NE 155, Classes 5-6, S16
Diffusion Equation
January 29 – February 1, 2016

Transport Equation

Largely from Lewis and Miller Chp. 1 [3] and Duderstadt and Hamilton Chp. 4 [1]. Note: Duderstadt and Martin [2] is a very good general reference. It goes through all of this same stuff, but from a slightly more generic point of view (since this applies to any collection of neutral particles).

Recap

The balance of neutrons: rate of change - production + loss = 0.

Suppressing dependencies to save space for the moment

$$\int_V d^3r \Big[\frac{\partial n}{\partial t} - \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \Sigma_s(E',\hat{\Omega}' \to E,\hat{\Omega}) v'n' \\ - \frac{\chi(E)}{4\pi}\int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \nu(E')\Sigma_f(E')v'n' - s + \Sigma_t vn + \hat{\Omega}\cdot\nabla vn\Big] = 0$$

We note that since the volume was arbitrarily chosen, the integral will only vanish if the integrand is zero

$$\int_{\text{any } V} d^3r f(\vec{r}) = 0 \to f(\vec{r}) = 0\,.$$

Now we have a balance relation that we can rearrange, substituting $\psi(\vec{r},E,\hat{\Omega},t) = vn(\vec{r},E,\hat{\Omega},t)$, to get what we usually call the Boltzmann Equation for neutron transport

$$\frac{1}{v}\frac{\partial\psi(\vec{r},E,\hat{\Omega},t)}{\partial t} + \hat{\Omega}\cdot\nabla\psi(\vec{r},E,\hat{\Omega},t) + \Sigma_t\psi(\vec{r},E,\hat{\Omega},t) = \\ \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\Sigma_s(E',\hat{\Omega}' \to E,\hat{\Omega})\psi(\vec{r},E',\hat{\Omega}',t) + \\ \frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu(E')\Sigma_f(E')\int_{4\pi} d\hat{\Omega}'\psi(\vec{r},E',\hat{\Omega}',t) + s(\vec{r},E,\hat{\Omega},t)$$

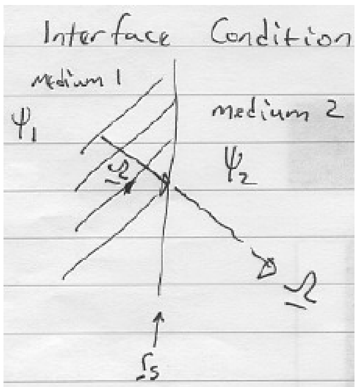
Initial and Boundary Conditions

1. Initial Condition: we start with some initial "known" state:

$$\psi(\vec{r}, E, \hat{\Omega}, 0) = \psi_0(\vec{r}, E, \hat{\Omega})$$

   for the problem domain. Note, the initial flux can be a functional expression.

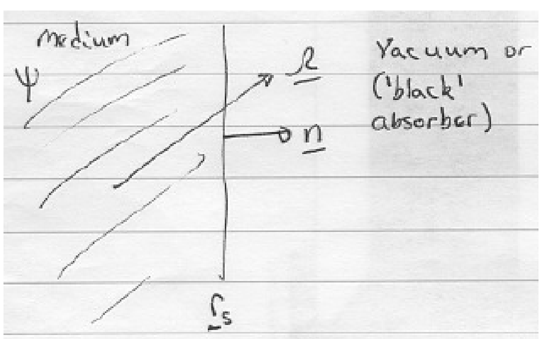
2. Interface Condition: the angular flux must be continuous along $\hat{\Omega}$ at all points, including material interfaces.



$$\psi_1(\vec{r}_S, E, \hat{\Omega}, t) = \psi_2(\vec{r}_S, E, \hat{\Omega}, t)$$

   $\forall E$ and $\hat{\Omega}$.

