

# Chapter 2

## Second-Order Neutron Transport Methods

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### 2.1 Introduction

Among the approaches to obtaining numerical solutions for neutral particle transport problems, those classified as second-order or even-parity methods have found increased use in recent decades. First-order and second-order methods differ in a number of respects. Following discretization of the energy variable, invariably through some form of the multigroup approximation, the time-independent forms of both are differential in the spatial variable and integral in angle. They differ in that the more conventional first-order equation includes only first derivatives in the spatial variables, but requires solution over the entire angular domain. Conversely, the second-order form includes second derivatives but requires solution over one half of the angular domain. The two forms in turn lead to contrasting approaches to reducing the differential–integral equations to sets of linear equations and in the formulation of iterative methods suitable for the numerical solution of large engineering design problems. In what follows, we explore the state of methods used to solve the second-order transport equation, comparing them, where possible, to first-order methods.

Historically, diffusion theory was the earliest and remains the most widely employed second-order computational method in reactor core design. Fine mesh spatial discretization has been performed through a variety of finite difference [1] and finite element techniques [2–4]. Along with the continuing advance of computing power, two events greatly influenced the development of methods that are emphasized in this work. The first was the translation in 1962 of Vladimirov’s variational formulation of the second-order form of the transport equation [5]. There followed increased interest in variational formulations and the systematic exploration of alternate variational principles and their interconnectedness [6]. The second was the rise of finite element methods, first in computational mechanics but then spreading to other fields [7–9]. The power of finite element methods largely supplanted

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earlier finite difference techniques not only in computational mechanics, but also in a number of related fields as well. Since finite element methods in computational mechanics were closely associated with variational principles, the method's application to transport problems was greatly facilitated by the variational framework that had been developed for the Boltzmann equation.

The first applications of finite element methods to neutronics problems appeared in the early 1970s, and not surprisingly to the diffusion approximation [2–4]. But soon thereafter finite element methods appeared coupled with spherical harmonics [10–14], discrete ordinates [14–20], and also with finite elements in angle [22, 23]. Through the 1970s and into the 1980s, however, second-order transport methods were largely limited to stand-alone codes applied to model problems. At that time, computer memory restrictions continued to favor very effective marching algorithms with which first-order discrete ordinates methods were able to solve large engineering problems with very limited memory [24, 25]. It has only been with the rapid expansion of computer memories since that time that second-order methods have become a viable alternative for engineering calculation, and production codes based on the methods became viable for large-scale engineering computations [11–14, 17–21, 26, 27].

To present the current state of even-parity computational methods, we begin in Section 2.2 by deriving the second-order form of the linear Boltzmann equation from its first-order counterpart. We then examine the weak and variational forms of these equations that are used almost without exception as the points of departure for numerical approximation. For brevity and clarity, isotropic scattering is assumed. Section 2.3 reduces these forms to the diffusion approximation and then discretizes the spatial variables. The simplicity of diffusion theory provides a convenient vehicle for introducing finite element methods, and for establishing notation that then carries over for use in conjunction with more accurate angular approximations. Following the inclusion of anisotropic scattering into the even-parity formulation, Section 2.4 treats angular approximations: spherical harmonics, discrete ordinates as well as their simplified forms. The section then combines these angular approximations with finite elements in space to obtain fully discretized forms of the even-parity equation. Section 2.5 examines two variants of even-parity approaches: a hybrid or nodal method and an integral even-parity method. Section 2.6 then offers concluding remarks.

## 2.2 The Transport Equation

The numerical algorithms of the following sections are based primarily on the variational form of the even-parity transport equation. We begin, however, with the standard first-order form of the equation and proceed to arrive at the variational principle. Along the way, we also present both the mixed and the second-order even- and odd-parity equations. Before proceeding to the variational formulation, we examine briefly the weak form of the even-parity equation and of the mixed

equations in their primal and dual weak forms. The even-parity weak form may be used interchangeably with the variational formulation. Mixed methods are less well developed but are included because of the future potential that they may hold.

In what follows, we assume the time-independent form of the neutron transport equation in which a multigroup discretization of the energy variable has already been performed. Thus, we need to deal only with the energy-independent or within-group form of the equation. For brevity, we also assume isotropic scattering in this section, reserving the introduction of anisotropic scattering to Section 2.4.

### 2.2.1 First- and Second-Order Forms

The first-order form of the transport equation is [28]

$$\hat{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \psi(\vec{r}, \hat{\Omega}) = \sigma_s(\vec{r}) \int d\Omega' \psi(\vec{r}, \hat{\Omega}') + s(\vec{r}), \quad \vec{r} \in V, \quad (2.1)$$

where  $\vec{r}$  is the spatial location, and  $\hat{\Omega}$  is the direction of neutron travel;  $\sigma$  and  $\sigma_s$  are the macroscopic total and scattering cross sections, respectively,  $s$  is the group source, and we normalize the angular integrals such that  $\int d\Omega = 1$ . Integrating over angle yields the neutron conservation equation

$$\vec{\nabla} \cdot \vec{J}(\vec{r}) + \sigma_t \phi(\vec{r}) = s(\vec{r}), \quad (2.2)$$

where

$$\phi(\vec{r}) = \int d\Omega \psi(\vec{r}, \hat{\Omega}) \quad (2.3)$$

and

$$\vec{J}(\vec{r}) = \int d\Omega \hat{\Omega} \psi(\vec{r}, \hat{\Omega}) \quad (2.4)$$

are the scalar flux and current, respectively, and

$$\sigma_t = \sigma - \sigma_s \quad (2.5)$$

defining the even- and odd-parity flux components as

$$\psi^\pm(\vec{r}, \hat{\Omega}) = 1/2 [\psi(\vec{r}, \hat{\Omega}) \pm \psi(\vec{r}, -\hat{\Omega})] \quad (2.6)$$

We may evaluate Eq. (2.1) at  $\hat{\Omega}$  and  $-\hat{\Omega}$  and add and subtract the results to obtain a set of coupled first-order equations

$$\hat{\Omega} \cdot \vec{\nabla} \psi^- + \sigma \psi^+ = \sigma_s \phi + s \quad (2.7)$$

and

$$\hat{\Omega} \cdot \vec{\nabla} \psi^+ + \sigma \psi^- = 0. \quad (2.8)$$

A pair of second-order equations may then be obtained. Eliminating  $\psi^-$  between Eqs. (2.7) and (2.8) yields the even-parity equation

$$-\hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ + \sigma \psi^+ = \sigma_s \phi + s \quad (2.9)$$

while eliminating  $\psi^+$  yields the odd-parity equation

$$-\hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^- + \sigma \psi^- = \hat{\Omega} \cdot \vec{\nabla} (\sigma - \sigma_s)^{-1} \left[ (\sigma_s / \sigma) \vec{\nabla} \cdot \vec{J} - s \right]. \quad (2.10)$$

These two equations contain only  $\psi^+$  and  $\psi^-$ , respectively, since the scalar flux and current may be expressed as

$$\phi = \int d\Omega \psi^+ \quad (2.11)$$

and

$$\vec{J} = \int d\Omega \hat{\Omega} \psi^-. \quad (2.12)$$

Finally, we may also write a second-order equation for the angular flux by first solving Eq. (2.1) for  $\psi = -\sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \psi - \sigma_s \phi - s)$  and substituting into Eq. (2.1) to obtain

$$-\hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi + \sigma \psi = (1 - \hat{\Omega} \cdot \vec{\nabla} \sigma^{-1}) (\sigma_s \phi + s). \quad (2.13)$$

### 2.2.2 Weak Forms

The starting point for most space-angle approximations is the weak form of the foregoing equations. To obtain the weak forms of the coupled equations (2.7) and (2.8) we multiply the two by even- and odd-parity test functions,  $\tilde{\psi}^+$  and  $\tilde{\psi}^-$ , respectively, and integrate over angle and space:

$$\int dV \int d\Omega \tilde{\psi}^+ \left( \hat{\Omega} \cdot \vec{\nabla} \psi^- + \sigma \psi^+ - \sigma_s \phi - s \right) = 0, \quad (2.14)$$

$$\int dV \int d\Omega \tilde{\psi}^- \left( \hat{\Omega} \cdot \vec{\nabla} \psi^+ + \sigma \psi^- \right) = 0. \quad (2.15)$$

Applying the divergence theorem to the first term of the two equations yield

$$\begin{aligned} \int dV \int d\Omega \left[ -(\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+) \psi^- + \sigma \tilde{\psi}^+ \psi^+ - \tilde{\phi} (\sigma_s \phi + s) \right] \\ + \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \psi^- = 0 \end{aligned} \quad (2.16)$$

and

$$\int dV \int d\Omega \left[ -(\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^-) \psi^+ + \sigma \tilde{\psi}^- \psi^- \right] + \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^- \psi^+ = 0. \quad (2.17)$$

where  $d\Gamma$  indicates integration over the surface of the spatial domain,  $V$ , and  $\hat{n}$  is the outward normal from  $d\Gamma$ .

Two classes of methods arise from these equations [8, 19]. Equation (2.16) is the basis for *primal* methods, and Eqs. (2.16) and (2.15) taken together constitute the *mixed-primal* formulation. Alternately, Eq. (2.8) may be used to eliminate  $\psi^-$  from the volume integral to obtain the second-order *even-parity primal* formulation:

$$\begin{aligned} \int dV \int d\Omega \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+) (\hat{\Omega} \cdot \vec{\nabla} \psi^+) + \sigma \tilde{\psi}^+ \psi^+ - \tilde{\phi} (\sigma_s \phi + s) \right] \\ + \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \psi^- = 0 \end{aligned} \quad (2.18)$$

This even-parity result may also be obtained directly by multiplying Eq. (2.9) by  $\tilde{\psi}^+$ , integrating over space and angle, and then applying the divergence theorem.

Equation (2.17) is the basis for *dual* methods. Taken together, Eqs. (2.17) and (2.14) constitute the *mixed dual* formulation. Alternately, Eq. (2.7) may be used to eliminate  $\psi^+$  from the volume integral in Eq. (2.17) to form the second-order *odd-parity dual* formulation:

$$\begin{aligned} \int dV \int d\Omega \left\{ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^-) (\hat{\Omega} \cdot \vec{\nabla} \psi^-) + \sigma \tilde{\psi}^- \psi^- \right. \\ \left. - (\sigma - \sigma_s)^{-1} (\vec{\nabla} \cdot \vec{J}) \left[ (\sigma_s / \sigma) \vec{\nabla} \cdot \vec{J} - s \right] \right\} + \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^- \psi^+ = 0 \end{aligned} \quad (2.19)$$

Multiplying Eq. (2.10) by  $\tilde{\psi}^-$ , integrating over space and angle and then applying the divergence theorem also leads to this result.

