Chapter 3

The Neutron Diffusion Equation

The neutron diffusion equation is an angular approximation to the transport equation. The benefit of the diffusion equation is that it only involves the scalar flux and not the angular flux. To get this equation we have to make a number of simplifications, that may or may not be justified for a given system. We will begin with a straightforward way to derive neutron diffusion equation, before delving deeper into when it is applicable.

3.1 Simple Derivation of the Neutron Diffusion Equation

We will begin with the multigroup form of the neutron transport equation using one of the methods of defining the multigroup cross-sections (P_1 consistent, extended Legendre, or separability assumption). This equation and it's boundary conditions are

$$\begin{aligned}\frac{1}{v_g}\frac{\partial \psi_g}{\partial t} + \hat{\Omega}\cdot\nabla\psi_g(\mathbf{x},\hat{\Omega},t) + \Sigma_{\mathrm{t}g}\psi_g(\mathbf{x},\hat{\Omega},t) = \\ \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\hat{\Omega})\sum_{g'=1}^{G}\Sigma_{\mathrm{s}l,g'\to g}(\mathbf{x},t)\phi_{lmg'}(\mathbf{x},t) + \\ \frac{\chi_g(\mathbf{x})}{4\pi}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{x},t)\phi_{g'}(\mathbf{x},t) + \frac{q_g(\mathbf{x},t)}{4\pi},\end{aligned} \tag{3.1}$$

$$\psi_g(\mathbf{x},\hat{\Omega},t) = F_g(\mathbf{x},\hat{\Omega},t), \qquad \text{for } \mathbf{x}\in\partial V \text{ and } \hat{n}\cdot\hat{\Omega} < 0.$$

We have included the time derivative term and assumed that the source is isotropic in angle.

We then, apropos of nothing, assume that the angular flux is linear in angle of the form

$$\psi_g(\mathbf{x},\hat{\Omega},t) = \frac{1}{4\pi}\phi_g(\mathbf{x},t) + \frac{3}{4\pi}\hat{\Omega}\cdot\mathbf{J}_g(\mathbf{x},t), \tag{3.2}$$

where ϕ_g and $\mathbf{J}_g$ are the group-integrated scalar flux and net current density given by

$$\phi_g(\mathbf{x},t) = \int_{4\pi} d\hat{\Omega}\,\psi_g(\mathbf{x},\hat{\Omega},t), \qquad \mathbf{J}_g(\mathbf{x},t) = \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\psi_g(\mathbf{x},\hat{\Omega},t).$$

Before we proceed, it will be useful to point out some identities from the spherical harmonics. The first involves Y_{00} times ϕ_{00g}:

$$Y_{00}(\hat{\Omega})\phi_{00g}(\mathbf{x},t) = \frac{1}{\sqrt{4\pi}}\int_{4\pi} d\hat{\Omega}\,\frac{1}{\sqrt{4\pi}}\psi_g(\mathbf{x},\hat{\Omega},t) = \frac{\phi_g(\mathbf{x},t)}{4\pi}. \quad (3.3)$$

The second identity involves $\hat{\Omega}$ written in spherical harmonics:

$$\hat{\Omega} \;=\; \begin{pmatrix} \sqrt{1-\mu^2}\cos\varphi \\ \sqrt{1-\mu^2}\sin\varphi \\ \mu \end{pmatrix} \;=\; \sqrt{\frac{4\pi}{3}}\begin{pmatrix} Y_{11}(\hat{\Omega}) \\ Y_{1,-1}(\hat{\Omega}) \\ Y_{10}(\hat{\Omega}) \end{pmatrix}. \quad (3.4)$$

Using this identity we can relate some spherical harmonics moments to $\mathbf{J}_g$:

$$Y_{10}(\hat{\Omega})\phi_{10g} = \sqrt{\frac{3}{4\pi}}\int_{4\pi} d\hat{\Omega}\,\sqrt{\frac{3}{4\pi}}\mu\psi_g(\mathbf{x},\hat{\Omega},t) = \frac{3}{4\pi}J_{zg}(\mathbf{x},t), \quad (3.5a)$$

$$Y_{11}(\hat{\Omega})\phi_{11g} = \sqrt{\frac{3}{4\pi}}\int_{4\pi} d\hat{\Omega}\,\sqrt{\frac{3}{4\pi}}\sqrt{1-\mu^2}\cos\varphi\psi_g(\mathbf{x},\hat{\Omega},t) = \frac{3}{4\pi}J_{xg}(\mathbf{x},t), \quad (3.5b)$$

and

$$Y_{1,-1}(\hat{\Omega})\phi_{1,-1g} = \sqrt{\frac{3}{4\pi}}\int_{4\pi} d\hat{\Omega}\,\sqrt{\frac{3}{4\pi}}\sqrt{1-\mu^2}\sin\varphi\psi_g(\mathbf{x},\hat{\Omega},t) = \frac{3}{4\pi}J_{yg}(\mathbf{x},t), \quad (3.5c)$$