3. Fixed Condition: you can specify incoming flux



   $\psi(\vec{r}_S, E, \hat{\Omega}, t) = \psi_{IN}(\vec{r}_S, E, \hat{\Omega}, t)$ for $\vec{e} \cdot \hat{\Omega} < 0$: specifying incoming neutrons. Note, the incoming flux can be a functional expression; it can also be zero.
   This is equivalent to specifying the incoming partial current,

$$\vec{j}^{\,-}(\vec{r}_S, E, t) = \int_{\vec{e}\cdot\hat{\Omega}<0} d\hat{\Omega}(\vec{e}\cdot\hat{\Omega})\psi(\vec{r}_S, E, \hat{\Omega}, t).$$

4. Reflective Condition: there is mirror symmetry at some surface:

$$\psi(\hat{\Omega}_{IN}) = \psi(\hat{\Omega}_{OUT}) \; .$$

5. Periodic Condition: you know there is a repetition in the system

$$\psi(\vec{r}_S, E, \hat{\Omega}, t) = \psi(\vec{r}_S \pm \vec{p}, E, \hat{\Omega}, t) \; .$$

6. Finiteness Condition: to by physically valid we need to meet the condition $0 < \psi(\vec{r}, E, \hat{\Omega}, t) < \infty$, with the possible exception of point sources,

7. which we handle with the Source Condition: localized sources are introduced as mathematical singularities at the location of the source.

For a source $s(\vec{r}_0, E, \hat{\Omega}, t)$:

$$\lim_{\vec{r}\to\vec{r}_0} \int_S dS\, \vec{e} \cdot \hat{\Omega}\psi(\vec{r}, E, \hat{\Omega}, t) = s(\vec{r}_0, E, \hat{\Omega}, t)\ ,$$
$$s(\vec{r}, E, \hat{\Omega}, t) = s(\vec{r}_0, E, \hat{\Omega}, t)\delta(\vec{r} - \vec{r}_0)\ .$$

Diffusion Equation Derivation

We will now derive the diffusion equation by **assuming the angular flux depends only weakly on direction**, $\hat{\Omega}$. Why derive the diffusion equation from the transport equation?

- Nuclear reactions and thus interaction rates only depend on the scalar flux; however,
- the angular flux lives in 7-D space (3 space, 2 angle, 1 energy, and 1 time) and
- the diffusion equation reduces this to 5-D space (3 space, 1 energy, and 1 time).

The diffusion equation is derived by starting with the transport equation and **integrating over all angles**. We'll use the <u>one-group</u> version for simplicity, but this assumption is not needed for the derivation.

Recall the definition of scalar flux and net current:

$$\phi(\vec{r}, t) = \int_{4\pi} d\hat{\Omega}\, \psi(\vec{r}, \hat{\Omega}, t)$$
$$\vec{J}(\vec{r}, t) = \int_{4\pi} d\hat{\Omega}\, \hat{\Omega}\psi(\vec{r}, \hat{\Omega}, t)$$

Neutron Continuity Equation

Now let's do the integration and go through it term by term:

$$\int_{4\pi} d\hat{\Omega} \left[\underbrace{\frac{1}{v}\frac{\partial\psi(\vec{r}, \hat{\Omega}, t)}{\partial t}}_{1} + \underbrace{\hat{\Omega} \cdot \nabla\psi(\vec{r}, \hat{\Omega}, t)}_{2} + \underbrace{\Sigma_t\psi(\vec{r}, \hat{\Omega}, t)}_{3} = \right.$$
$$\left. \underbrace{\int_{4\pi} d\hat{\Omega}'\, \Sigma_s(\hat{\Omega}' \to \hat{\Omega})\psi(\vec{r}, \hat{\Omega}', t)}_{4} + \underbrace{\frac{\nu\Sigma_f}{4\pi} \int_{4\pi} d\hat{\Omega}'\, \psi(\vec{r}, \hat{\Omega}', t)}_{5} + \underbrace{s(\vec{r}, \hat{\Omega}, t)}_{6} \right]$$

This is called the zeroeth order moment w.r.t. $\hat{\Omega}$.