The surface terms in the above equations determine the form of the boundary conditions [9, 28]. Setting them equal to zero yields the homogeneous form of the natural boundary conditions. Thus  $\psi^- = 0$ , and  $\psi^+ = 0$  for  $\vec{r} \in \Gamma$  are the natural boundary conditions, respectively, in the primal and dual formulations. Inhomogeneous natural conditions may be obtained by setting  $\psi^- = \psi_\lambda^-$ , in the primal and  $\psi^+ = \psi_\lambda^+$ , in the dual formulation; hereafter, we employ the subscript  $\lambda$  to indicate a known function on the boundary. Conversely, if the boundary conditions specify  $\psi^+$  in the primal or  $\psi^-$  in the dual formulations, they are essential; the surface integral is deleted, and they are imposed directly on the solution.

Classically, it is the incoming angular flux that is known on the boundary. Hence

$$\psi^+(\vec{r}, \hat{\Omega}) + \psi^-(\vec{r}, \hat{\Omega}) - \psi_\lambda(\vec{r}, \hat{\Omega}) = 0, \vec{r} \in \Gamma, \hat{n} \cdot \hat{\Omega} < 0, \quad (2.20)$$

and in particular the vacuum boundary  $\psi_\lambda(\vec{r}, \hat{\Omega}) = 0$ ,  $\vec{r} \in \Gamma$ ,  $\hat{n} \cdot \hat{\Omega} < 0$  is the homogeneous form of this condition. These conditions may be treated as modified natural conditions by first forming weighted residuals

$$2 \int d\Gamma \int_{\hat{n} \cdot \hat{\Omega} < 0} d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^\pm (\psi^+ + \psi^- - \psi_\lambda) = 0 \quad (2.21)$$

for primal and dual formulations, respectively. By making use of angular parity arguments, it can be written

$$\begin{aligned} \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^\pm \psi^\mp &= \int d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^\pm \psi^\pm + 2 \int d\Gamma \\ &\int_{\hat{n} \cdot \hat{\Omega} < 0} d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^\pm \psi_\lambda. \end{aligned} \quad (2.22)$$

By employing this expression to eliminate the surface integral on the left of Eq. (2.22) from the primal or dual formulations in Eq. (2.16) or (2.17), modified natural boundary conditions may be obtained for a known incoming flux distribution. Reflected boundary conditions, which have the form  $\psi(\vec{r}, \hat{\Omega}') = \psi(\vec{r}, \hat{\Omega})$ , where  $\hat{\Omega}$  and  $\hat{\Omega}'$  are the angles of incidence and reflection are essential since they apply directly to  $\psi$ , with no contribution from its derivatives.

Until quite recently, the vast majority of second-order transport work has applied to the even-parity form of the equation given by Eq. (2.9), whose weak form is given by Eq. (2.18). Thus, we focus our attention on it. With the incoming flux boundary conditions, Eq. (2.18) becomes

$$\begin{aligned} \int dV \int d\Omega \left[ \sigma^{-1}(\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+)(\hat{\Omega} \cdot \vec{\nabla} \psi^+) + \sigma \tilde{\psi}^+ \psi^+ - \tilde{\phi}(\sigma_s \phi + s) \right] \\ + \int d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^+ \psi^+ + 2 \int d\Gamma \int_{\hat{n} \cdot \hat{\Omega} < 0} d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \psi_\lambda = 0, \end{aligned} \quad (2.23)$$

where for vacuum boundary conditions we set  $\psi_\lambda = 0$ . For most computations, the problem domain is bounded by some combinations of reflected and vacuum boundaries. We indicate this by dividing the boundary as  $\Gamma = \Gamma_r + \Gamma_v$ . Then, instead of Eq. (2.23), we have

$$\begin{aligned} \int dV \int d\Omega \left[ \sigma^{-1}(\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+)(\hat{\Omega} \cdot \vec{\nabla} \psi^+) + \sigma \tilde{\psi}^+ \psi^+ - \tilde{\phi}(\sigma_s \phi + s) \right] \\ + \int_{\Gamma_v} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^+ \psi^+ = 0, \end{aligned} \quad (2.24)$$

since no surface integral appears for  $\Gamma_r$ , where the essential reflected conditions are applied.

### 2.2.3 Variational Formulation

Both coupled and second-order forms of the primal and dual formulations may also be formulated as variational principles, and surface terms are added to impose modified natural boundary conditions. Here, we restrict attention to the primal second-order form, since it was the original variational principal of Vladimirov [5] and is that upon which virtually all second-order methods are based.

The variational principle corresponding to Eq. (2.24) derives from the requirement that the following functional be stationary with respect to variations in  $\psi^+$ :

$$F[\psi^+] = \int dV \int d\Omega \left[ \sigma^{-1} \left( \hat{\Omega} \cdot \vec{\nabla} \psi^+ \right)^2 + \sigma \psi^{+2} - \sigma_s \phi^2 - 2\phi s \right] + \int_{\nu} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \psi^{+2}. \quad (2.25)$$

To illustrate, suppose we make the substitution  $\psi^+ \rightarrow \psi^+ + \delta \tilde{\psi}^+$  where  $\delta$  is a very small number, and  $\tilde{\psi}^+$  is an arbitrary deviation about the true solution  $\psi^+$ . We then have

$$\begin{aligned} F[\psi^+ + \delta \tilde{\psi}^+] &= \int dV \int d\Omega \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \psi^+)^2 + \sigma \psi^{+2} - \sigma_s \phi^2 - 2\phi s \right] \\ &+ \int_{\nu} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \psi^{+2} + 2\delta \left\{ \int dV \int d\Omega \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+) (\hat{\Omega} \cdot \vec{\nabla} \psi^+) \right. \right. \\ &+ \tilde{\psi}^+ (\sigma \psi^+ - \sigma_s \phi - s)] + \int_{\nu} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^+ \psi^+ \left. \right\} + \delta^2 \left\{ \int dV \int d\Omega \right. \\ &\times \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+)^2 + \sigma \tilde{\psi}^{+2} - \sigma_s \tilde{\phi}^2 \right] + \int_{\nu} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^{+2} \left. \right\}. \quad (2.26) \end{aligned}$$

For the functional to be stationary, the linear term in  $\delta$  must vanish. This term, however, is identical to Eq. (2.24) derived from the weak form. Applying the divergence theorem to Eq. (2.24), or to the linear term in  $\delta$  in Eq. (2.26), yields:

$$\begin{aligned} &\int dV \int d\Omega \tilde{\psi}^+ \left( -\hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ + \sigma \psi^+ - \sigma_s \phi - s \right) \\ &+ \int_{\nu} d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ + \int_{\nu} d\Gamma \int d\Omega |\hat{\Omega} \cdot \hat{n}| \tilde{\psi}^+ \psi^+ = 0. \quad (2.27) \end{aligned}$$

For this expression to hold, both the volume and surface integrals must vanish. Since  $\tilde{\psi}^+$  is an arbitrary function, the expression in parentheses must vanish. Thus, the even-parity transport equation given by Eq. (2.9) is satisfied. This is the

Euler–Lagrange equation. On the vacuum boundary the two surface integral terms may be rewritten as

$$\begin{aligned} & \int_r d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ \\ & + 2 \int_v d\Gamma \int_{\hat{\Omega} \cdot \hat{n} < 0} d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ (\sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ - \psi^+). \end{aligned} \quad (2.28)$$

Since from Eqs. (2.8) and (2.6) we have  $\psi^- = -\sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+$  and  $\psi = \psi^+ - \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+$ , the first term in Eq. (2.28) yields the natural boundary condition  $\psi^- = 0$ . However, on reflected boundary condition we take  $\tilde{\psi}^+ = 0$  on  $\Gamma_r$  and impose the essential boundary condition on the solution. From the second term, the modified natural boundary condition on the vacuum ( $\psi = 0$ , for  $\hat{n} \cdot \hat{\Omega} < 0$  on  $\Gamma_v$ ) is satisfied.

## 2.3 The Discretized Diffusion Equation

The diffusion approximation may be viewed as arising naturally as the lowest-order angular approximation to the even-parity equation. Indeed a straightforward exercise is to eliminate the angular variables from the weak or variational forms discussed in Section 2.2 by using the diffusion approximation. Here, a simple statement of the diffusion equation in variational form serves as a vehicle for introducing the finite element method. Finite element notation established for use in conjunction with the diffusion equation then allows for a more straightforward discretization of the spatial variable in conjunction with the higher order angular approximations treated in Section 2.4.

### 2.3.1 The Diffusion Formulation

The diffusion approximation may be obtained by making the approximations  $\psi^+ \approx \phi$ ,  $\psi^- \approx 3\hat{\Omega} \cdot \vec{J}$  and then operating on Eqs. (2.7) and (2.8) with  $\int d\Omega$  and  $\int d\Omega \hat{\Omega}$ , respectively, to obtain

$$\vec{\nabla} \cdot \vec{J} + \sigma_r \phi = s \quad (2.29)$$

and

$$\frac{1}{3} \vec{\nabla} \phi + \sigma \vec{J} = 0. \quad (2.30)$$

The second-order form of the diffusion equation is obtained by eliminating  $\vec{J}$  between Eqs. (2.29) and (2.30):

$$-\vec{\nabla}(3\sigma)^{-1} \cdot \vec{\nabla}\phi + (\sigma - \sigma_s)\phi = s. \quad (2.31)$$

Alternately, we may obtain this equation directly from the even-parity transport equation, or from its variational form. Let

$$\psi^+ \approx \phi. \quad (2.32)$$

Then operating on Eq. (2.9) with  $\int d\Omega$  yields Eq. (2.31). The approximation  $\psi^+ \approx \phi$  likewise reduces the even-parity functional  $F[\psi^+]$ , given by Eq. (2.25), to its diffusion form

$$F[\phi] = \int dV \left[ \frac{1}{3}\sigma^{-1} (\vec{\nabla}\phi)^2 + \sigma_r\phi^2 - 2\phi s \right] + \frac{1}{2} \int_{\nu} d\Gamma \phi^2. \quad (2.33)$$

The diffusion equation can be shown to be the Euler–Lagrange equation by letting  $\phi \rightarrow \phi + \delta\tilde{\phi}$ , where  $\tilde{\phi}$  is an arbitrary deviation from the solution  $\phi$  and requiring the linear term in  $\delta$  to vanish:

$$\int dV \left[ \frac{1}{3}\sigma^{-1} (\vec{\nabla}\tilde{\phi}) (\vec{\nabla}\phi) + \sigma_r\tilde{\phi}\phi - \tilde{\phi}s \right] + \frac{1}{2} \int_{\nu} d\Gamma \tilde{\phi}\phi = 0. \quad (2.34)$$

This is identical to the diffusion approximation’s weak form obtainable by inserting Eq. (2.32) into Eq. (2.27). If we apply the divergence theorem to Eq. (2.34), we obtain

$$\begin{aligned} \int dV \tilde{\phi} \left( -\vec{\nabla} \cdot \frac{1}{3}\sigma^{-1} \vec{\nabla}\phi + \sigma_r\phi - s \right) + \int_{\Gamma} d\Gamma \tilde{\phi} \frac{1}{3}\sigma^{-1} \hat{n} \cdot \vec{\nabla}\phi \\ + \int_{\nu} d\Gamma \tilde{\phi} \left( \frac{1}{3}\sigma^{-1} \hat{n} \cdot \vec{\nabla}\phi + \frac{1}{2}\phi \right) = 0. \end{aligned} \quad (2.35)$$

For arbitrary  $\tilde{\phi}$ , the quantity in parentheses in the first term must vanish, yielding Eq. (2.31) as the Euler–Lagrange equation. The surface integral over  $\Gamma_r$  yields the reflected or zero current condition  $\hat{n} \cdot \vec{\nabla}\phi = 0$  as the natural boundary condition, and in diffusion theory this corresponds to the reflected boundary condition. (Recall, however, that for the transport equation more generally reflective boundary conditions are essential.) Requiring the quantity in parentheses in the last term to vanish yields the modified natural boundary condition; it approximates the vacuum condition extrapolating the flux to zero at a distance of  $\frac{2}{3}\sigma^{-1}$  outside of  $\Gamma_{\nu}$ .

