilde{\mathbf{f}}_i, \quad (2-213)$$

$$\mathbf{f}_d = \sum_i \beta_i^l \tilde{\mathbf{f}}_i. \quad (2-214)$$

We then have for the kinetics equations,

$$\mathbf{V}^{-1} \frac{\partial \psi}{\partial t} + \mathbf{H}\psi = \chi_p \mathbf{f}_p^T \int d\Omega \psi + \sum_l \chi_l \lambda_l C_l + \mathbf{q}^e \quad (2-215)$$

and

$$\frac{\partial C_l}{\partial t} = \mathbf{f}_d^T \int d\Omega \psi - \lambda_l C_l. \quad (2-216)$$

Under some circumstances the time-dependent behavior of Eq. 2-215 is so rapid that the more sluggish behavior of the delayed neutrons has little effect on the transient. This occurs when the reactor is superprompt critical, which means that the neutron population will increase even if the contribution of the delayed neutrons is neglected. Roughly speaking, this condition exists when the fission term is larger than the streaming-collision scattering term  $\mathbf{H}\psi$ . More precisely, if the prompt eigenvalue problem

$$\mathbf{H}\psi = \frac{1}{k_p} \chi_p \mathbf{f}_p^T \int d\Omega \psi \quad (2-217)$$

has a largest eigenvalue  $k_p > 1$  for  $\psi > 0$  in the reactor volume, the reactor is said to be superprompt critical. For such situations we obtain the prompt neutron approximation simply by setting the decay constants equal to zero in Eq. 2-215:

$$\mathbf{V}^{-1} \frac{\partial \psi}{\partial t} + \mathbf{H}\psi = \chi_p \mathbf{f}_p^T \int d\Omega \psi + \mathbf{q}^e. \quad (2-218)$$

Significant gains in accuracy often are obtained if delayed neutrons are included while assuming that the time derivative of  $C_i$  can be taken to be so small, relative to the derivative of  $\psi$ , that the delayed neutron term in the kinetics equation remains essentially constant. This approximation is easily accommodated in the prompt neutron approximation by replacing  $\mathbf{q}^e$  in Eq. 2-218 by

$$\mathbf{q}^e + \left. \sum_i \chi_i \lambda_i C_i \right|_{t=0}. \quad (2-219)$$

### Differencing of the Prompt Neutron Approximation

The two most straightforward methods for discretizing the time variable are explicit and fully implicit differencing.<sup>11, 24</sup> These techniques as well as the other method described in the following subsection may be formulated in a common framework by defining the time steps according to

$$t_{j+1} = t_j + \Delta_j \quad (2-220)$$

and integrating the kinetics equations between  $t_j$  and  $t_{j+1}$ ,

$$\mathbf{V}^{-1}(\psi_{j+1} - \psi_j) = \int_{t_j}^{t_{j+1}} dt \left\{ -\mathbf{H}\psi + \chi_p \mathbf{f}_p^T \int d\Omega \psi + \mathbf{q}^e \right\}, \quad (2-221)$$

where we have introduced the time discretization as

$$\psi_j \approx \psi(\vec{r}, \hat{\Omega}, t_j). \quad (2-222)$$

Explicit and implicit methods differ in the manner in which the time integral on the right of Eq. 2-221 is evaluated. For explicit differencing we approximate the integral as  $\Delta_j$  multiplied by the bracketed integrand evaluated at  $t_j$ . In this manner everything on the right of the equations is known from the previous time step and we may march forward in time according to

$$\psi_{j+1} = \psi_j + \Delta_j \mathbf{V} \left\{ -\mathbf{H}\psi_j + \chi_p \mathbf{f}_p^T \int d\Omega \psi_j + \mathbf{q}_j^e \right\}. \quad (2-223)$$

In the fully implicit method the right-hand side of Eq. 2-221 is approximated as  $\Delta_j$  multiplied by the bracketed integrands evaluated at  $t_{j+1}$ . Since the terms on the right now depend on  $\psi_{j+1}$ , solution of the resulting equation has the implicit form

$$\left\{ \frac{1}{\Delta_j} \mathbf{V}^{-1} + \mathbf{H} - \chi_p \mathbf{f}_p^T \int d\Omega \right\} \psi_{j+1} = \mathbf{q}_{j+1}^e + \frac{1}{\Delta_j} \mathbf{V}^{-1} \psi_j. \quad (2-224)$$