1. No approximations

$$\frac{1}{v}\frac{\partial}{\partial t} \int_{4\pi} d\hat{\Omega}\, \psi(\vec{r}, \hat{\Omega}, t) = \boxed{\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r}, t)}$$

3. No approximations

$$\Sigma_t \int_{4\pi} d\hat{\Omega}\, \psi(\vec{r}, \hat{\Omega}, t) = \boxed{\Sigma_t \phi(\vec{r}, t)}$$

5. No approximations; but we will make use of the identity

$$\int_{4\pi} d\hat{\Omega} = \int_0^{\pi} \sin(\theta) d\theta \int_0^{2\pi} d\varphi = 4\pi$$

Thus

$$\int_{4\pi} d\hat{\Omega}\, \frac{\nu\Sigma_f}{4\pi} \int_{4\pi} d\hat{\Omega}'\, \psi(\vec{r}, \hat{\Omega}', t) =$$
$$4\pi \frac{\nu\Sigma_f}{4\pi} \int_{4\pi} d\hat{\Omega}'\, \psi(\vec{r}, \hat{\Omega}', t) = \boxed{\nu\Sigma_f \phi(\vec{r}, t)}$$

6. No approximations

$$\int_{4\pi} d\hat{\Omega}\, s(\vec{r}, \hat{\Omega}, t) \equiv \boxed{S(\vec{r}, t)}$$

4. Further investigate the scattering cross section

Let's interchange the order of integrations over $\hat{\Omega}$ and $\hat{\Omega}'$:

$$\int_{4\pi} d\hat{\Omega} \int_{4\pi} d\hat{\Omega}'\, \Sigma_s(\hat{\Omega}' \to \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}', t)$$
$$= \int_{4\pi} d\hat{\Omega}' \left[\int_{4\pi} d\hat{\Omega}\, \Sigma_s(\hat{\Omega}' \to \hat{\Omega}) \right] \psi(\vec{r}, \hat{\Omega}', t)$$

Then we can simplify the scattering term with the assumption (which is often true) that $\Sigma_s(\hat{\Omega}' \to \hat{\Omega})$ is **azimuthally symmetric**, meaning it only depends on the angle of the scattering cosine $\mu = \hat{\Omega}' \cdot \hat{\Omega}$. This implies

$$\int_{4\pi} d\hat{\Omega}\, \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) = 2\pi \int_{-1}^{1} d\mu\, \Sigma_s(\mu) = \Sigma_s$$

And therefore:

$$\begin{aligned} \text{scattering integral } &= \Sigma_s \int_{4\pi} d\hat{\Omega}'\, \psi(\vec{r}, \hat{\Omega}', t) \\ &= \boxed{\Sigma_s \phi(\vec{r}, t)} \end{aligned}$$

2. Finally, we get to the trouble term: streaming

$$\int_{4\pi} d\hat{\Omega}\, \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, t) = \nabla \cdot \int_{4\pi} d\hat{\Omega}\, \hat{\Omega} \psi(\vec{r}, \hat{\Omega}, t) = \nabla \cdot \vec{J}(\vec{r}, t)\,.$$

When we put all of the terms together we get the **neutron continuity equation**. You can see that we have 1 equation, but 2 unknowns (technically 3 equations and 4 unknowns b/c $\vec{J}$ has 3 spatial components):

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},t) + \nabla \cdot \vec{J}(\vec{r},t) + \Sigma_t\phi(\vec{r},t) = \Sigma_s\phi(\vec{r},t) + \nu\Sigma_f\phi(\vec{r},t) + S(\vec{r},t)\ . \tag{1}$$

We at least have a relationship between ϕ and $\vec{J}$.

First Angular Moment

The next step is to take the first angular moment of the transport equation to try to develop additional relationships that we can use to solve for ϕ. Thus, we multiply the one-group TE by $\hat{\Omega}$ and integrate over angle (with the zeroth moment, which is what we took to get the continuity equation, we didn't do the multiplication).

NOTE: at this point I'm dropping the fission term for simplicity (the extension is straightforward). We will assume any fission neutrons are included in our source term, S.