To these two identities based on spherical harmonics, we also will need some identities related to integrals over the unit sphere:

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega} = 0, \qquad\qquad \int_{4\pi} d\hat{\Omega}\,\Omega_i\Omega_j = \frac{4\pi}{3}\delta_{ij}. \quad (3.6)$$

The derivation of the diffusion equation will replace ψ_g in Eq. (3.1) with the linear-in-angle form from Eq. (3.2), and then integrate the equation over all $\hat{\Omega}$. Some of the terms simplify using the above identities to get

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} + \nabla \cdot \mathbf{J}_g(\mathbf{x}, t) + \Sigma_{\mathrm{t}g}\phi_g(\mathbf{x}, t) = \sum_{g'=1}^{G} \Sigma_{\mathrm{s}g' \to g}(\mathbf{x}, t)\phi_{g'}(\mathbf{x}, t) + \chi_g(\mathbf{x}) \sum_{g'=1}^{G} \bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{x}, t)\phi_{g'}(\mathbf{x}, t) + q_g(\mathbf{x}, t), \quad (3.7)$$

we have dropped the subscript "0" from the scattering cross-section that is the zeroth Legendre moment. The simplification of the scattering term comes from the orthogonality of the spherical harmonics functions. This is an equation involving only the scalar flux and current density. We will need another equation to close the system. To get this equation we multiply Eq. (3.1) by $\hat{\Omega}$ and integrate over the unit sphere to get:

$$\frac{1}{v_g}\frac{\partial \mathbf{J}_g}{\partial t} + \frac{1}{3}\nabla\phi_g(\mathbf{x}, t) + \Sigma_{\mathrm{t}g}\mathbf{J}_g(\mathbf{x}, t) = \sum_{g'=1}^{G} \Sigma_{\mathrm{s}1,g' \to g}(\mathbf{x}, t)\mathbf{J}_{g'}(\mathbf{x}, t). \quad (3.8)$$

The next approximation we make is that the scattering into group G is the same as the scattering out of group G. This approximation means

$$\sum_{g'=1}^{G} \Sigma_{\mathrm{s}1,g' \to g}(\mathbf{x}, t))\mathbf{J}_{g'}(\mathbf{x}, t) = \sum_{g'=1}^{G} \Sigma_{\mathrm{s}1,g \to g'}(\mathbf{x}, t)\mathbf{J}_g(\mathbf{x}, t).$$

To proceed we define a quantity $\bar{\mu}$ as

$$\bar{\mu}_g(\mathbf{x}) = \frac{\sum_{g'=1}^{G} \Sigma_{\mathrm{s1},g\to g'}(\mathbf{x},t)}{\sum_{g'=1}^{G} \Sigma_{\mathrm{s}g\to g'}(\mathbf{x},t)}. \tag{3.9}$$

This quantity is the average cosine of the scattered angle for neutrons in group g. We also note that the sum over all g' of $\Sigma_{\mathrm{s}l,g\to g'} = \Sigma_{\mathrm{s}l,g}$, and that $\Sigma_{\mathrm{s}g} = \Sigma_{\mathrm{s}0,g}$. This allows us to write Eq. (3.8) as

$$\frac{1}{v_g}\frac{\partial \mathbf{J}_g}{\partial t} + \frac{1}{3}\nabla\phi_g(\mathbf{x},t) + \Sigma_{\mathrm{t}g}\mathbf{J}_g(\mathbf{x},t) = \Sigma_{\mathrm{s}g}\bar{\mu}_g\mathbf{J}_g. \tag{3.10}$$