A comparison of the explicit and the fully implicit differencing is instructive. As indicated in Appendix B the accuracy of the time differencing in both cases is of order  $\Delta_j$ , meaning that very small time steps must be taken in both cases if adequate accuracy is to be obtained. In the explicit method relatively little effort need be expended at each time step since no inversion of the transport operator  $\mathbf{H}$  is required. Conversely the implicit method requires that we invert the operator on the left of Eq. 2-224; this may involve an amount of work comparable to solving an eigenvalue problem, such as Eq. 2-137, at each time step.

While the explicit method is desirable from the standpoint of computational effort per time step, another criterion may be overriding: stability. As discussed in Appendix B, we must be concerned not only with the discretization errors introduced at each time step in the calculation, but also with the propagation of the errors from step to step. For if the errors grow faster than the solution, the algorithm is unstable. To study such stability in detail one must examine the equations, not in the form that they are written above, but rather after the discretization of the space and angular variables has been completed. For systems of such time-dependent differential equations, fully implicit methods usually are found to be stable regardless of the

time step  $\Delta_j$ .<sup>24</sup> The spatially differenced forms of explicit methods, however, become unstable if the time step is too large. Moreover, the criterion for explicit methods that  $\Delta_j/\Delta_x$ , or  $\Delta_j/\Delta_x^2$  (where  $\Delta_x$  is the spatial mesh spacing) be less than some characteristic number often places a stringent criterion on the size of the time step, and one that becomes more severe as the spatial grid is refined.<sup>25-27</sup> Thus one must weigh the increased effort per time spent with implicit methods against the requirements for smaller time steps with explicit methods.

We next examine the so-called diamond differencing method for time discretization. It has the desirable property that the time differencing may be shown to be accurate to order  $\Delta_j^2$  as opposed to  $\Delta_j$  for the preceding schemes. Moreover, use of the technique in conjunction with discrete ordinates approximations had indicated that its stability properties are better than those of the explicit scheme, even though the time step may be severely limited if nonphysical oscillations in the flux are to be avoided.<sup>26</sup>

We begin with Eq. 2-221 and approximate the integral on the right as  $\Delta_j$  times the integrand evaluated at  $t_{j+1/2}$ :

$$\mathbf{V}^{-1}(\psi_{j+1} - \psi_j) = \Delta_j \left\{ -\mathbf{H}\psi_{j+1/2} + \mathbf{x}_p \mathbf{f}_p^T \int d\Omega \psi_{j+1/2} + \mathbf{q}_{j+1/2}^e \right\}. \quad (2-225)$$

To eliminate one of the unknowns the diamond differencing relationship,

$$\psi_{j+1/2} = \frac{1}{2}(\psi_j + \psi_{j+1}), \quad (2-226)$$

is used. By rewriting this relationship as

$$\psi_{j+1} = 2\psi_{j+1/2} - \psi_j \quad (2-227)$$

we may eliminate  $\psi_{j+1}$  from Eq. 2-225 to yield

$$\left[ \frac{2}{\Delta_j} \mathbf{V}^{-1} + \mathbf{H} - \mathbf{x}_p \mathbf{f}_p^T \int d\Omega \right] \psi_{j+1/2} = \mathbf{q}_{j+1/2}^e + \frac{2}{\Delta_j} \mathbf{V}^{-1} \psi_j. \quad (2-228)$$

Thus Eqs. 2-228 and 2-227 may be solved alternately for  $\psi_{1/2}$ ,  $\psi_1$ ,  $\psi_{3/2}$ , and so on. Note that the transport operator on the left of Eq. 2-228 must be inverted, however, at each time step.

## Delayed Neutron Kinetics

When delayed neutron behavior must be considered the foregoing techniques are complicated by the need also to follow the precursor equations

and to follow transients for longer time periods. As a result, the following semi-implicit method has been implemented with the objective of preserving some of the stability benefits of the fully implicit method without requiring time-consuming iteration methods for the inversion of the transport operator at each time step.<sup>28</sup> The method—unlike diamond differencing, however—is accurate only to order  $\Delta_j$  in the time variable.