We will use the following identities in this part of the derivation:

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega} = 0 \qquad \text{because } \hat{\Omega} \text{ is an odd function}$$

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega} = \frac{4\pi}{3}\bar{\bar{I}} \qquad \bar{\bar{I}} \text{ is the identity tensor, which means}$$

$$\begin{aligned}\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}_i\hat{\Omega}_j &= 0 \qquad i \neq j\\ &= \frac{4\pi}{3} \qquad i = j\end{aligned}$$

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\hat{\Omega} = 0$$

Multiplying by $\hat{\Omega}$ and dropping dependencies when appropriate:

$$\begin{aligned}&\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\frac{1}{v}\frac{\partial\psi}{\partial t} + \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\cdot\nabla\psi + \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\Sigma_t\psi = \\ &\qquad \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\int_{4\pi} d\hat{\Omega}'\,\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}',t) + \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}s(\vec{r},\hat{\Omega},t)\ .\end{aligned}$$

Now we can go through term by term, just like how we got the continuity equation.

1.

$$\frac{1}{v}\frac{\partial}{\partial t}\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\psi(\vec{r},\hat{\Omega},t) = \boxed{\frac{1}{v}\frac{\partial \vec{J}}{\partial t}}$$

3.

$$\Sigma_t \int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\psi(\vec{r},\hat{\Omega},t) = \boxed{\Sigma_t \vec{J}(\vec{r},t)}$$

5. (was 6)

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}s(\vec{r},\hat{\Omega},t) \equiv \boxed{S_1(\vec{r},t)}$$

This is the definition of the first angular moment of the source term.

4. For the scattering term we will do some mathematical manipulation. There are several ways to do this, but this one makes the most sense to me (different from Duderstadt and Hamilton).

Expand the scattering cross section in Legendre Polynomials, which are a sequence of orthogonal polynomials:

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}\left[\left(x^2-1\right)^n\right].$$

Use the polynomials as follows and take the first two terms of the expansion:

$$\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\Sigma_{sl}P_l(\hat{\Omega}')P_l(\hat{\Omega})$$

$l=0$ is isotropic; (note $P_0(\hat{\Omega})=1$)

$$\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) \cong \frac{1}{4\pi}\Sigma_{s0}$$

$l=1$ is linearly isotropic; (note $P_1(\hat{\Omega})=\hat{\Omega}$)

$$\Sigma_s(\hat{\Omega}'\cdot\hat{\Omega}) \cong \frac{1}{4\pi}\left(\Sigma_{s0}+3\hat{\Omega}'\hat{\Omega}\Sigma_{s1}\right)$$

We're going to **assume that scattering is at most linearly anisotropic**, so we will stop expanding here.

Substitute the $l=1$ linearly anisotropic truncation into the equation and use some of our identities:

$$\begin{aligned}
&\frac{1}{4\pi}\int_{4\pi}\hat{\Omega}d\hat{\Omega}\int_{4\pi}d\hat{\Omega}'\left[\Sigma_{s0}+3\hat{\Omega}'\hat{\Omega}\Sigma_{s1}\right]\psi(\vec{r},\hat{\Omega}',t) = \\
&\qquad \underbrace{\frac{1}{4\pi}\int_{4\pi}d\hat{\Omega}\,\hat{\Omega}}_{0}\underbrace{\int_{4\pi}d\hat{\Omega}'\,\Sigma_{s0}\psi(\vec{r},\hat{\Omega}',t)}_{\Sigma_{s0}\phi(\vec{r},t)} + \frac{1}{4\pi}\underbrace{\int_{4\pi}d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}}_{4\pi/3\bar{\bar{I}}}\underbrace{\int_{4\pi}d\hat{\Omega}'\,\hat{\Omega}'3\Sigma_{s1}\psi(\vec{r},\hat{\Omega}',t)}_{3\Sigma_{s1}\vec{J}(\vec{r},t)} \\
&\qquad = \boxed{\Sigma_{s1}\vec{J}(\vec{r},t)}
\end{aligned}$$