### 2.3.2 Finite Element Discretization

We discretize the spatial variable employing the finite element method. For clarity, we illustrate using simple triangular elements in two-dimensional Cartesian geometry [7]. We first divide the problem domain into elemental volumes  $V_e$ :

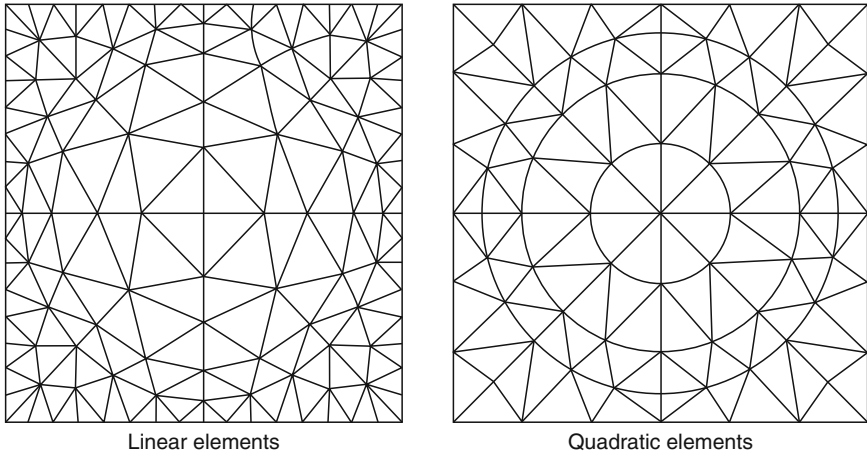
$$V = \sum_e V_e. \quad (2.36)$$

In two dimensions, these may appear, for example, as the triangles in Fig. 2.1.

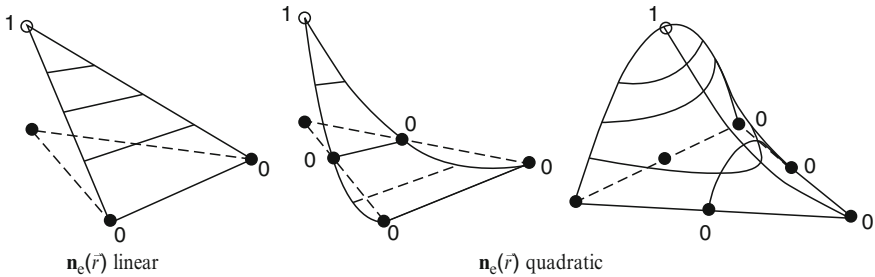
Within each element, we approximate  $\phi(\vec{r})$  as the scalar product of a vector of polynomial trial functions,  $\mathbf{n}_e(\vec{r})$ , and unknown coefficient vector,  $\xi_e$ :

$$\phi(\vec{r}) \approx \mathbf{n}_e^T(\vec{r})\xi_e, \quad \vec{r} \in V_e. \quad (2.37)$$

Representative linear and quadratic trial functions for triangular elements, for which the length of  $\mathbf{n}_e(\vec{r})$  is 3 for the linear element and 6 for the quadratic element,



**Fig. 2.1** Triangular finite element grids



**Fig. 2.2** Triangular finite element trial functions

respectively, are shown in Fig. 2.2. (These and other classes of finite elements are discussed in detail elsewhere [7]). They have the properties that  $\left[\mathbf{n}_e(\vec{r}_i)\right]_j = \delta_{ij}$  so that the components of  $\xi_e$  are equal to  $\phi$  at  $\vec{r}_i$ ,  $i = 1, \dots, 3$  or  $6$ , the mesh points shown in Fig 2.2. Moreover, if the same sets of trial functions are used in adjoining elements, the flux approximation will be continuous across the interfaces.

Provided continuity is maintained, the functional given by Eq. (2.33) may be written as the sum of elemental contributions.

$$F[\xi_e] = \sum_e \xi_e^T \mathbf{A}_e \xi_e - 2 \sum_e \xi_e^T \mathbf{q}_e, \quad (2.38)$$

where the elemental matrices involve integrals of the known trial functions,

$$\mathbf{A}_e = 1/3 \sigma_e^{-1} \int_e dV (\vec{\nabla} \mathbf{n}_e) \cdot (\vec{\nabla} \mathbf{n}_e^T) + \sigma_{re} \int_e dV \mathbf{n}_e \mathbf{n}_e^T + 1/2 \int_{ve} d\Gamma \mathbf{n}_e \mathbf{n}_e^T, \quad (2.39)$$

with the last term present only where one or more of the element surfaces lie along a vacuum boundary; the source term is given by

$$\mathbf{q}_e = \int_e dV \mathbf{n}_e s. \quad (2.40)$$

We may formally assemble the global functional from its elemental contributions as follows. The continuity of the trial functions across element interfaces allows the elemental unknowns to be mapped on to a globally numbered vector of  $N$  unknowns:

$$\xi_e = \Xi_e \xi. \quad (2.41)$$

where  $\Xi_e$  is  $3 \times N$  or  $6 \times N$  Boolean transformation matrices. Inserting this equation into Eq. (2.38), we obtain the algebraic functional

$$F[\xi] = \xi^T \mathbf{A} \xi - 2 \xi^T \mathbf{q}, \quad (2.42)$$

where

$$\mathbf{A} = \sum_e \Xi_e^T \mathbf{A}_e \Xi_e, \quad (2.43)$$

and

$$\mathbf{q} = \sum_e \Xi_e^T \mathbf{q}_e. \quad (2.44)$$

We obtain a set of linear equations for  $\xi$  by requiring the reduced functional  $F[\xi]$  to be stationary with respect to variations:  $\xi \rightarrow \xi + \delta \xi$ . Hence

$$F[\xi + \delta \xi] = (\xi^T \mathbf{A} \xi - 2 \xi^T \mathbf{q}) + 2 \delta \xi^T (\mathbf{A} \xi - \mathbf{q}) + \delta^2 \xi^T \mathbf{A} \xi, \quad (2.45)$$

and since the linear terms in  $\delta$  must vanish we have

$$\mathbf{A}\xi = \mathbf{q}. \quad (2.46)$$

Here,  $\mathbf{A}$  is a symmetric matrix. Provided a consistent numbering scheme has been applied to the mesh points the matrix will also be banded. Solution may be obtained using any number of direct methods for smaller problems, or iterative techniques such as preconditioned conjugate gradients for large problems [29–31].

## 2.4 The Discretized Transport Equation

In this section, we first write Eq. (2.1) with anisotropic scattering included, and then derive the corresponding form of the even-parity equation as well as stating the variational principle that provides the starting point for numerical approximation. We then derive spherical harmonic and discrete ordinates angular approximations (referred to frequently as  $Pn$  and  $Sn$  methods, respectively) along with their simplified spherical harmonic and discrete ordinates ( $SPn$  and  $SSn$ ) counterparts. For each approximation, the result is a coupled set of second-order partial differential equations. The sets differ only in the structure of their coefficient matrices. Thus, we can apply the finite element methods discussed in Section 2.3 to discretize the spatial variables for all of the approximations simultaneously.

### 2.4.1 Anisotropic Scattering

With anisotropic scattering included, the form of the second-order equation becomes more complex [15, 17, 32]. To obtain it, we begin with the first-order form of the equation:

$$\hat{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \psi(\vec{r}, \hat{\Omega}) = \int d\Omega' \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi(\vec{r}, \hat{\Omega}') + s(\vec{r}, \hat{\Omega}), \quad (2.47)$$

where  $\sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}')$  is the macroscopic differential scattering cross section. In the multigroup approximation the group source is given by

$$s(\vec{r}, \hat{\Omega}) = \sum_{g' \neq g} \int d\Omega' \sigma_{sgg'}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi_{g'}(\vec{r}, \hat{\Omega}') + S_{fg}(\vec{r}) \quad (2.48)$$

where  $g$  designates the group under consideration,  $\sigma_{sgg'}$  represents scattering from group  $g'$  to  $g$ , and  $S_{fg}$  includes the isotropic fission and external sources.