The two properties to be introduced into the equations are as follows. First, we wish to proceed successively through the energy group structure from  $g = 1$  to  $g = G$  only once per time step, eliminating the repeated iteration on the fission source that would be required in the fully implicit method. Second, within each energy group we do not want to invert  $\mathbf{H}_{gg}$ , for this often must involve a within-group or inner iteration that can be very time consuming. To avoid this, we split the transport matrix into streaming-collision and scattering contributions as in Eq. 2-76 and invert only the streaming-collision contribution  $\mathbf{H}^0$  at each time step.

To implement these properties, we begin with Eqs. 2-215 and 2-216, and integrate over a time step to obtain a flux equation analogous to Eq. 2-221. Using Eq. 2-76 to separate streaming-collision from scattering terms, and combining the scattering and prompt fission operators as

$$\mathbf{R} = \mathbf{H}^1 + \chi_p \mathbf{f}_p^T \int d\Omega, \quad (2-229)$$

we obtain

$$\mathbf{V}^{-1}(\psi_{j+1} - \psi_j) = \int_{t_j}^{t_{j+1}} dt \left\{ -\mathbf{H}^0 \psi + \mathbf{R} \psi + \sum_l \chi_l \lambda_l C_l + \mathbf{q}^e \right\}. \quad (2-230)$$

We evaluate the integral on the right by multiplying  $\Delta_j$  by an integrand. For the streaming-collision and external source terms the integrand is evaluated at  $t_{j+1}$ , while the delayed neutron term is evaluated at  $t_j$ . Hence

$$\left[ \frac{1}{\Delta_j} \mathbf{V}^{-1} + \mathbf{H}^0 \right] \psi_{j+1} = \frac{1}{\Delta_j} \int_{t_j}^{t_{j+1}} dt \mathbf{R} \psi + \frac{1}{\Delta_j} \mathbf{V}^{-1} \psi_j + \sum_l \chi_l \lambda_l C_{lj} + \mathbf{q}_{j+1}^e. \quad (2-231)$$

We now divide the scattering-prompt fission term into two contributions:

$$\mathbf{R} = \mathbf{U} + \mathbf{L}, \quad (2-232)$$

where  $\mathbf{U}$  is the upper triangular matrix operator,

$$[\mathbf{U}]_{gg'} = \begin{cases} [\mathbf{R}]_{gg'}, & g \leq g', \\ \mathbf{0}, & g > g', \end{cases} \quad (2-233)$$

and  $\mathbf{L}$  is the strictly lower triangular matrix,

$$[\mathbf{L}]_{gg'} = \begin{cases} \mathbf{0}, & g \leq g', \\ [\mathbf{R}]_{gg'}, & g > g'. \end{cases} \quad (2-234)$$

We then evaluate the integral in Eq. 2-231 by evaluating the upper triangular term at  $t_j$  and the strictly lower triangular term at  $t_{j+1}$ . The sought-after kinetics equation is then

$$\left[ \frac{1}{\Delta_j} \mathbf{V}^{-1} + \mathbf{H}^0 \right] \Psi_{j+1} = \mathbf{L} \Psi_{j+1} + \mathbf{q}_{j+1}^e + \left[ \mathbf{U} + \frac{1}{\Delta_j} \mathbf{V}^{-1} \right] \Psi_j + \sum_l \chi_l \lambda_l C_{lj}. \quad (2-235)$$

Since the Eqs. 2-216 governing the time-dependent behavior of  $C_l(t)$  have a simpler structure we can use fully implicit differencing to determine the  $C_{lj}$  at each time step:

$$C_{l,j+1} = \frac{1}{1 + \Delta_j \lambda_l} \left( C_{lj} + \Delta_j \mathbf{f}_d^T \int d\Omega \Psi_j \right). \quad (2-236)$$