2. And once again, the trouble term: streaming

$$\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\cdot\nabla\psi(\vec{r},\hat{\Omega},t) = \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\psi(\vec{r},\hat{\Omega},t)$$

All together this is the **current continuity equation**:

$$\frac{1}{v}\frac{\partial\vec{J}}{\partial t} + \nabla\cdot\int_{4\pi} d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\psi(\vec{r},\hat{\Omega},t) + \Sigma_t\vec{J}(\vec{r},t) = \Sigma_{s1}\vec{J}(\vec{r},t) + S_1(\vec{r},t)\ . \qquad (2)$$

Now we have 2 moment equations that give us 4 total equations (neutron continuity and 3 tensor equations) and 10 unknowns (ϕ, 3 from the $\vec{J}$, and 6 from the new tensor term).

Taking higher moments by repeating the multiply by $\hat{\Omega}$ and integrating isn't going to help matters.

Linearly Anisotropic Approximation

And finally, we introduce an approximation about the angular flux (so far we have only approximated the scattering as linearly anisotropic). We now **assume that the angular flux is at most linearly anisotropic** as well.

To implement this assumption, the angular flux is expanded in angle and only the first two terms are retained (similar to what we just did with scattering):

$$\begin{aligned}
\psi(\hat{\Omega}) &\cong \frac{1}{4\pi}\big(\psi_0 + 3\hat{\Omega}\cdot\vec{\psi}_1\big) \qquad l = 1;\text{ linearly isotropic}\\
\psi(\hat{\Omega}) &\cong \frac{1}{4\pi}\big(\phi(\vec{r},t) + 3\hat{\Omega}\cdot\vec{J}(\vec{r},t)\big)\ .
\end{aligned}$$

The truncated angular flux expansion is then inserted into the streaming term in the current continuity equation, Eqn. (2), giving

$$\begin{aligned}
\nabla\cdot\frac{1}{4\pi}\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\big(\phi(\vec{r},t) + 3\hat{\Omega}\cdot\vec{J}(\vec{r},t)\big) &= \nabla\cdot\frac{1}{4\pi}\Big[\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\phi(\vec{r},t) + 3\underbrace{\int d\hat{\Omega}\,\hat{\Omega}\hat{\Omega}\hat{\Omega}\cdot\vec{J}(\vec{r},t)}_{0}\Big]\\
&= \nabla\cdot\frac{1}{4\pi}\frac{4\pi}{3}\bar{\bar{I}}\phi(\vec{r},t)\\
&= \frac{1}{3}\nabla\phi(\vec{r},t)\ .
\end{aligned}$$

With this approximation, the current continuity equation becomes:

$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} + \frac{1}{3}\nabla\phi(\vec{r},t) + \Sigma_t \vec{J}(\vec{r},t) = \Sigma_{s1}\vec{J}(\vec{r},t) + S_1(\vec{r},t)$$

Next we'll define:

$$\begin{aligned} \Sigma_a &\equiv \Sigma_t - \Sigma_{s0} && \text{“absorption” cross section} \\ \Sigma_{tr} &\equiv \Sigma_t - \Sigma_{s1} && \text{“transport” cross section} \end{aligned}$$

Let's substitute these into our equation set: equations (1) and (2), neutron and current continuity, respectively:

$$\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},t) + \nabla\cdot\vec{J}(\vec{r},t) + \Sigma_a\phi(\vec{r},t) = \nu\Sigma_f\phi(\vec{r},t) + S(\vec{r},t)$$
$$\frac{1}{v}\frac{\partial \vec{J}}{\partial t} + \frac{1}{3}\nabla\phi(\vec{r},t) + \Sigma_{tr}\vec{J}(\vec{r},t) = S_1(\vec{r},t)$$

These are the P_1 equations because they are derived from the 0th and 1st Legendre polynomial expansions of the angular flux. And we now have 4 equations with 4 unknowns!