We may evaluate Eq. (2.47) at  $\hat{\Omega}$  and  $-\hat{\Omega}$  and add and subtract the results to obtain a pair of coupled first-order equations

$$\hat{\Omega} \cdot \vec{\nabla} \psi^\mp(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \psi^\pm(\vec{r}, \hat{\Omega}) = \int d\Omega' \sigma_s^\pm(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi^\pm(\vec{r}, \hat{\Omega}') + s^\pm(\vec{r}, \hat{\Omega}), \quad (2.49)$$

where

$$\sigma_s^\pm(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') = 1/2 \left[ \sigma_s(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \pm \sigma_s(\vec{r}, -\hat{\Omega} \cdot \hat{\Omega}') \right] \quad (2.50)$$

and

$$s^\pm(\vec{r}, \hat{\Omega}) = 1/2 \left[ s(\vec{r}, \hat{\Omega}) \pm s(\vec{r}, -\hat{\Omega}) \right]. \quad (2.51)$$

Here,  $\sigma_s^\pm$  and  $s^\pm$  indicate the even- and odd-parity components of the anisotropic scattering cross section and source, respectively. We next express the anisotropic scattering cross sections as expansions in an orthonormal set of spherical harmonics [28, 33]

$$Y_{lm}(\hat{\Omega}) = C_{lm} P_l^m(\mu) \begin{cases} \cos(m\omega) \\ \sin(m\omega) \end{cases}, \quad l = 0, 1, 2, \dots, \quad |m| = 0, 1, 2, \dots, l \quad (2.52)$$

where  $P_l^m(\mu)$  are the associated Legendre polynomials, and the  $C_{lm}$  are chosen such that  $\int d\Omega Y_{lm}(\hat{\Omega}) Y_{l'm'}(\hat{\Omega}) = \delta_{ll'} \delta_{mm'}$ ; we follow the convention that  $m \geq 0$  signifies the cosine series and  $m < 0$  the sine series. We first write  $\sigma_s^\pm(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}')$  as expansions in Legendre polynomials

$$\sigma_s^\pm(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') = \sum_{\substack{l \\ \text{even} \\ \text{odd}}} \sigma_l(\vec{r}) P_l(\hat{\Omega} \cdot \hat{\Omega}'). \quad (2.53)$$

The Legendre addition theorem [33]

$$P_l(\hat{\Omega} \cdot \hat{\Omega}') = \sum_{m=-l}^l Y_{lm}(\hat{\Omega}) Y_{lm}(\hat{\Omega}') \quad (2.54)$$

then allows Eq. (2.53) to be written in the convenient vector form

$$\sigma_s^\pm(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') = \mathbf{y}_\pm^T(\hat{\Omega}) \boldsymbol{\Sigma}_\pm(\vec{r}) \mathbf{y}_\pm(\hat{\Omega}'), \quad (2.55)$$

where we have formed vectors of the even- and odd-parity spherical harmonics

$$\mathbf{y}_+^T(\hat{\Omega}) = [Y_{00}, Y_{2-2}, Y_{2-1}, Y_{20}, Y_{21}, Y_{22}, Y_{4-4}, \dots], \quad (2.56)$$

$$\mathbf{y}_-^T(\hat{\Omega}) = [Y_{1-1}, Y_{10}, Y_{11}, Y_{3-3}, Y_{3-2}, Y_{3-1}, Y_{30}, Y_{31}, \dots], \quad (2.57)$$

with  $\int d\Omega \mathbf{y}_{\pm}(\hat{\Omega}) \mathbf{y}_{\pm}^T(\hat{\Omega}) = \mathbf{I}$  and  $\int d\Omega \mathbf{y}_{\pm}(\hat{\Omega}) \mathbf{y}_{\mp}^T(\hat{\Omega}) = \mathbf{0}$ . The diagonal matrices are defined by

$$\Sigma_+ = \text{diag}[\sigma_0, \sigma_2, \sigma_2, \sigma_2, \sigma_2, \sigma_2, \sigma_4, \dots], \quad (2.58)$$

$$\Sigma_- = \text{diag}[\sigma_1, \sigma_1, \sigma_1, \sigma_3, \sigma_3, \sigma_3, \sigma_3, \dots]. \quad (2.59)$$

The coupled pair of even- and odd-parity equations given by Eq.(2.49) then becomes

$$\begin{aligned} \hat{\Omega} \cdot \vec{\nabla} \psi^-(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \psi^+(\vec{r}, \hat{\Omega}) \\ = \mathbf{y}_+^T(\hat{\Omega}) \Sigma_+(\vec{r}) \int d\Omega' \mathbf{y}_+(\hat{\Omega}') \psi^+(\vec{r}, \hat{\Omega}') + s^+(\vec{r}, \hat{\Omega}), \end{aligned} \quad (2.60)$$

and

$$\begin{aligned} \hat{\Omega} \cdot \vec{\nabla} \psi^+(\vec{r}, \hat{\Omega}) + \sigma(\vec{r}) \psi^-(\vec{r}, \hat{\Omega}) \\ = \mathbf{y}_-^T(\hat{\Omega}) \Sigma_-(\vec{r}) \int d\Omega' \mathbf{y}_-(\hat{\Omega}') \psi^-(\vec{r}, \hat{\Omega}') + s^-(\vec{r}, \hat{\Omega}). \end{aligned} \quad (2.61)$$

To obtain the even-parity equation, we employ Eq.(2.61) to obtain the odd-parity moments in terms of the even-parity moments:

$$[\mathbf{I} - \sigma^{-1} \Sigma_-] \int d\Omega \mathbf{y}_-(\hat{\Omega}) \psi^-(\hat{\Omega}) = \sigma^{-1} \mathbf{s}^- - \sigma^{-1} \vec{\nabla} \cdot \int d\Omega \hat{\Omega} \mathbf{y}_-(\hat{\Omega}) \psi^+(\hat{\Omega}), \quad (2.62)$$

where we define the even- and odd-parity group-source moments as

$$\mathbf{s}^{\pm}(\vec{r}) = \int d\Omega \mathbf{y}_{\pm}(\hat{\Omega}) s^{\pm}(\vec{r}, \hat{\Omega}). \quad (2.63)$$

Using Eq.(2.62) to eliminate the integral of  $\psi^-$  on the right side of Eq.(2.61), we may solve for  $\psi^-$  in terms of  $\psi^+$  and the group-source terms:

$$\begin{aligned} \psi^-(\hat{\Omega}) = -\sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+(\hat{\Omega}) + \sigma^{-1} s^-(\hat{\Omega}) \\ - \sigma^{-2} \mathbf{y}_-^T(\hat{\Omega}) \tilde{\Sigma}_- \int d\Omega' \mathbf{y}_-(\hat{\Omega}') \hat{\Omega}' \cdot \vec{\nabla} \psi^+(\hat{\Omega}') + \sigma^{-2} \mathbf{y}_-^T(\hat{\Omega}) \tilde{\Sigma}_- \mathbf{s}^-, \end{aligned} \quad (2.64)$$

where

$$\tilde{\Sigma}_{\pm} = \Sigma_{\pm} [\mathbf{I} - \sigma^{-1} \Sigma_{\pm}]^{-1}. \quad (2.65)$$

Finally, substituting Eq.(2.64) into Eq.(2.60) we obtain the second-order even-parity equation;

$$\begin{aligned} -\hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \hat{\Omega} \cdot \vec{\nabla} \psi^+ + \sigma \psi^+ = \mathbf{y}_+^T \left[ \Sigma_+ \int d\Omega' \mathbf{y}_+(\hat{\Omega}') \psi^+(\hat{\Omega}') + \mathbf{s}^+ \right] \\ + \hat{\Omega} \cdot \vec{\nabla} \sigma^{-1} \mathbf{y}_-^T \left[ \sigma^{-1} \tilde{\Sigma}_- \int d\Omega' \mathbf{y}_-(\hat{\Omega}') \hat{\Omega}' \cdot \vec{\nabla} \psi^+(\hat{\Omega}') - (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-) \mathbf{s}^- \right], \end{aligned} \quad (2.66)$$

where we have also expanded the group source in harmonic moments

$$\mathbf{s}^+ = \sum_{g' \neq g} \boldsymbol{\Sigma}_{+gg'} \int d\Omega \mathbf{y}_+(\hat{\Omega}) \psi_{g'}^+(\hat{\Omega}) + \mathbf{s}_{fg}, \quad (2.67)$$

$$\mathbf{s}^- = \sum_{g' \neq g} \boldsymbol{\Sigma}_{-gg'} \sigma_{g'}^{-1} [\mathbf{I} - \sigma_{g'}^{-1} \boldsymbol{\Sigma}_{-g'g'}]^{-1} \left[ \mathbf{s}_{g'}^- - \vec{\nabla} \cdot \int d\Omega \hat{\Omega} \mathbf{y}_-(\hat{\Omega}) \psi_{g'}^+(\hat{\Omega}) \right]. \quad (2.68)$$

Comparing Eq. (2.9) to Eq. (2.66), it is apparent that the second-order forms of the equation appear to be considerably more complex than the first-order form when anisotropic scattering is included.

The weak form of Eq. (2.66) may be obtained by integrating over angle and volume and then applying the divergence theorem:

$$\begin{aligned} \int dV \Big\{ & \int d\Omega \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+) (\hat{\Omega} \cdot \vec{\nabla} \psi^+) + \sigma \tilde{\psi}^+ \psi^+ \right] \\ & - \left( \int d\Omega \mathbf{y}_+ \tilde{\psi}^+ \right)^T \boldsymbol{\Sigma}_+ \left( \int d\Omega \mathbf{y}_+ \psi^+ \right) - \left( \int d\Omega \mathbf{y}_+ \tilde{\psi} \right)^T \mathbf{s}^+ \\ & + \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+ \right)^T \sigma^{-2} \tilde{\boldsymbol{\Sigma}}_- \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \psi^+ \right) \\ & - \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \tilde{\psi}^+ \right)^T \sigma^{-2} (\mathbf{I} + \sigma^{-1} \tilde{\boldsymbol{\Sigma}}_-) \mathbf{s}^- \Big\} \\ & + \int d\Gamma \int d\Omega \hat{\Omega} \cdot \hat{n} \tilde{\psi}^+ \psi^- = 0, \end{aligned} \quad (2.69)$$

where  $\psi^-$  is given by Eq. (2.64).

Alternately, a variational principle may be written, which yields Eq. (2.66) as the Euler–Lagrange equation. Variational formulation of the within-group problem is

$$\begin{aligned} F[\psi^+] = \int dV \Big\{ & \int d\Omega \left[ \sigma^{-1} (\hat{\Omega} \cdot \vec{\nabla} \psi^+)^2 + \sigma \psi^{+2} \right] \\ & - \left( \int d\Omega \mathbf{y}_+ \psi^+ \right)^T \boldsymbol{\Sigma}_+ \left( \int d\Omega \mathbf{y}_+ \psi^+ \right) - \left( \int d\Omega \mathbf{y}_+ \psi^+ \right)^T 2\mathbf{s}^+ \\ & + \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \psi^+ \right)^T \sigma^{-2} \tilde{\boldsymbol{\Sigma}}_- \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \psi^+ \right) \\ & - \left( \int d\Omega \mathbf{y}_- \hat{\Omega} \cdot \vec{\nabla} \psi^+ \right)^T \sigma^{-2} 2(\mathbf{I} + \sigma^{-1} \tilde{\boldsymbol{\Sigma}}_-) \mathbf{s}^- \Big\}. \end{aligned} \quad (2.70)$$

The natural boundary condition remains  $\psi^- = 0$ , but where  $\psi^-$  is defined by Eq. (2.64).

## 2.4.2 Angular Approximations

We next use Eq. (2.70) as the point of departure for deriving spherical harmonics and discrete ordinates approximations.