The properties of these equations are noteworthy. The operator on the left of Eq. 2-235 is diagonal, with the term for the  $g$ th energy group being

$$\vec{\Omega} \cdot \vec{\nabla} + \left[ \sigma_g(\vec{r}) + \frac{1}{\Delta_j v_g} \right]. \quad (2-237)$$

Consequently, within each group, inversion of this operator is equivalent to a problem with no scattering, but for which  $1/(\Delta_j v_g)$  has been added to the absorption cross section. Since  $\mathbf{L} \Psi_{j+1}$  is strictly lower triangular, it includes only neutrons that are scattered from and are produced by fission in higher energy groups. Thus the equations can be solved successively for  $g = 1, 2, \dots, G$ . Neutrons entering group  $g$  from scattering or fission in the same or lower energy groups are evaluated as  $\mathbf{U} \Psi_i$  with the flux at the preceding time step.

Even with the improvements in this mixed method, the complexity of transport calculations and the time-step limitation imposed by the small

prompt lifetime of neutrons, have limited its implementation to one-dimensional, few energy-group problems in which the total time over which the calculation must proceed is relatively short.<sup>28</sup> When multidimensional problems over larger time periods are considered, computational economy usually requires that the diffusion approximation be imposed. As stated earlier, further approximations usually are made to achieve a quasi-separation of space and time through an adiabatic or quasi-static approximation. These methods allow space-energy calculations to be carried out at relatively infrequent intervals compared to the time steps used in the calculation. The methods that may be used depend strongly on the physics of the problems; they are treated elsewhere.<sup>1,2</sup>

## REFERENCES

1. G. I. Bell and S. Glasstone, *Nuclear Reactor Theory*, Van Nostrand Rienhold, New York, 1970.
2. A. F. Henry, *Nuclear-Reactor Analysis*, MIT Press, Cambridge, 1975.
3. G. I. Bell, G. E. Hansen, and H. A. Sandmeier, "Multitable Treatments of Anisotropic Scattering in  $S_N$  Multigroup Transport Calculations," *Nucl. Sci. Eng.* **28**, 376 (1967).
4. H. Goldstein, *Fundamental Aspects of Reactor Shielding*, Addison-Wesley, Reading, Mass., 1959.
5. A. Radkowsky (ed.), *Naval Reactors Physics Handbook*, Vol. 1, U.S. Atomic Energy Commission, Washington, DC., 1964.
6. F. G. Tricomi, *Integral Equations*, Wiley, New York, 1957.
7. B. G. Carlson and K. D. Lathrop, "Transport Theory—The Method of Discrete Ordinates," in *Computing Methods in Reactor Physics*, H. Greenspan, C. N. Kelber, and D. Okrent (eds.), Gordon and Breach, New York, 1968.
8. L. A. Hageman, "Numerical Methods and Techniques Used in the Two-Dimensional Neutron Transport Program TPT," *WAPD-TM-1125(6)*, Bettis Atomic Power Laboratory (1973).
9. K. D. Lathrop, "DTF-IV, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," *LA-3373*, Los Alamos Scientific Laboratory (1965).
10. R. S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, N.J., 1962.
11. S. Nakamura, *Computational Methods in Engineering and Science*, Wiley, New York, 1977.
12. K. D. Lathrop and F. W. Brinkley, "TWOTRAN-II: An Interfaced, Exportable Version of the TWOTRAN Code for Two-Dimensional Transport," *LA-4848-MS*, Los Alamos Scientific Laboratory (1973).
13. W. A. Rhoades and F. R. Mynatt, "The DOT-III Two-Dimensional Discrete Ordinates Transport Code," *ORNL-TM-4280*, Oak Ridge National Laboratory (1973).
14. W. H. Reed, "The Effectiveness of Acceleration Techniques for Iterative Methods in Transport Theory," *Nucl. Sci. Eng.* **45**, 245 (1971).