The final assumption we make is that the time derivative term can be neglected. This could be for two reasons: the neutron speed could be very large or the current has reached steady-state. Upon neglecting the time derivative term, we get an equation that is known as Fick's law, which relates the current to the gradient of the scalar flux:

$$\mathbf{J}_g(\mathbf{x},t) \approx -D_g(\mathbf{x},t)\nabla\phi_g, \tag{3.11}$$

where the diffusion coefficient, D_g, is given by

$$D_g(\mathbf{x},t) = \frac{1}{3\left(\Sigma_{\mathrm{t}g} - \bar{\mu}_g\Sigma_{\mathrm{s}g}\right)} = \frac{1}{3\Sigma_{\mathrm{tr}g}}. \tag{3.12}$$

The diffusion coefficient is often given in terms of the "transport" cross-section $\Sigma_{\mathrm{tr}g}$, which is defined as

$$\Sigma_{\mathrm{tr}g}(\mathbf{x}) = \Sigma_{\mathrm{t}g} - \bar{\mu}_g\Sigma_{\mathrm{s}g}.$$

The last step is to use Fick's law in Eq. (3.7) to get a single equation for the scalar flux:

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} - \nabla\cdot D_g(\mathbf{x},t)\nabla\phi_g(\mathbf{x},t) + \Sigma_{\mathrm{r}g}\phi_g(\mathbf{x},t) = \sum_{g'=1,g'\neq g}^{G} \Sigma_{\mathrm{s},g'\to g}\phi_{g'} + \chi_g\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'} + Q_g, \tag{3.13}$$

where the removal cross-section, Σ_{rg}, represents the total cross-section corrected for the scattering of neutrons that stay in group g:

$$\Sigma_{\mathrm{r}g}(\mathbf{x}) = \Sigma_{\mathrm{t}g} - \Sigma_{\mathrm{s}g'\to g}.$$

3.1.1 Summary of Approximations made to get the diffusion equation

To get the diffusion equation we had to make several approximations:

1. The angular flux is linear in angle,
2. The neutron current is weakly time-dependent, and
3. The in-scattering to group g is approximately the same as the out-scattering from group g.

Approximation 2 is no longer an approximation when we look at eigenvalue or steady-state problems, though it does make the idea of time-dependent diffusion a bit strange. We assumed $\mathbf{J}_g$, which depends on ϕ_g, to be approximately constant in time and at the same time we say that the scalar flux is time dependent.

The in and out scattering assumption actually goes away as we coarsen the groups, that is, make G smaller. With coarse groups, the leakage out and into a group would be smaller than if the groups were fine. Moreover, when we only have a single group, $G = 1$, there is no approximation here at all.

The approximation of the angular flux being linearly dependent on $\hat{\Omega}$ is hard to justify without some additional discussion. We cannot say why such a nice form for the angular flux should exist. We can justify this assumption, in particular cases, using an asymptotic analysis.

3.2 Asymptotic Derivation of the Diffusion Equation

We can derive the diffusion equation without making approximations pell mell. Rather we characterize the problem we are looking at using a positive parameter, ϵ. We will then look at how the solution to the transport equation behaves as $\epsilon \to 0$. The problem we will consider has in each group a large scattering cross-section, small absorption, and small sources. The time-evolution of the solution is also assumed to be slow; this is equivalent to assuming that any fast transients in the system has passed. We will represent this problem using by scaling terms in the transport equation as

$$\Sigma_{\mathrm{s}g} \to \frac{\Sigma_{\mathrm{s}g}}{\epsilon},$$

$$\Sigma_{\mathrm{t}g} \to \epsilon\Sigma_{\mathrm{a}g} + \frac{\Sigma_{\mathrm{s}g}}{\epsilon},$$

$$\frac{1}{v_g} \to \frac{\epsilon}{v_g},$$

and

$$q_g \to \epsilon q_g.$$

Because fission is an absorption reaction, we also have

$$\bar{\nu}\Sigma_{\mathrm{f}g'} \to \epsilon\bar{\nu}\Sigma_{\mathrm{f}g'}.$$

In the problem we are interested in, the scattering is only weakly anisotropic, and that within group scattering is large so that

$$\Sigma_{\mathrm{s}l,g'\to g} \to \epsilon^{l-\delta_{l0}-2\delta_{l1}-\delta_{gg'}}\Sigma_{\mathrm{s}l,g'\to g}.$$