### 2.4.2.1 Spherical Harmonics Expansions

The spherical harmonics approximations may be expressed as the scalar product of a row and a column vector, where  $\mathbf{y}_+(\hat{\Omega})$  is given by Eq. (2.56)

$$\psi^+(\vec{r}, \hat{\Omega}) \approx \mathbf{y}_+^T(\hat{\Omega}) \Psi^+(\vec{r}). \quad (2.71)$$

From the orthonormality of the  $\mathbf{y}_+(\hat{\Omega})$ , we then have the space-dependent coefficients to be

$$\Psi^+(\vec{r}) = \int d\Omega \mathbf{y}_+(\hat{\Omega}) \psi^+(\vec{r}, \hat{\Omega}). \quad (2.72)$$

Likewise, we may write

$$\mathbf{U}_{k'} \nabla_{k'} \Psi^+(\vec{r}) = \int d\Omega \mathbf{y}_-(\hat{\Omega}) \hat{\Omega} \cdot \vec{\nabla} \psi^+(\vec{r}, \hat{\Omega}), \quad (2.73)$$

where

$$\mathbf{U}_k = \int d\Omega \hat{\Omega} \cdot \hat{k} \mathbf{y}_-(\hat{\Omega}) \mathbf{y}_+^T(\hat{\Omega}). \quad (2.74)$$

and hereafter repeated  $k$  or  $k'$  in the same term indicates summation over the spatial directions.

We next substitute Eq. (2.71) into the functional given by Eq. (2.70) to obtain:

$$\begin{aligned} F[\Psi^+] = \int dV \Big\{ & (\mathbf{U}_k \nabla_k \Psi^+)^T \sigma^{-1} (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-) (\mathbf{U}_{k'} \nabla_{k'} \Psi^+) \\ & + \Psi^{+T} \sigma (\mathbf{I} - \sigma^{-1} \Sigma_+) \Psi^+ - 2 \Psi^{+T} \mathbf{s}^+ - 2 (\nabla_k \Psi^+)^T \sigma^{-2} (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-) \mathbf{s}^- \Big\}, \end{aligned} \quad (2.75)$$

where we have used the orthonormal properties of  $\mathbf{y}_+(\hat{\Omega})$  to obtain the identity

$$\mathbf{U}_k^T \mathbf{U}_{k'} = \int d\Omega \hat{\Omega} \cdot \hat{k} \hat{\Omega} \cdot \hat{k}' \mathbf{y}_+(\hat{\Omega}) \mathbf{y}_+^T(\hat{\Omega}) \quad (2.76)$$

and thus simplify the streaming term in the reduced functional. Requiring the functional to be stationary with respect to variations in  $\Psi^+(\vec{r})$  yields the spherical harmonics approximation as the Euler–Lagrange equation:

$$\begin{aligned} -\nabla_k \mathbf{U}_k^T \sigma^{-1} [\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-] \mathbf{U}_{k'} \nabla_{k'} \Psi^+ + (\sigma \mathbf{I} - \Sigma_+) \Psi^+ \\ = \mathbf{s}^+ - \nabla_k \mathbf{U}_k^T \sigma^{-1} (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-) \mathbf{s}^-. \end{aligned} \quad (2.77)$$

### 2.4.2.2 Discrete Ordinates Approximations

The discrete ordinates equation may be obtained from the Functional, Eq. (2.70), by evaluating all the quantities at discrete directions  $\hat{\Omega}_n$  and replacing integrals over angle with an appropriate quadrature approximation

$$\int d\Omega f(\vec{r}, \hat{\Omega}) \approx \sum_n w_n f(\vec{r}, \hat{\Omega}_n), \quad (2.78)$$

where  $w_n$  are the weights and  $\hat{\Omega}_n$  are the discrete ordinates directions. The even-parity flux is then evaluated in the discrete ordinates directions by  $\psi^+(\vec{r}, \hat{\Omega}_n)$ . Thus, to reduce the functional we create a vector of the even-parity flux approximated in the discrete ordinates directions:

$$\Psi^{+T}(\vec{r}) \approx \left[ \psi^+(\vec{r}, \hat{\Omega}_1), \psi^+(\vec{r}, \hat{\Omega}_2), \psi^+(\vec{r}, \hat{\Omega}_3), \dots, \psi^+(\vec{r}, \hat{\Omega}_n), \dots \right]. \quad (2.79)$$

To apply the quadrature rule of Eq. (2.78) to the functional, we also define two diagonal matrices

$$\mathbf{\Omega}_k = \text{diag} \left[ \hat{\Omega}_1 \cdot \hat{k}, \hat{\Omega}_2 \cdot \hat{k}, \hat{\Omega}_3 \cdot \hat{k}, \dots, \hat{\Omega}_n \cdot \hat{k}, \dots \right] \quad (2.80)$$

and

$$\mathbf{W} = \text{diag}[w_1, w_2, w_3, \dots, w_n, \dots]. \quad (2.81)$$

We also employ matrices made up of the  $\mathbf{y}_{\pm}(\hat{\Omega})$  column vectors evaluated in the ordinates directions:

$$\mathbf{Y}_{\pm} = \left[ \mathbf{y}_{\pm}(\hat{\Omega}_1), \mathbf{y}_{\pm}(\hat{\Omega}_2), \mathbf{y}_{\pm}(\hat{\Omega}_3), \dots, \mathbf{y}_{\pm}(\hat{\Omega}_n), \dots \right]. \quad (2.82)$$

Utilizing the angular quadrature approximation and Eqs. (2.79) through (2.82), the Functional reduces to the form

$$\begin{aligned} F[\Psi^+] = \int dV \left\{ (\mathbf{\Omega}_k \nabla_k \Psi^+)^T \sigma^{-1} \mathbf{W} (\mathbf{I} + \sigma^{-1} \mathbf{Y}_{-}^T \tilde{\Sigma} - \mathbf{Y}_{-} \mathbf{W}) (\mathbf{\Omega}_{k'} \nabla_{k'} \Psi^+) \right. \\ \left. + \Psi^{+T} \sigma \mathbf{W} (\mathbf{I} - \sigma^{-1} \mathbf{Y}_{+}^T \Sigma + \mathbf{Y}_{+} \mathbf{W}) \Psi^+ - 2 \Psi^{+T} \mathbf{W} \mathbf{Y}_{+}^T \mathbf{s}^+ \right. \\ \left. - 2 (\mathbf{\Omega}_k \nabla_k \Psi^+)^T \mathbf{W} \mathbf{Y}_{-}^T \sigma^{-2} (\mathbf{I} + \sigma^{-1} \tilde{\Sigma} -) \mathbf{s}^- \right\}, \quad (2.83) \end{aligned}$$

where the group sources are obtained by applying the quadrature formula to Eqs. (2.67) and (2.68). If we require  $F[\Psi^+]$  to be stationary by taking  $F[\Psi^+ + \delta \tilde{\Psi}^+]$  and requiring the linear term in  $\delta$  to vanish, we obtain an Euler-Lagrange equation

$$\begin{aligned} -\nabla_k \mathbf{\Omega}_k \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \mathbf{Y}_{-}^T \tilde{\Sigma} - \mathbf{Y}_{-} \mathbf{W} \right] \mathbf{\Omega}_{k'} \nabla_{k'} \Psi^+ + [\sigma \mathbf{I} - \mathbf{Y}_{+}^T \Sigma + \mathbf{Y}_{+} \mathbf{W}] \Psi^+ \\ = \mathbf{Y}_{+}^T \mathbf{s}^+ - \mathbf{\Omega}_k \nabla_k \sigma^{-1} \mathbf{Y}_{-}^T (\mathbf{I} + \sigma^{-1} \tilde{\Sigma} -) \mathbf{s}^-, \quad (2.84) \end{aligned}$$

which is just the even-parity form of the discrete ordinates equations.

Both the spherical harmonics and discrete ordinates approximations can be written in forms that are identical except for the coefficient matrices. The variational principle has the form

$$F[\Psi^+] = \int dV \{ (\nabla_k \Psi^+)^T \mathbf{H}_{kk'} (\nabla_{k'} \Psi^+) + \Psi^{+T} \mathbf{K} \Psi^+ - 2 \Psi^{+T} \mathbf{G}_+ \mathbf{s}^+ - 2 (\nabla_k \Psi^+)^T \mathbf{G}_{k-} \mathbf{s}^- \}, \quad (2.85)$$

and the corresponding even-parity equations are

$$-\nabla_k \mathbf{H}_{kk'} \nabla_{k'} \Psi^+ + \mathbf{K} \Psi^+ = \mathbf{G}_+ \mathbf{s}^+ - \nabla_k \mathbf{G}_{k-} \mathbf{s}^-. \quad (2.86)$$

The coefficient matrices are given in Table 2.1, along with those for the simplified approximations treated in the following section.

Thus far, the derivations hold for three dimensions. For one or two dimensions they may be appropriately reduced by eliminating terms in the spherical harmonics or discrete ordinates expansions. In spherical harmonics all terms with  $m < 0$  for  $x$ - $y$  geometry and all terms with  $m \neq 0$  for plane geometry are eliminated from Eqs. (2.71) through (2.77). The duplicate directions are likewise eliminated from discrete ordinates approximations (polar axis in  $x$  direction, and azimuthal angle measured from  $y$  direction  $k = 1, 2, 3$  for  $x, y$ , and  $z$  axes). The plane-geometry spherical harmonics equation, in which the forgoing matrices are expressed in terms of Legendre polynomials, is particularly relevant here as the basis for the simplified spherical harmonics approximation.