15. R. Froehlich, "A Theoretical Foundation for Coarse Mesh Variational Techniques," *GA-7870*, General Atomic (1967).
16. H. J. Kopp, "Synthetic Method Solution of the Transport Equation," *Nucl. Sci. Eng.* **17**, 65 (1963).
17. E. M. Gelbard and L. A. Hageman, "The Synthetic Method Applied to the  $S_N$  Equations," *Nucl. Sci. Eng.* **37**, 288 (1969).
18. E. A. Larsen, "Diffusion-Synthetic Acceleration Methods for the Discrete-Ordinates Equations," *Proc. ANS Topical Meeting on Advances in Reactor Computations*, Salt Lake City, March 28–30, 1983, American Nuclear Society (1983).
19. E. L. Wachspress, *Iterative Solution of Elliptic Systems*, Prentice-Hall, Englewood Cliffs, N.J., 1966.
20. E. M. Gelbard, C. H. Adams, D. R. McCoy, and E. W. Larsen, "Acceleration of Transport Eigenvalue Problems," *Trans. Am. Nucl. Soc.* **41**, 309 (1982).
21. R. E. Alcouffe, "Diffusion-Synthetic Acceleration Methods for the Diamond-Differenced Discrete-Ordinates Equations," *Nucl. Sci. Eng.* **64**, 344 (1977).
22. W. F. Miller, Jr., R. E. Alcouffe, G. E. Bosler, F. W. Brinkley, Jr., and R. D. O'Dell, "A Timing Comparison of Two-Dimensional Discrete-Ordinates Codes for Criticality Calculations," *Proc. ANS Topical Meeting on Computational Methods in Nuclear Engineering*, Williamsburg, Va., April 23–25, 1979, American Nuclear Society (1979).
23. G. R. Keepin, *Physics of Nuclear Kinetics*, Addison-Wesley, Reading, Mass., 1965.
24. R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial Value Problems*, Wiley, New York, 1967.
25. S. A. Dupree, H. A. Sandmeier, G. E. Hansen, W. W. Engle, Jr., and F. R. Mynatt, "Time-Dependent Neutron and Photon Transport Calculations Using the Method of Discrete Ordinates," *LA-4557*, Los Alamos Scientific Laboratory (1971).
26. K. D. Lathrop, R. E. Anderson, and F. W. Brinkley, "TRANZIT: A Program for Multigroup Time-Dependent Transport in  $(\rho, z)$  Cylindrical Geometry," *LA-4575*, Los Alamos Scientific Laboratory (1971).
27. Wm. H. Reed, "A Non-Iterative Method for Time-Dependent Transport," *Proc. Conf. New Developments in Reactor Math. Applications*, Idaho Falls, March 29–31, 1971, CONF-710302, Vol. 2, U.S. Atomic Energy Commission (1971).
28. T. R. Hill and Wm. H. Reed, "TIMEX: A Time-Dependent Explicit Discrete Ordinates Program for the Solution of Multigroup Transport Equations with Delayed Neutrons," *LA-6201-MS*, Los Alamos Scientific Laboratory (1976).

## PROBLEMS

- 2-1.** Derive Eq. 2-14 without assuming Eq. 2-6. Use instead the assumption that all of the cross sections are piecewise constants, changing values only at the  $E_g$ .
- 2-2.** For a uniform, infinite medium show that Eq. 2-31 reduces to

$$\sigma_g \phi_g = \sum_{g'} \sigma_{0gg'} \phi_{g'} + \frac{\chi_g}{k} \sum_{g'} \nu \sigma_{fg'} \phi_{g'},$$

then derive the multigroup approximation to the expression for  $k$  given in Problem 1-10.

- 2-3. Use energy separability to derive the multigroup approximation to Eq. 1-109.
- 2-4. Derive the multigroup approximation to the adjoint equation (1-141). Then derive the multigroup approximation to the perturbation expression (1-154).
- 2-5. With anisotropic scattering in the laboratory system, assume Eq. 2-14 has a source term of the form  $q_g^e = S_0 \exp(i\vec{B} \cdot \vec{r})$  and  $\nu\sigma_{fg} = 0$ . Find the scalar flux  $\phi_0 \exp(i\vec{B} \cdot \vec{r})$  in terms of  $S_0$  and  $\vec{B}$ . The cross sections are space-independent.
- 2-6. For isotropic scattering and sources the within-group transport equation is

$$\hat{\Omega} \cdot \vec{\nabla} \psi + \sigma \psi = \sigma_s \phi + S, \quad \phi \equiv \int d\Omega \psi,$$

and the diffusion approximation is

$$-\vec{\nabla} \cdot D \vec{\nabla} \phi + \sigma_s \phi = S.$$

Consider a system where all of the boundaries are parallel to the  $z$  axis and let  $s(\vec{r}) = \tilde{s}(x, y) \exp(iBz)$  where  $\tilde{s}$  and  $B$  are real. Assume a source-free vacuum surrounds the  $x-y$  domain of the problem.