Inserting these substitutions into the neutron transport equation gives the following equation

$$\begin{aligned}\frac{\epsilon}{v_g}\frac{\partial\psi_g}{\partial t} + \hat{\Omega}\cdot\nabla\psi_g + \left(\epsilon\Sigma_{\mathrm{a}g} + \frac{\Sigma_{\mathrm{s}g}}{\epsilon}\right)\psi_g = \\ \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\hat{\Omega})\sum_{g'=1}^{G}\epsilon^{l-\delta_{l0}-2\delta_{l1}-\delta_{gg'}}\Sigma_{\mathrm{s}l,g'\to g}(\mathbf{x},t)\phi_{lmg'} + \\ \frac{\epsilon\chi_g(\mathbf{x})}{4\pi}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{x},t)\phi_{g'} + \frac{\epsilon q_g}{4\pi}.\end{aligned} \tag{3.14}$$

The next step in our derivation is to write the solution as the sum of functions that have a magnitude of powers of ϵ. This means we write the angular flux as

$$\psi_g(\mathbf{x},\hat{\Omega},t) = \sum_{m=0}^{\infty}\epsilon^m\psi_g^{(m)}(\mathbf{x},\hat{\Omega},t). \tag{3.15}$$

This power series in ϵ partitions the solution so that as ϵ goes to zero we know that

$$\psi_g^{(0)}(\mathbf{x},\hat{\Omega},t) \gg \epsilon\psi_g^{(1)}(\mathbf{x},\hat{\Omega},t) \gg \epsilon^2\psi_g^{(2)}(\mathbf{x},\hat{\Omega},t) \gg \dots$$

Ergo, if ϵ is small, which corresponds to the problem set up we have described above, then if we can get an equation for $\psi_g^{(0)}$, we have captured the lion's share of the behavior of the angular flux. In more formal notation $\psi_g = \psi_g^{(0)} + O(\epsilon)$. Given that moments of the angular flux do not affect the power series representation in Eq. (3.15), we can also write the moments as

$$\phi_g(\mathbf{x},t) = \sum_{m=0}^{\infty} \epsilon^m \phi_g^{(m)}(\mathbf{x},t), \qquad \phi_{lmg}(\mathbf{x},t) = \sum_{m=0}^{\infty} \epsilon^m \phi_{lmg}^{(m)}(\mathbf{x},t). \tag{3.16}$$

The way that we proceed is to substitute the power series into Eq. (3.14) and look at the terms that are particular powers of ϵ. The terms in Eq. (3.14) that are multiplied by ϵ^{-1} are

$$\Sigma_{\mathrm{s}g}\psi_g^{(0)} = \frac{1}{4\pi}\left[\Sigma_{\mathrm{s}g}\phi_g^{(0)} + 3\Sigma_{\mathrm{s}1,g}\hat{\Omega}\cdot\mathbf{J}_g^{(0)}\right]. \tag{3.17}$$

To get this result we have used the following $O(\epsilon)$ approximations

$$\Sigma_{\mathrm{s}g} = \Sigma_{\mathrm{s}g'\to g} + O(\epsilon), \qquad \Sigma_{\mathrm{s}1,g} = \Sigma_{\mathrm{s}1,g'\to g} + O(\epsilon). \tag{3.18}$$

This equation tells that to leading order in ϵ, ψ_g is linear in angle. Looking at the terms in Eq. (3.14) that are multiplied by ϵ^0 are

$$\hat{\Omega}\cdot\nabla\psi_g^{(0)} + \Sigma_{\mathrm{s}g}\psi_g^{(1)} = \frac{1}{4\pi}\left[\Sigma_{\mathrm{s}g}\phi_g^{(1)} + 3\Sigma_{\mathrm{s}1,g}\hat{\Omega}\cdot\mathbf{J}_g^{(1)}\right] \tag{3.19}$$

If we multiply this equation by Ω and integrate over the unit sphere we get

$$\frac{1}{3}\nabla\phi_g^{(0)} + \Sigma_{\mathrm{s}g}\mathbf{J}_g^{(1)} = \Sigma_{\mathrm{s}1,g}\mathbf{J}_g^{(1)}, \tag{3.20}$$

which we can rearrange into Fick's law

$$\mathbf{J}_g^{(1)} = \frac{-1}{3(\Sigma_{\mathrm{s}g} - \Sigma_{\mathrm{s}1,g})}\nabla\phi_g^{(0)} = \frac{-1}{3(\Sigma_{\mathrm{t}g} - \Sigma_{\mathrm{s}1,g})}\nabla\phi_g^{(0)} + O(\epsilon^2). \tag{3.21}$$