**Table 2.1** Uniform notation for Eqs. (2.84) and (2.85)

|     | $\mathbf{H}_{kk'}$                                                                                                                            | $\mathbf{K}$                                                                     | $\mathbf{G}_+$   | $\mathbf{G}_{k-}$                                                                                   |
|-----|-----------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|------------------|-----------------------------------------------------------------------------------------------------|
| Pn  | $\mathbf{U}_k^T \sigma^{-1} [\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-] \mathbf{U}_{k'}$                                                      | $\sigma \mathbf{I} - \Sigma_+$                                                   | $\mathbf{I}$     | $\mathbf{U}_k^T \sigma^{-1} \times (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-)$                     |
| Sn  | $\Omega_k \sigma^{-1} [\mathbf{W} + \sigma^{-1} \mathbf{W} \mathbf{Y}_-^T \tilde{\Sigma}_- \mathbf{Y}_- \mathbf{W}] \Omega_{k'}$              | $\sigma \mathbf{W} - \mathbf{W} \mathbf{Y}_+^T \Sigma_+ \mathbf{Y}_+ \mathbf{W}$ | $\mathbf{Y}_+^T$ | $\Omega_k \sigma^{-1} \mathbf{W} \mathbf{Y}_-^T \times (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-)$ |
| SPn | $\mathbf{U}_0 \sigma^{-1} [\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-] \mathbf{U}_0^T \delta_{kk'}$                                            | $\sigma \mathbf{I} - \Sigma_+$                                                   | $\mathbf{I}$     | $\mathbf{U}_0^T \sigma^{-1} \times (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-)$                     |
| SSn | $\Omega_k \sigma^{-1} [\mathbf{W} + \sigma^{-1} \mathbf{W} \mathbf{Y}_-^T \tilde{\Sigma}_- \mathbf{Y}_- \mathbf{W}] \Omega_{k'} \delta_{kk'}$ | $\sigma \mathbf{W} - \mathbf{W} \mathbf{Y}_+^T \Sigma_+ \mathbf{Y}_+ \mathbf{W}$ | $\mathbf{Y}_+^T$ | $\Omega_k \sigma^{-1} \mathbf{W} \mathbf{Y}_-^T \times (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-)$ |

### 2.4.2.3 Simplified Angular Approximations

Cross-derivative terms  $\nabla_k(\cdots)\nabla_{k'}$  with  $k \neq k'$  appear in both the spherical harmonics and discrete ordinates approximations. Eliminating them greatly simplifies the spatial discretization. The widely employed simplified spherical harmonics, or *SPn*, approximation provides such simplification and reduces the number of coupled differential equations that must be solved, often without substantial loss of accuracy [34–41]. We obtain the *SPn* equations by taking the one-dimensional form of the *Pn* equations, given by Eq. (2.77)

$$\begin{aligned} & -\frac{\partial}{\partial x} \mathbf{U}_1^T \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \tilde{\Sigma}_- \right] \mathbf{U}_1 \frac{\partial}{\partial x} \Psi^+ + (\sigma \mathbf{I} - \Sigma_+) \Psi^+ \\ & = \mathbf{s}^+ - \frac{\partial}{\partial x} \mathbf{U}_1^T \sigma^{-1} \left( \mathbf{I} + \sigma^{-1} \tilde{\Sigma}_- \right) \mathbf{s}^- \end{aligned} \quad (2.87)$$

and replacing the derivatives with gradient and divergence operators

$$\begin{aligned} & -\nabla_k \mathbf{U}_1^T \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \tilde{\Sigma}_- \right] \mathbf{U}_1 \nabla_k \Psi^+ + (\sigma \mathbf{I} - \Sigma_+) \Psi^+ \\ & = \mathbf{s}^+ - \sum_k \nabla_k \mathbf{U}_1^T \sigma^{-1} \left( \mathbf{I} + \sigma^{-1} \tilde{\Sigma}_- \right) \mathbf{s}^-. \end{aligned} \quad (2.88)$$

The resulting equation may also be written in variational form and expressed as coupled partial differential equations; the coefficient matrices are included in Table 2.1. More importantly, Eq. (2.88) can be written as coupled sets of diffusion equations, allowing highly developed diffusion computational methods to be used to obtain solutions with great computational efficiency.

The simplified discrete ordinates approximation is much more recent [42], and to date not widely employed. It simply eliminates the cross-derivative terms from Eq. (2.84) by letting

$$\Omega_k \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \mathbf{Y}_-^T \tilde{\Sigma}_- \mathbf{Y}_- \mathbf{W} \right] \Omega_{k'} \rightarrow \Omega_k \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \mathbf{Y}_-^T \tilde{\Sigma}_- \mathbf{Y}_- \mathbf{W} \right] \Omega_{k'} \delta_{kk'} \quad (2.89)$$

to yield

$$\begin{aligned} & -\nabla_k \Omega_k \sigma^{-1} \left[ \mathbf{I} + \sigma^{-1} \mathbf{Y}_-^T \tilde{\Sigma}_- \mathbf{Y}_- \mathbf{W} \right] \Omega_k \nabla_k \Psi^+ + [\sigma \mathbf{I} - \mathbf{Y}_+^T \Sigma_+ \mathbf{Y}_+ \mathbf{W}] \Psi^+ \\ & = \mathbf{Y}_+^T \mathbf{s}^+ - \Omega_k \nabla_k \sigma^{-1} \mathbf{Y}_-^T (\mathbf{I} + \sigma^{-1} \tilde{\Sigma}_-) \mathbf{s}^-. \end{aligned} \quad (2.90)$$

The *SSn* equations may also be written as coupled sets of partial differential equations as indicated in Table 2.1.

Before proceeding, it is instructive to briefly compare *Pn* and *Sn* solutions for which the spatial discretization error is insignificant. Figure 2.3 shows results for the widely used Azmy benchmark [43], which consists of a fixed source located in a highly absorbing medium. The flux plots along the surface far from the source accentuate errors in angular approximations. The  $P_{11}$  solution is converged in angle, and may be used as a reference.

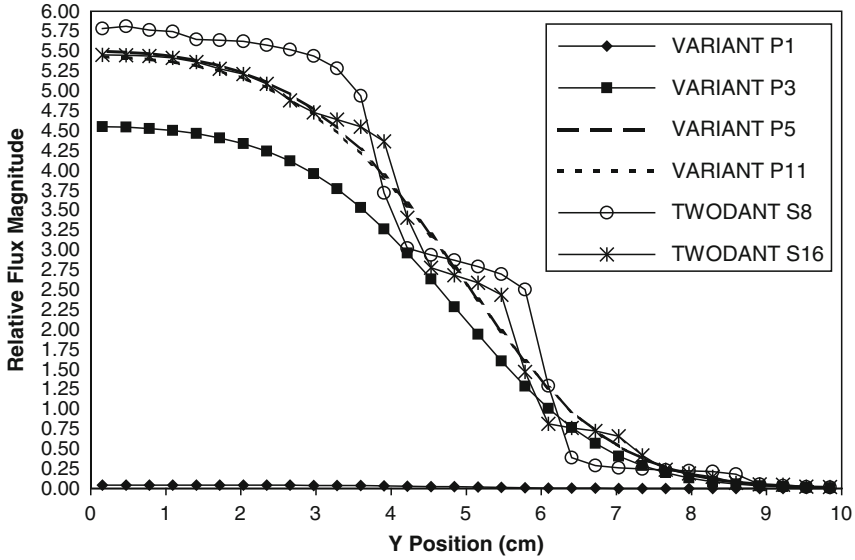


Fig. 2.3 Flux plots from  $S_n$  and  $P_n$  calculations

Note that the  $S_n$  solutions oscillate about the reference demonstrating the well-known ray effects. Low order  $P_n$  solutions appear more physically plausible, since they are smooth curves and their errors tend to be either systematically low (as in this problem) or high. For this problem,  $SP_n$  solutions, which are not shown, closely track the corresponding  $P_n$  solutions. Since  $SP_n$  has fewer angular degrees of freedom, computational algorithms for  $SP_n$  solutions run faster and use less memory than those for the same level  $P_n$  approximation. Unlike discrete ordinates or spherical harmonics methods, however,  $SP_n$  calculations do not converge to the true solution as  $n$  is increased. In many cases, however, the residual errors are acceptably small. The circumstances under which  $SP_n$  solutions may be expected to reasonably approximate the transport equation are well examined elsewhere [34, 35, 39, 40].

### 2.4.3 Spatial Discretization

We spatially discretize the foregoing angular approximations using the same finite element techniques employed in Section 2.3. Thus, we begin by subdividing the problem domain into a finite number of volume elements.

$$V = \sum_e V_e. \quad (2.91)$$

Then, provided we consider only spatial trial functions that are continuous across element interfaces, we may write the functional given by Eq. (2.85) as a superposition of elemental contributions:

$$F[\Psi^+] = \sum_e \int_e dV \left\{ (\nabla_k \Psi^+)^T \mathbf{H}_{kk'}^e (\nabla_{k'} \Psi^+) + \Psi^{+T} \mathbf{K}^e \Psi^+ - 2\Psi^{+T} \mathbf{G}_+^e \mathbf{s}^+ - 2(\nabla_k \Psi^+)^T \mathbf{G}_{k-}^e \mathbf{s}^- \right\}. \quad (2.92)$$

Within each element, we represent the spatial distribution trial functions, designated by the vector  $\mathbf{n}_e(\vec{r})$ , and a vector of unknown magnitudes  $\xi_e$ . The even-parity flux moments become

$$\Psi^+(\vec{r}) = \mathbf{I} \otimes \mathbf{n}_e^T(\vec{r}) \xi_e, \quad \vec{r} \in V_e. \quad (2.93)$$

Then, using the properties of the tensor product, we may write

$$\Psi^{+T} \mathbf{K}^e \Psi^+ = (\mathbf{I} \otimes \mathbf{n}_e^T \xi_e)^T \mathbf{K}^e \mathbf{I} \otimes \mathbf{n}_e^T \xi_e = \xi_e^T \mathbf{I} \otimes \mathbf{n}_e \mathbf{K}^e \otimes \mathbf{n}_e^T \xi_e = \xi_e^T \mathbf{K}^e \otimes \mathbf{n}_e \mathbf{n}_e^T \xi_e. \quad (2.94)$$

Similarly, it follows that

$$(\nabla_k \Psi^+)^T \mathbf{H}_{kk'}^e (\nabla_{k'} \Psi^+) = \xi_e^T \mathbf{H}_{kk'}^e \otimes (\nabla_k \mathbf{n}_e) (\nabla_{k'} \mathbf{n}_e^T) \xi_e. \quad (2.95)$$

The functional given by Eq. (2.92) reduces to a superposition of subelement contributions:

$$F[\xi_e] = \sum_e \xi_e^T \mathbf{A}_e \xi_e - 2 \sum_e \xi_e^T \mathbf{q}_e, \quad (2.96)$$

where the coefficient matrices are given in terms of the known trial functions of space and angle

$$\mathbf{A}_e = \mathbf{H}_{kk'}^e \otimes \int_e dV (\nabla_k \mathbf{n}_e) (\nabla_{k'} \mathbf{n}_e^T) + \mathbf{K}^e \otimes \int_e dV \mathbf{n}_e \mathbf{n}_e^T. \quad (2.97)$$

Here, the superscripts on  $\mathbf{H}_{kk'}^e$  and  $\mathbf{K}^e$  indicate that the cross sections are evaluated for element  $V_e$ . The source term is

$$\mathbf{q}_e = \mathbf{G}_+^e \int_e dV \mathbf{s}^+ \otimes \mathbf{n}_e + \mathbf{G}_{k-}^e \int_e dV \mathbf{s}^- \otimes \nabla_k \mathbf{n}_e. \quad (2.98)$$

With piecewise polynomial trial functions for the finite elements, the components of  $\xi_e$  are just the approximate values of  $\Psi^+$  at the element vertices [7]. Since these trial functions must be continuous across element interfaces, the process for assembling the elemental contributions and determining a set of linear equations is completely analogous to that of Eqs. (2.38) through (2.46): The components of  $\xi_e$  corresponding to the same physical location on either side of a subelement must have the same value. This continuity condition is enforced by creating a Boolean

matrix  $\Xi_e$  for each subelement that maps the  $\xi_e$  onto  $\xi$ , a node wide vector of coefficients:  $\xi_e = \Xi_e \xi$ . This transformation allows us to write the discretized functional in the form of Eq. (2.38). The set of algebraic equations is again obtained by requiring the discretized functional to be stationary. The result, once again, is a set of equations with the form  $\mathbf{A}\xi = \mathbf{q}$ , but where the elemental contributions to  $\mathbf{A}$  and  $\mathbf{q}$  are now given by Eqs. (2.97) and (2.98). Regardless of the angular approximation employed, the  $\mathbf{A}$  matrix is sparse and symmetric. For smaller problems, direct methods may be used for solving the matrix problem. For large problems, an array of sparse matrix iterative techniques may be employed [29–31].