Fick's Law

If we also assume steady state (or weak temporal dependence) and an isotropic source ($S_1 = 0$), the current continuity equation becomes

$$\frac{1}{3}\nabla\phi(\vec{r},t) + \Sigma_{tr}\vec{J}(\vec{r}) = 0$$

$$\boxed{\vec{J}(\vec{r}) = -\frac{1}{3\Sigma_{tr}}\nabla\phi(\vec{r},t) = -D\nabla\phi(\vec{r},t)} \qquad \text{Fick's Law}$$

where

$$D = \frac{1}{3\Sigma_{tr}} = \frac{1}{3(\Sigma_t(\vec{r}) - \Sigma_{s1}(\vec{r}))}$$

is the diffusion coefficient.

Aside: $\Sigma_{s1} = \int d\hat{\Omega}\,\hat{\Omega}\Sigma_s$. When we include the azimuthally symmetric assumption we get $\Sigma_{s1} = \bar{\mu}_0\Sigma_s$, where $\bar{\mu}_0$ is the average cosine of the scattering angle.

For elastic scattering from stationary nuclei when s-wave scattering is present in the center of mass frame, $\bar{\mu}_0 = \frac{2}{3A}$, where A is atomic mass number.

With all of this, $\Sigma_{tr} = \Sigma_t - \bar{\mu}_0\Sigma_s$.

Punchline: Fick's Law gives us a clear relationship between current and scalar flux. Now we can write the diffusion equation in terms of only ϕ!

$$\boxed{\frac{1}{v}\frac{\partial}{\partial t}\phi(\vec{r},t) - \nabla \cdot D\nabla\phi(\vec{r},t) + \Sigma_a\phi(\vec{r},t) = \nu\Sigma_f\phi(\vec{r},t) + S(\vec{r},t)}\,.$$

We can also re-write our angular flux expansion as

$$\psi(\vec{r},\hat{\Omega},t) \cong \frac{1}{4\pi}\Big(\phi(\vec{r},t) - \frac{1}{\Sigma_{tr}}\nabla\phi(\vec{r},t)\Big)\,.$$

The physical interpretation of the diffusion process is that the "flow" of neutrons is driven by a spatial gradient of flux. Or rather, neutrons diffuse from high to low concentration areas. You can see the driving function in Fick's Law:

- Equilibrium is at any location where $\vec{J} = 0$; there are an equal number of neutrons crossing the interface in both directions.
- When we're not in equilibrium, more neutrons will be scattered from the side with larger ϕ to the side with lower ϕ. Hence the net migration is opposed to the gradient (matching the negative sign).

Initial and Boundary Conditions

We now need one initial condition and two boundary conditions. We will also use some other information.

Mean free path is the mean distance from the last collision.

$$\lambda_t = \frac{1}{\Sigma_t} \qquad \lambda_{tr} = \frac{1}{\Sigma_{tr}}$$

If scattering is

- isotropic, then $\bar{\mu}_0 = 0$ and $\lambda_{tr} = \lambda_t$
- forward peaked, then $\bar{\mu}_0 > 0$ and $\lambda_{tr} > \lambda_t$

Initial conditions are pretty easy:

$$\phi(\vec{r},0) = \phi_0(\vec{r}) \qquad \forall\vec{r} \in V\,.$$

Basic requirements: still need

- the flux to be real and positive: $0 \leq \phi$
- and bounded: $\phi < \infty$ except near mathematical approximations (the source condition).

Interface Conditions

These are also fairly straightforward. We take the 0th and 1st moments of our TE condition,

$$\psi_1(\vec{r}_S, \hat{\Omega}, t) = \psi_2(\vec{r}_S, \hat{\Omega}, t) \qquad \forall \hat{\Omega} \ ,$$

and we get two equations rather than one. Now

$$\begin{aligned} \phi_1(\vec{r}, t) &= \phi_2(\vec{r}, t) \\ \vec{J}_1(\vec{r}, t) &= \vec{J}_2(\vec{r}, t) \end{aligned}$$