We can write this version of Fick's law using the average scattering angle cosine, $\bar{\mu}_g$, by recognizing

$$\bar{\mu}_g = \frac{\Sigma_{\mathrm{s}1,g}}{\Sigma_{\mathrm{s}g}}.$$

The last step is to take the scaled-transport equation and look at the $O(\epsilon)$ terms. These are

$$\frac{1}{v_g}\frac{\partial \psi_g^{(0)}}{\partial t} + \hat{\Omega}\cdot\nabla\psi_g^{(1)} + \Sigma_{\mathrm{a}g}\psi_g^{(0)} + \Sigma_{\mathrm{s}g}\psi_g^{(2)} = \frac{1}{4\pi}\left[\Sigma_{\mathrm{s}g}\phi_g^{(2)} + 3\Sigma_{\mathrm{s}1,g}\hat{\Omega}\cdot\mathbf{J}_g^{(2)}\right]$$
$$+\frac{1}{4\pi}\sum_{g'=1,g'\neq g}^{G}\left[\Sigma_{\mathrm{s}g'\to g}\phi_{g'}^{(0)} + 3\Sigma_{\mathrm{s}1,g'\to g}\hat{\Omega}\cdot\mathbf{J}_{g'}^{(0)}\right]+$$
$$\frac{\chi_g}{4\pi}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'}^{(0)} + \frac{q_g}{4\pi}. \quad (3.22)$$

Once again we integrate over the unit sphere:

$$\frac{1}{v_g}\frac{\partial \phi_g^{(0)}}{\partial t} + \nabla\cdot\mathbf{J}_g^{(1)} + \Sigma_{\mathrm{a}g}\phi_g^{(0)} + \Sigma_{\mathrm{s}g}\phi_g^{(2)} = \Sigma_{\mathrm{s}g}\phi_g^{(2)}$$
$$\sum_{g'=1,g'\neq g}^{G}\Sigma_{\mathrm{s}g'\to g}\phi_{g'}^{(0)}+$$
$$\chi_g\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'}^{(0)} + q_g. \quad (3.23)$$

To finish our derivation we will use Fick's law from Eq. (3.21) and the following asymptotic relation for the removal cross-section:

$$\Sigma_{\mathrm{r}g} = \Sigma_{\mathrm{t}g} - \Sigma_{\mathrm{s}g\to g} = \Sigma_{\mathrm{t}g} - \Sigma_{\mathrm{s}g} + O(\epsilon) = \Sigma_{\mathrm{a}g} + O(\epsilon). \quad (3.24)$$

Therefore, we can write Eq. (3.23) as the diffusion equation that we derived in the previous section:

$$\frac{1}{v_g}\frac{\partial \phi_g^{(0)}}{\partial t} - \nabla \cdot D_g \nabla \phi_g^{(0)} + \Sigma_{\mathrm{r}g}\phi_g^{(0)} = \sum_{g'=1, g'\neq g}^{G} \Sigma_{\mathrm{s}g'\to g}\phi_{g'}^{(0)} + \chi_g \sum_{g'=1}^{G} \bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'}^{(0)} + q_g. \quad (3.25)$$

This equation says that to leading order in ϵ the scalar flux will satisfy the diffusion equation if the problem has the following features:

1. The cross-sections are scattering dominated, i.e., $(\Sigma_{\mathrm{s}g} \gg \Sigma_{\mathrm{a}g})$,
2. Group to group scattering is small, i.e., $\Sigma_{\mathrm{s}g} \approx \Sigma_{\mathrm{s}g\to g}$,
3. The scattering is weakly anisotropic, i.e., $\Sigma_{sl,g} = O(\epsilon^{l-1})$ for $l > 1$, and
4. The source strength is small.

These are the approximations that we need for the diffusion equation to be valid. The suppositions on the material properties (cross-sections, etc.) can be justified for some light-water reactor systems, especially if the fuel and moderator are homogenized. Moreover, the group to group scattering being small can be assured by having a coarse group structure[1].

3.3 Boundary Conditions for the Diffusion Equation

There is one more approximation that we need to handle for the diffusion equation: boundary conditions. Because the diffusion equation only deals with the scalar flux, which is an integral over all angles and the transport equation has boundary conditions in terms of incoming angles, there is a mismatch. This results in a situation where we cannot specify the correct transport boundary conditions for diffusion and near a boundary the diffusion solution will differ from the transport solution. In the following discussion we will assume that we have a boundary condition for the transport problem of the form

$$\psi_g(\mathbf{x}, \hat{\Omega}, t) = F(\mathbf{x}, \hat{\Omega}, t), \qquad \text{for } \mathbf{x} \in \partial V, \quad \hat{n}\cdot\hat{\Omega} < 0.$$

[1] This is one of those times in computational science where coarser resolution can give you a better answer than a higher resolution discretization. This is important to understand when someone shows you a result with many groups using diffusion: the actual spectrum may not be better than a few group calculation.