- a. Look for a solution of the transport equation in the form

$$\psi(\vec{r}, \hat{\Omega}) = [\psi_r(x, y, \hat{\Omega}) + i\psi_i(x, y, \hat{\Omega})] \exp(iBz)$$

and find the equations governing the real and imaginary components,  $\psi_r$  and  $\psi_i$ .

- b. Look for a solution of the diffusion equation in the analogous form

$$\phi(\vec{r}) = [\phi_r(x, y) + i\phi_i(x, y)] \exp(iBz)$$

and compare the resulting equations to those in part a.

- c. In a expand

$$\psi_r = \psi_{r0} + B\psi_{r1} + B^2\psi_{r2} + \dots,$$

$$\psi_i = \psi_{i0} + B\psi_{i1} + B^2\psi_{i2} + \dots,$$

and find the coupled equations governing  $\psi_{rl}$  and  $\psi_{il}$ ,  $l = 0, 1, 2$ .

d. Repeat c for  $\phi_r$  and  $\phi_i$  in the diffusion equation, and compare your results with those of part c.

- 2-7.** Equation 2-37 gives an expression for the group total cross section obtained from fine mesh calculations. For isotropic scattering, find the corresponding expressions for  $\sigma_{gg'}$  the group-to-group scattering cross section. Repeat the calculation with  $f(E) \propto 1/E$ .
- 2-8.** The homogenized group cross section, averaged over the fine energy groups, is given by Eq. 2-42. Derive the analogous expression for the group-to-group scattering cross section  $\sigma_{gg'}$ .
- 2-9.** Verify Eq. 2-48.
- 2-10.** Use Eq. 2-51 and the properties of the Legendre polynomial to show that

$$a_{00j} = \gamma_j^{-1} \tanh^{-1} \gamma_j,$$

$$\gamma_j^{-1} (2l + 1) a_{nlj} - (l + 1) a_{n,l+1,j} - l a_{n,l-1,j} = \gamma_j^{-1} \delta_{nl}$$

and

$$a_{nlj} = a_{lnj},$$

where

$$\gamma_j = iB/\sigma_j^{\ddagger}.$$

- 2-11.** Suppose iteration on the scattering source is applied to a uniform infinite medium in the one-group approximation. The source is uniform and isotropic. If the initial flux guess is  $\phi_0 = 0$ , how many iterations will be required to achieve 1% accuracy when  $\sigma_s/\sigma = 0.0, 0.5, 0.75, 0.9, 0.95$ , and  $0.99$ ? Discuss the physical significance of the case where  $(\sigma_s/\sigma) = 1.0$ .
- 2-12.** Verify Eq. 2-181.
- 2-13.** Suppose that synthetic acceleration (with  $\sigma_r \equiv \sigma - \sigma_s$ ) is applied after each iteration on the scattering source used in Problem 2-11. Show that regardless of the initial guess  $\phi_0$ , an exact solution is obtained after one accelerated iteration.

- 2-14.** Show that for a source-free infinite medium with no scattering or fission, Eq. 2-215 reduces to

$$\frac{1}{v_g} \frac{d}{dt} \psi_g(t) + \sigma_g \psi_g(t) = 0.$$

Then do the following:

- a. Solve this equation analytically, when  $\psi_g(0)$  is known.
- b. Solve the equation using the difference approximations contained in Eq. 2-223, Eq. 2-224, and in Eqs. 2-227 and 2-228.
- c. Plot your results from a and b for  $0 \leq t \leq 6/(\sigma_g v_g)$  with  $\Delta_j \sigma_g v_g = 0.25, 0.5, 1,$  and  $2.$