Vacuum Boundary Condition

These aren't quite so simple. We start by thinking about the transport non-reentrant condition:

$$\psi(\vec{r}_s, \hat{\Omega}, t) = 0 \text{ for } \hat{\Omega} \cdot \hat{e}_s < 0 \ ,$$

which is a mathematical statement that there are no neutrons entering our volume. Also written as

$$J_-(\vec{r}, t) = \int_{\hat{\Omega} \cdot \hat{e}_s < 0} d\hat{\Omega} \, \hat{\Omega} \cdot \hat{e}_s \psi(\vec{r}_s, \hat{\Omega}, t) = 0 \ .$$

However, with diffusion theory

$$\psi(\vec{r}_s, \hat{\Omega}, t) \cong \frac{1}{4\pi} \big(\phi(\vec{r}_s, t) - \frac{1}{\Sigma_{tr}} \nabla \phi(\vec{r}_s, t) \big)$$

and our partial currents become

$$\begin{aligned} J_\pm = & \int_{2\pi^\pm} d\hat{\Omega} \, \hat{\Omega} \cdot \hat{e}_s \psi(\vec{r}_s, \hat{\Omega}, t) = \\ & \cong \frac{1}{4} \phi(\vec{r}, t) \mp \frac{D}{2} \hat{e}_s \cdot \nabla \phi(\vec{r}_s, t) = 0 \ . \end{aligned}$$

For a 1-D slab with a vacuum boundary at $x = x_s$:

$$J_-(\vec{r}_s, t) = J_-(x_s, t) = \frac{1}{4} \phi(x_s, t) + \frac{D}{2} \frac{d\phi}{dx} \Big|_{x_s} = 0$$

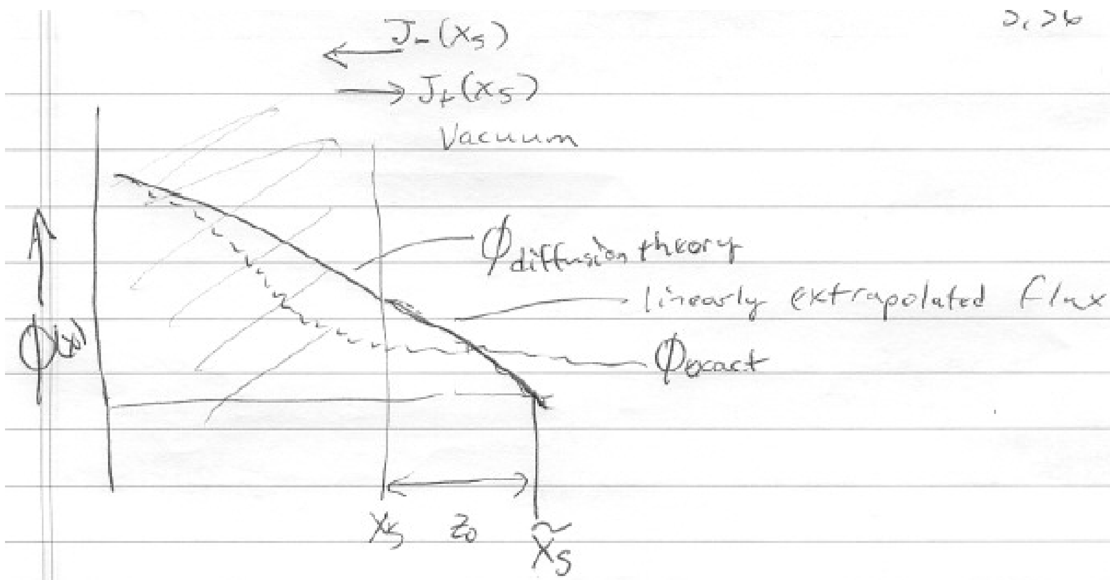
$$\text{Or} \qquad \frac{1}{\phi(x_s, t)} \frac{d\phi}{dx} \Big|_{x_s} = -\frac{1}{2D}$$

This relationship implies that linearly extrapolating the flux beyond the vacuum boundary would lead to a vanishing flux at the point

$$\tilde{x}_s = x_s + 2D = x_s + \frac{2}{3}\lambda_{tr} \; .$$

Thus, the vacuum condition $J_-(x_s) = 0$ is usually replaced with $\phi(\tilde{x}_s) = 0$. Additionally, computation with more detailed transport theory leads to an **extrapolation distance** of $0.7104\lambda_{tr} = z_0$ rather than $\frac{2}{3}\lambda_{tr}$.