The most typical way to treat boundary conditions with diffusion is to use what are known as Marshak boundary conditions. In this case equate a half-range moment of the incoming angular flux to the half-range moment of the linear-in-angle expansion used in diffusion. In particular we equate

$$\int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}\psi_g(\mathbf{x},\hat{\Omega},t) = \int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}F(\mathbf{x},\hat{\Omega},t), \qquad \mathbf{x}\in\partial V,. \tag{3.26}$$

Using the linear-in-angle form of the angular flux used in the diffusion approximation, the half-range integral of the angular flux becomes

$$\int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}\psi_g(\mathbf{x},\hat{\Omega},t) = \int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}\left(\frac{\phi_g}{4\pi} + \frac{3}{4\pi}\hat{\Omega}\cdot\mathbf{J}_g\right) \tag{3.27}$$

$$= \frac{\phi_g}{4} - \frac{1}{2}\hat{n}\cdot\mathbf{J}_g$$

$$= \frac{\phi_g}{4} + \frac{D_g}{2}\left(\hat{n}\cdot\nabla\phi_g\right), \qquad \mathbf{x}\in\partial V.$$

Therefore, the Marshak boundary condition can be written for diffusion as

$$\frac{\phi_g}{4} + \frac{D_g}{2}\left(\hat{n}\cdot\nabla\phi_g\right) = \int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}F(\mathbf{x},\hat{\Omega},t), \qquad \mathbf{x}\in\partial V. \tag{3.28}$$

Another type of boundary condition that we use is known as the Mark boundary condition. In this boundary condition we enforce the angular flux to be equal to the incoming flux at a particular direction. The direction we choose is $\hat{n}\cdot\hat{\Omega} = -1/\sqrt{3}$. This angle is chosen because it is the root of the second Legendre moment (the one we neglect in the linear expansion of the angular flux). There is an entire circle of angles that have this dot product with the boundary normal, therefore we need to integrate the boundary flux around this circle to get the Mark boundary condition is then

$$\frac{\phi_g}{2}+\frac{D_g\sqrt{3}}{2}\left(\hat{n}\cdot\nabla\phi_g\right)=\int_{\hat{n}\cdot\hat{\Omega}=-1/\sqrt{3}} d\hat{\Omega}\, F\left(\mathbf{x},\hat{\Omega},t\right), \qquad \mathbf{x}\in\partial V. \tag{3.29}$$

Sometimes it is useful to specify the scalar flux on the boundary as a Dirichlet boundary condition. In some sense this does not make sense physically, but there may be times when for code testing purposes this is useful. Additionally, if there are no incoming neutrons into the problem, then we can expect that somewhere just outside the boundaries the scalar flux will go to zero. This is the type of boundary condition used in elementary reactor theory. A Dirichlet boundary condition is simply specified as

$$\phi_g(\mathbf{x})=G(\mathbf{x}), \qquad \text{for } \mathbf{x}\in\partial V \text{ or } \mathbf{x}\in\partial V^+, \tag{3.30}$$

where we have denoted a position some distance beyond the boundary as ∂V^+ to allow for extrapolated boundary conditions.

The previous three boundary conditions dealt with specifying the solution on the boundary. In some cases there will be a plane of symmetry in the problem and we want to specify that the problem is symmetric across some boundary. One can show that in this case the net current density across this boundary is zero. We usually call this a reflecting boundary because both the system can be reflected across this boundary *and* neutrons in effect bounce (i.e., reflect) on this boundary. To specify a reflecting boundary we write

$$\mathbf{J}_g(\mathbf{x})=0, \qquad \text{for } \mathbf{x}\in\partial V. \tag{3.31}$$

The final boundary condition we will consider is the albedo boundary condition. This condition specifies that some fraction of the outgoing neutron current density returns. This fraction is given as α. In particular we write

$$\int\limits_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}\psi_g(\mathbf{x},\hat{\Omega},t)=\alpha\int\limits_{\hat{\Omega}\cdot\hat{n}>0} d\hat{\Omega}\,\hat{\Omega}\psi_g(\mathbf{x},\hat{\Omega},t), \qquad \text{for } \mathbf{x}\in\partial V. \tag{3.32}$$