## 2.5 Hybrid and Integral Methods

Thus far, we have examined a number of angular approximations to the even-parity transport equations coupled with the use of finite elements in space. There are, of course, other possibilities for the discretization of the second-order equations. Here, we briefly examine two of these, the variational nodal method [11, 13, 32, 41] and an integral method [44], and then discuss recent work in combining nodal, finite element, and integral methods.

### 2.5.1 A Variational Nodal Method

The variational forms of the even-parity equation that we have utilized have incoming flux, vacuum, or reflected boundary conditions. Suppose, however, that we create a functional that is easily shown to be equivalent to the weighted residual, Eq. (2.69), which has an inhomogeneous natural boundary condition on the odd-parity flux. We simply append the following surface term to the functional given by Eq. (2.70):

$$F_v[\psi^+, \psi^-] = F_v[\psi^+] + 2 \int_v d\Gamma \int d\Omega \hat{n} \cdot \hat{\Omega} \psi^+ \psi^-. \quad (2.99)$$

The subscript  $v$  is appended to denote that the problem domain is a volume  $V_v$  bounded by  $\Gamma_v$ . By requiring this functional to be stationary with respect to variations in  $\psi^+$  within  $V_v$  we obtain the Euler–Lagrange equation (2.66). Variations on the boundary,  $\Gamma_v$ , yield the relationship, Eq. (2.64), giving  $\psi^-$  in terms of  $\psi^+$ . Thus, we may consider solving the transport problem within  $V_v$ , assuming that the odd-parity flux  $\psi^-$  is known at the boundary. In the finite element literature the following would be classified as a hybrid element approach [7, 8].

Suppose we consider  $V_v$  to be the volume of one “node” of the problem domain, and the volume of the entire domain to be the sum of the nodes’ volumes:

$$V = \sum_v V_v, \quad (2.100)$$

Then, we may write the functional for the entire domain as

$$F[\psi^+, \psi^-] = \sum_v F_v[\psi^+, \psi^-], \quad (2.101)$$

where  $\psi^-$  now appears as a Lagrange multiplier at the nodal interfaces. Requiring  $F[\psi^+, \psi^-]$  to be stationary with respect to variations in  $\psi^+$  within  $V_v$ , just yields Eq. (2.66) within each  $V_v$ . Requiring it to be stationary with respect to  $\psi^- \rightarrow \psi^- + \delta\psi^-$  yields the condition

$$\int d\Gamma \int d\Omega \hat{n} \cdot \hat{\Omega} (\psi^+ - \psi'^+) \tilde{\psi}^- = 0, \quad (2.102)$$

where  $\hat{n}$  and  $\hat{n}' = -\hat{n}$  are the outward normal vectors from nodes  $V_v$  and  $V'_v$  on either side of  $\Gamma$ . Thus,  $\psi^+$  must be continuous across the interfaces.

In the neutronics literature, a nodal method is generally defined as one in which neutron conservation is enforced for each node or subregion  $V_v$  [45]. The variational method described here may be shown to meet this condition as follows: suppose we let  $\bar{\phi} = V_v^{-1} \int_v dV \int d\Omega \psi^+$  be the scalar flux averaged over node  $V_v$ . We may then write  $\psi^+ = \bar{\phi} + \psi_0^+$  where  $\int_v dV \int d\Omega \psi_0^+ = 0$  and substitute this expression into Eq. (2.99) to obtain

$$\begin{aligned} F_v[\psi^+, \psi^-] &= (\sigma - \sigma_s) V_v \bar{\phi}^2 - 2V_v \bar{\phi} \bar{s} + 2\bar{\phi} \int_v d\Gamma \hat{n} \cdot \vec{J} \\ &+ \text{terms independent of } \bar{\phi}, \end{aligned} \quad (2.103)$$

where  $\bar{s}$  is the group source averaged over  $V_v$  and angle. If we require the functional to be stationary with respect to variations  $\bar{\phi} \rightarrow \bar{\phi} + \delta\bar{\phi}$  we obtain the nodal balance condition

$$(\sigma - \sigma_s) V_v \bar{\phi} + \int_v d\Gamma \hat{n} \cdot \vec{J} = V_v \bar{s}. \quad (2.104)$$

This enforcement of neutron conservation over each  $V_v$  allows larger nodes to be used than typical in the case of fine mesh methods that do not enforce such balance.

To proceed, we apply spherical harmonics, discrete ordinates, or one of the simplified angular approximations given in Section 2.4 to  $F_v[\psi^+]$  given by Eq. (2.99). We must consistently discretize the surface term. We first divide the surface  $\Gamma$  into a number of flat surfaces,  $\Gamma_\gamma$ . In the spherical harmonics approximation, we let

$$\psi^-(\vec{r}, \hat{\Omega}) \approx \mathbf{y}_{-\gamma}^T(\hat{\Omega}) \Psi_\gamma^-(\vec{r}), \quad \vec{r} \in \Gamma_\gamma. \quad (2.105)$$

Here, the subscript  $\gamma$  is attached to  $\mathbf{y}_{-\gamma}(\hat{\Omega})$  to indicate that the odd-parity spherical harmonics are rotated such that the polar axis is perpendicular to the surface. In

addition, the  $Y_{ll}$  are deleted from  $\mathbf{y}_{-\gamma}(\hat{\Omega})$ ; this is necessary to obtain the correct number of linearly independent coupling conditions [14]. Employing Eqs. (2.71) and (2.105), we get

$$\int_v d\Gamma \int d\Omega \hat{n}_\gamma \cdot \hat{\Omega} \psi^+ \psi^- = \sum_\gamma \int_\gamma d\Gamma \Psi^{+T} \mathbf{C}_\gamma \Psi_\gamma^-, \quad (2.106)$$

with  $\mathbf{C}_\gamma = \int d\Omega \hat{n}_\gamma \cdot \hat{\Omega} \mathbf{y}_+ \mathbf{y}_{-\gamma}^T$ , while for the  $SPn$  approximation  $\mathbf{C}_\gamma = \mathbf{U}_1^T$ .

For discrete ordinates, we approximate the odd-parity flux on  $\Gamma_\gamma$  by using Eqs. (2.79) through (2.81) with

$$\Psi^{-T}(\vec{r}) \approx \left[ \psi^-(\vec{r}, \hat{\Omega}_{1\cdot}), \psi^-(\vec{r}, \hat{\Omega}_{2\cdot}), \psi^-(\vec{r}, \hat{\Omega}_{3\cdot}), \dots, \psi^-(\vec{r}, \hat{\Omega}_{n\cdot}), \dots \right] \quad (2.107)$$

and

$$\mathbf{\Omega}_\gamma = \text{diag} \left[ \hat{\Omega}_1 \cdot \hat{n}_\gamma, \hat{\Omega}_2 \cdot \hat{n}_\gamma, \hat{\Omega}_3 \cdot \hat{n}_\gamma, \dots, \hat{\Omega}_n \cdot \hat{n}_\gamma, \dots \right]. \quad (2.108)$$

The result is again Eq. (2.106), but with  $\mathbf{C}_\gamma = \mathbf{W} \mathbf{\Omega}_\gamma$ ; this equality remains unchanged in the  $SSn$  approximation.

Next, we rewrite the reduced form of the functional given by Eq. (2.99) with the angularly discretized variables discretized in a form similar to Eq. (2.92):

$$\begin{aligned} F_v [\Psi^+, \Psi_\gamma^-] = & \int_v dV \{ (\nabla_k \Psi^+)^T \mathbf{H}_{kk'} (\nabla_{k'} \Psi^+) + \Psi^{+T} \mathbf{K} \Psi^+ - 2 \Psi^{+T} \mathbf{G}_+ \mathbf{s}^+ \\ & - 2 (\nabla_k \Psi^+)^T \mathbf{G}_{k-} \mathbf{s}^- \} + 2 \sum_\gamma \int_\gamma d\Gamma \Psi^{+T} \mathbf{C}_\gamma \Psi_\gamma^-. \end{aligned} \quad (2.109)$$

Within the node, we approximate the spatial dependence of the even-parity flux by a vector  $\mathbf{f}(\vec{r})$  containing the orthonormal components of a complete polynomial, and on the interfaces the spatial dependence of the odd-parity flux is given by a second set of orthonormal polynomials,  $\mathbf{h}_\gamma(\vec{r})$ , defined only on the interface. Thus,

$$\Psi^+(\vec{r}) = \mathbf{I} \otimes \mathbf{f}^T(\vec{r}) \xi \quad \vec{r} \in V_v \quad (2.110)$$

and

$$\Psi_\gamma^-(\vec{r}) = \mathbf{I} \otimes \mathbf{h}_\gamma^T(\vec{r}) \chi_\gamma \quad \vec{r} \in \Gamma_\gamma, \quad (2.111)$$

where  $\xi$  and  $\chi_\gamma$  are the unknown coefficients. The reduced functional then becomes

$$F_v[\xi, \chi] = \xi^T \mathbf{A} \xi - 2 \xi^T \mathbf{q} + 2 \xi^T \sum_\gamma \mathbf{M}_\gamma \chi_\gamma, \quad (2.112)$$

where

$$\mathbf{A} = \mathbf{H}_{kk'} \otimes \int_{\mathbf{v}} dV (\nabla_k \mathbf{f}) (\nabla_{k'} \mathbf{f}^T) + \mathbf{K} \otimes \int_{\mathbf{v}} dV \mathbf{f} \mathbf{f}^T, \quad (2.113)$$

$$\mathbf{q} = \mathbf{G}_+ \int_{\mathbf{v}} dV \mathbf{s}^+ \otimes \mathbf{f} + \mathbf{G}_{k-} \int_{\mathbf{v}} dV \mathbf{s}^- \otimes \nabla_k \mathbf{f} \quad (2.114)$$

and

$$\mathbf{M}_\gamma = \mathbf{C}_\gamma \otimes \int_{\gamma} d\Gamma \mathbf{f} \mathbf{h}_\gamma^T. \quad (2.115)$$