DRAW PICTURE



In reality, though, $\lambda_{tr} \sim 0$ [cm] compared to the size of a reactor core [m].

Helmholtz Form

In steady state we can write the diffusion equation this way:

$$-\nabla \cdot D\nabla\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = Q(\vec{r}) \; ,$$
$$\text{where} \qquad Q(\vec{r}) = \nu\Sigma_f\phi(\vec{r}) + S(\vec{r}) \; ,$$

which can be written as the Helmholtz equation of applied mathematics:

$$\nabla^2\phi(\vec{r}) - \frac{1}{L^2}\phi(\vec{r}) = \frac{-Q(\vec{r})}{D} \; ,$$
$$\text{where} \qquad L \equiv \sqrt{\frac{D}{\Sigma_a}} \; .$$

L is called the neutron diffusion length. This is "how far a neutron diffuses from a source prior to absorption".

In the Helmholtz formulation, ϕ is amplitude and $\frac{1}{L}$ is wave number.

This formulation is useful because we know how to solve it. We write

$$\phi(\vec{r}) = \phi_H(\vec{r}) + \phi_P(\vec{r}) \, ,$$

For example, we often have:

$$\phi_H(\vec{r}) = A \exp\big(-\frac{|\vec{r}|}{L}\big) + B \exp\big(-\frac{|\vec{r}|}{L}\big) \, .$$

Going through how to solve this analytically in a variety of circumstances, geometries, etc. is another class (NE 150/250). We're going to focus on numerical solution techniques. But first, one more thing.

Criticality Calculations

We can write our DE in steady state for a nuclear reactor core:

$$\begin{gathered} -\nabla \cdot D \nabla \phi(\vec{r}) + \Sigma_a \phi(\vec{r}) = \nu \Sigma_f \phi(\vec{r}) \, , \\ \text{with} \qquad \phi(\tilde{x}_s) = 0 \, . \end{gathered}$$

Unless we have the proper combination of core composition (Σ_a, Σ_f, D) and geometry ($\vec{r}$,$\vec{r_s}$) details, there is no general solution.

To deal with this, we introduce a parameter k into the equation:

$$-\nabla \cdot D \nabla \phi(\vec{r}) + \Sigma_a \phi(\vec{r}) = \frac{1}{k} \nu \Sigma_f \phi(\vec{r}) \, .$$

Then, for any value of k we assert that there is always a solution. We use an iterative process to find the condition when $k = 1$, called "critical".

A reactor is called **"critical"** if the chain reaction is self-sustaining and time-independent. Another way to think of the addition of k is to assume ν can be adjusted to obtain a time-independent solution by replacing it with $\frac{\nu}{k}$, where k is the parameter expressing the deviation from critical.

This substitution changes the transport equation into an **eigenvalue problem.** A spectrum of eigenvalues can be found, but at **long times only the non-negative solution corresponding to the largest real eigenvalue will dominate**, and that's k.

k can also be thought of as the asymptotic ratio of the number of neutrons in one generation to the number in the next.

References

[1] James J. Duderstadt and Louis J. Hamilton. *Nuclear Reactor Analysis*. John Wiley & Sons, Inc., New York, 1 edition, 1976.

[2] James J. Duderstadt and William R. Martin. *Transport Theory*. John Wiley & Sons, Inc., New York, 1979.

[3] E. E. Lewis and Jr. W. F. Miller. *Computational Methods of Neutron Transport*. American Nuclear Society, La Grange Park, IL, 1 edition, 1993.