Table 3.1: Constants in the Brunner boundary condition given by Eq. (3.35)

Boundary Condition	$\mathcal{A}$	$\mathcal{B}$	$\mathcal{C}$
Marshak	$\frac{1}{4}$	$\frac{1}{2}$	$\int_{\hat{\Omega}\cdot\hat{n}<0} d\hat{\Omega}\,\hat{\Omega}F(\mathbf{x},\hat{\Omega},t)$
Mark	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$\int_{\hat{\Omega}\cdot\hat{n}=-1/\sqrt{3}} d\hat{\Omega}\,F\left(\mathbf{x},\hat{\Omega},t\right)$
Dirichlet	1	0	G
Reflecting	0	1	0
Albedo	$\frac{1-\alpha}{2(1+\alpha)}$	1	0

With the linear-in-angle expansion of the angular flux, this relationship becomes

$$\frac{\phi_g}{4}+\frac{D_g}{2}\left(\hat{n}\cdot\nabla\phi_g\right)=\alpha\left[\frac{\phi_g}{4}-\frac{D_g}{2}\left(\hat{n}\cdot\nabla\phi_g\right)\right], \qquad \text{for } \mathbf{x}\in\partial V. \tag{3.33}$$

We can rearrange this equation to get the more common form of the albedo boundary condition

$$\frac{1-\alpha}{2(1+\alpha)}\phi_g+D_g\left(\hat{n}\cdot\nabla\phi_g\right)=0, \qquad \text{for } \mathbf{x}\in\partial V. \tag{3.34}$$

Notice that for $\alpha = 1$ we recover the reflecting boundary condition. The albedo boundary condition is useful for modeling objects that are outside the system of interest that return some neutrons to the system. This could be the case for a shield outside a reactor where a fraction of neutrons that leak into the shield are returned to the reactor. It is also possible to derive albedo boundary conditions that couple groups, e.g., a fraction neutrons that leak out in group g are returned in group $g+1$, but such conditions are not commonly used.

3.3.1 The Brunner Boundary Conditions

Brunner [4] formulated a compact and general form for diffusion boundary conditions for high-energy density physics radiative transfer problems. We borrow his notation here to write a general boundary condition for the neutron transport equation as

$$\mathcal{A}\phi_g+\mathcal{B}D_g\left(\hat{n}\cdot\nabla\phi_g\right)=\mathcal{C}, \qquad \text{for } \mathbf{x}\in\partial V. \tag{3.35}$$

The constants, $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are given for the various boundary conditions we have discussed in Table 3.1.

3.4 Other forms of the diffusion equation

To this point we have only discussed time-dependent diffusion problems with general boundary conditions. There is also a diffusion version of the two eigenvalue problems we discussed in Chapter 1. The α-eigenvalue problem seeks the rightmost value of α in the complex plane for which a non-trivial solution, $\phi_g(\mathbf{x})$ to the following equation exists:

$$-\nabla \cdot D_g \nabla \phi_g + \left(\frac{\alpha}{v_g} + \Sigma_{\mathrm{a}g}\right)\phi_g = \sum_{g'=1, g'\neq g}^{G} \Sigma_{\mathrm{s}g'\to g}\phi_{g'} + \chi_g \sum_{g'=1}^{G} \bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'}, \quad (3.36)$$

with boundary conditions that are either zero incoming neutrons (either as Marshak, Mark, or Dirichlet) or reflecting/albedo. In terms of Brunner boundary conditions, for α eigenvalue problems $\mathcal{C} = 0$.

The form of k-eigenvalue problems is similar. Here we seek the largest value of k such that there exists a non-trivial solution $\phi_g(\mathbf{x})$ to the equation

$$-\nabla \cdot D_g \nabla \phi_g + \Sigma_{\mathrm{a}g}\phi_g = \sum_{g'=1, g'\neq g}^{G} \Sigma_{\mathrm{s}g'\to g}\phi_{g'} + \frac{\chi_g}{k} \sum_{g'=1}^{G} \bar{\nu}\Sigma_{\mathrm{f}g'}\phi_{g'}, \quad (3.37)$$

with the same boundary conditions as the α-eigenvalue problem. We call this largest eigenvalue k_{eff} and the associated eigenfunction the fundamental mode.