Requiring Eq. (2.112) to be stationary with respect to variations in  $\xi$  yields

$$\mathbf{A}\xi = \mathbf{q} - \sum_{\gamma} \mathbf{M}_\gamma \chi_\gamma, \quad (2.116)$$

or equivalently

$$\xi = \mathbf{A}^{-1} \mathbf{q} - \mathbf{A}^{-1} \mathbf{M} \chi, \quad (2.117)$$

where  $\mathbf{M} = [\mathbf{M}_1, \mathbf{M}_2, \dots]$  and  $\chi^T = [\chi_1^T, \chi_2^T, \dots]$ . To obtain the interface continuity conditions we first note that

$$F[\xi, \chi] = \sum_{\mathbf{v}} F_{\mathbf{v}}[\xi, \chi] \quad (2.118)$$

Requiring that the functional be stationary with respect to the variations  $\chi_{\mathbf{v}} \rightarrow \chi_{\mathbf{v}} + \delta \tilde{\chi}_{\mathbf{v}}$ , we obtain the condition

$$\sum_{\gamma} \xi^T \mathbf{M}_\gamma \tilde{\chi}_\gamma = 0 \quad (2.119)$$

where the sum is now over all interfaces in the problem domain. This condition can be met for arbitrary  $\tilde{\chi}_{\mathbf{v}}$  only if the even-parity moments

$$\phi_\gamma = \mathbf{M}_\gamma^T \xi \quad (2.120)$$

are continuous across the interfaces. Thus for each node, we may combine this expression with Eq. (2.117) to express the even-parity interface moments in terms of the node source and the odd-parity interface moments

$$\phi_\gamma = \mathbf{M}_\gamma^T \mathbf{A}^{-1} \mathbf{q}_{\mathbf{v}} - \mathbf{M}_\gamma^T \mathbf{A}^{-1} \mathbf{M} \chi. \quad (2.121)$$

Letting  $\phi^T = [\phi_1^T, \phi_2^T, \dots]$ , and therefore  $\phi = \mathbf{M}^T \xi$ , we may write for each node

$$\phi = \mathbf{M}^T \mathbf{A}^{-1} \mathbf{q}_{\mathbf{v}} - \mathbf{M}^T \mathbf{A}^{-1} \mathbf{M} \chi. \quad (2.122)$$

A convenient way to solve these equations is to convert them to response matrix form. We make a linear transformation of variables

$$\mathbf{j}^{\pm} = 1/4\boldsymbol{\varphi} \pm 1/2\boldsymbol{\chi}, \quad (2.123)$$

which in the diffusion approximation correspond to the partial currents. We then may rewrite Eq. (2.122) in response matrix form

$$\mathbf{j}^{+} = \mathbf{R}\mathbf{j}^{-} + \mathbf{B}\mathbf{q}, \quad (2.124)$$

where the matrices are defined by  $\mathbf{R} = \left[ 1/2\mathbf{M}^T\mathbf{A}^{-1}\mathbf{M} + \mathbf{I} \right]^{-1} \left[ 1/2\mathbf{M}^T\mathbf{A}^{-1}\mathbf{M} - \mathbf{I} \right]$  and  $\mathbf{B} = \left[ 1/2\mathbf{M}^T\mathbf{A}^{-1}\mathbf{M} + \mathbf{I} \right]^{-1} 1/2\mathbf{M}^T\mathbf{A}^{-1}$ .

Red-black iteration or other methods, then, may be applied to the solution of the resulting equations. Partitioning algorithms, over-relaxation methods, and other techniques have also been developed to accelerate the iterative solutions of the systems of nodal response matrix equations [46,47].

### 2.5.2 An Even-Parity Integral Method

The functional given by Eq. (2.25) may also be used to derive an even-parity integral transport method [28, 44]. The treatment is restricted to isotropic scattering, and we also eliminate the surface term from Eq. (2.25) by assuming essential boundary conditions. To obtain the integral method, we reverse the discretization order used in the preceding sections and first discretize the spatial variables, using finite elements, while leaving the unknowns functions of angle. Dividing the problem domain into elements, Eq. (2.25) reduces to

$$F[\psi^{+}] = \sum_e \int_e dV \int d\Omega \left[ \sigma_e^{-1} (\Omega_k \nabla_k \psi^{+})^2 + \sigma_e \psi^{+2} - \sigma_{se} \phi^2 - 2\phi s \right]. \quad (2.125)$$

Then, employing the same finite element trial functions,  $\mathbf{n}_e(\vec{r})$ , used in Sections 2.4 and 2.5, we get

$$\psi^{+}(\vec{r}, \hat{\Omega}) = \mathbf{n}_e^T(\vec{r}) \boldsymbol{\varphi}_e(\hat{\Omega}), \quad (2.126)$$

and correspondingly

$$\phi(\vec{r}) = \mathbf{n}_e^T(\vec{r}) \boldsymbol{\phi}_e. \quad (2.127)$$

Here, the vectors  $\boldsymbol{\varphi}_e(\hat{\Omega})$  and  $\boldsymbol{\phi}_e$  approximate the even-parity angular flux and the scalar flux, respectively, at the spatial mesh points. Combining these approximations with Eq. (2.125) then yields

$$F[\boldsymbol{\varphi}_e] = \sum_e \left\{ \int d\Omega \boldsymbol{\varphi}_e^T(\hat{\Omega}) \left[ \Omega_k \Omega_{k'} \sigma_e^{-1} \int_e dV (\nabla_k \mathbf{n}_e) (\nabla_{k'} \mathbf{n}_e^T) \right. \right. \\ \left. \left. + \sigma_e \int_e dV \mathbf{n}_e \mathbf{n}_e^T \right] \boldsymbol{\varphi}_e(\hat{\Omega}) - \boldsymbol{\phi}_e^T \sigma_{se} \int_e dV \mathbf{n}_e \mathbf{n}_e^T \boldsymbol{\phi}_e - 2 \boldsymbol{\phi}_e^T \mathbf{s}_e \right\} \quad (2.128)$$

where  $\mathbf{s}_e = \int_e dV \mathbf{n}_e s$ . As in Eqs. (2.38) through (2.46), we assemble the elemental contributions into global vectors of angularly dependent coefficients through the use of the Boolean transformations  $\boldsymbol{\varphi}_e(\hat{\Omega}) = \Xi_e \boldsymbol{\varphi}(\hat{\Omega})$  and  $\boldsymbol{\phi}_e = \Xi_e \boldsymbol{\phi}$ . The reduced functional is then

$$F[\boldsymbol{\varphi}] = \int d\Omega \boldsymbol{\varphi}^T(\hat{\Omega}) \mathbf{A}_I(\hat{\Omega}) \boldsymbol{\varphi}(\hat{\Omega}) - \boldsymbol{\phi}^T \mathbf{B}_I \boldsymbol{\phi} - 2 \boldsymbol{\varphi}^T \mathbf{s}_I, \quad (2.129)$$

where

$$\mathbf{A}_I(\hat{\Omega}) = \Omega_k \Omega_{k'} \sum_e \Xi_e^T \sigma_e^{-1} \int_e dV (\nabla_k \mathbf{n}_e) (\nabla_{k'} \mathbf{n}_e^T) \Xi_e \\ + \sum_e \Xi_e^T \sigma_e \int_e dV \mathbf{n}_e \mathbf{n}_e^T \Xi_e, \quad (2.130)$$

$$\mathbf{B}_I = \sum_e \Xi_e^T \sigma_{se} \int_e dV \mathbf{n}_e \mathbf{n}_e^T \Xi_e, \quad (2.131)$$

and

$$\mathbf{s}_I = \sum_e \Xi_e^T \mathbf{s}_e. \quad (2.132)$$

Requiring Eq. (2.129) to be stationary with regard to variations in  $\boldsymbol{\varphi}(\hat{\Omega})$  then yields the Euler–Lagrange equation

$$\mathbf{A}_I(\hat{\Omega}) \boldsymbol{\varphi}(\hat{\Omega}) = \mathbf{B}_I \boldsymbol{\phi} + \mathbf{s}_I. \quad (2.133)$$

We may obtain scalar flux equations by first inverting  $\mathbf{A}$  and then integrating over angle. We obtain

$$\left[ \mathbf{I} - \int d\Omega \mathbf{A}_I^{-1}(\hat{\Omega}) \mathbf{B}_I \right] \boldsymbol{\phi} = \int d\Omega \mathbf{A}_I^{-1}(\hat{\Omega}) \mathbf{s}_I. \quad (2.134)$$

This equation has a number of similarities to those obtained using collision probability theory [28]. The dimension of the problem is only that of the number of spatial nodes, but the coefficient matrix on the left is both dense and nonsymmetric. Moreover, since analytical inversion of  $\mathbf{A}_I(\hat{\Omega})$  represents an intractable task, numerical quadrature must be used, inviting comparison to the ray tracing methods used in integral transport schemes. Treating curved boundaries and other irregular features is straightforward using isoparametric finite elements. Moreover, the truncation errors

are order  $h^2$  for the lowest-order finite elements (triangles with piecewise linear trial functions), compared to  $h$  for collision probability methods, allowing coarser element meshes to be used.

### 2.5.3 Combined Methods

The variational nodal method as described in Section 2.5.1 is applicable to homogeneous nodes. However, by using finite element trial functions within the nodes, heterogeneous nodes may also be treated. Recently, this has been accomplished in what is called the subelement nodal method and applied to reactor problems in which each node corresponds to one pin-cell [48]. Likewise, the integral method described in Section 2.5.2 may be placed within the nodal framework, and this too has resulted in the ability to treat heterogeneous nodes, often times with substantial savings in memory over what is required using the corresponding differential method [49].

## 2.6 Discussion

The foregoing sections attempt to provide an overview of the second-order methods that are finding increased use in neutron transport calculations. The focus has been placed upon the discretization of the transport equation rather than on the algorithms that are employed to solve the resulting sets of linear equations. The vast literature on iterative methods used to solve large sets of sparse matrix equations, and in particular the intense efforts being made to effectively utilize parallel computing to speed such computations, lies beyond the scope of this overview. In addition, the foregoing exposition has been limited to the linear neutron transport equation. No attempt has been made to include recent work in which second-order transport methods are combined with computational fluid mechanics or other techniques to include nonlinear thermal-hydraulic feedback mechanisms into neutronics calculations. Likewise, the scope of this work has not included techniques needed specifically in treating the unique characteristics of thermal radiation or of electron transport problems.

Work in progress seems destined to expand significantly the value of second-order methods. In particular, interest in the primal and dual coupled forms of the transport equations is beginning to break down the sharp distinction between first- and second-order methods. Perhaps the greatest challenge facing the expanded use of second-order methods, however, is in the treatment of void regions. Since the total cross section appears in the denominator of the even-parity equations, they cannot be applied directly to vacuum regions. Rather, they must be coupled with ray tracing or other techniques in situations, where neutron streaming in voids must be incorporated into second-order computations.

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