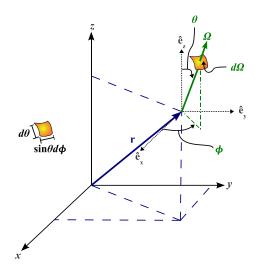
NE 155, Classes 4-5, S21 TE January 28, 2021

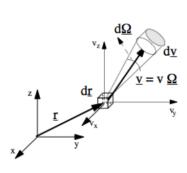
Transport Equation

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).

Definitions

Spatial logistics





- $d\vec{r} = d^3r$ = ordinary volume = $r^2\sin(\theta)d\theta d\varphi dr$
- v = speed (scaler)
- \vec{v} = velocity (vector)
- $d\vec{v} = d^3v$ = velocity volume = $v^2\sin(\theta')d\theta'd\varphi'dr$

- $v = \sqrt{(2E)/m}$ where m is the rest mass of the particle. Thus, we can relate energy and speed.
- $\hat{\Omega}$: unit directional vector in velocity space, $\vec{v} = v\hat{\Omega}$
- $d\hat{\Omega} = \sin(\theta')d\theta'd\varphi' = d^2\Omega$

These are the possible reactions we're generally going to worry about:

total (t): all interactions. We can break total into:

- scattering (s): a neutron interacts with an atom and bounces off either elastically or inelastically.
- absorption (a): a neutron is absorbed by a nucleus. If this happens it might
- fission (f): cause the nucleus to split into two pieces, releasing more neutrons.

Physics terms we will use:

- 1. **microscopic x-sec** $(\sigma, [cm^2])$: measure of the probability that an incident neutron will collide with a specific nucleus; σ_j indicates a specific reaction, e.g. j = f is fission.
- 2. **macroscopic x-sec** (Σ [cm^{-1}]): measure of the probability per unit path length that an incident neutron will collide with a target

$$\Sigma_j = \sigma_j N \; ,$$

where N is the atomic density of the target.

- 3. **double-differential scattering x-sec** $(\sigma_s(E,\hat{\Omega}\to E',\hat{\Omega}')dE'd\hat{\Omega}')$: measure of the probability that a neutron of energy E and moving in direction $\hat{\Omega}$ scatters off of a specific nucleus into energy range [E',E'+dE'] and direction range $[\hat{\Omega}',\hat{\Omega}'+d\hat{\Omega}']$.
- 4. **fission yield** $(\nu(E))$: average # of neutrons released by a fission induced by a neutron of energy E.
- 5. **fission spectrum** ($\chi(E)dE$): average # of neutrons produced from fission that are born with energy in [E, E+dE]. This is normalized such that

$$\int_0^\infty \chi(E)dE = 1.$$

6. **particle angular density** $(n(\vec{r}, E, \hat{\Omega}, t)d\vec{r}d\hat{\Omega}dE)$: expected number of particles in volume element d^3r at \vec{r} whose energies are in [E, E+dE] and direction of motion is in $[\hat{\Omega}, \hat{\Omega}+d\hat{\Omega}]$ at time t.

Note:

$$n(\vec{r}, E, \hat{\Omega}, t) = \frac{1}{mv} n(\vec{r}, v, \hat{\Omega}, t)$$
$$n(\vec{r}, v, \hat{\Omega}, t) = v^2 n(\vec{r}, \vec{v}, t)$$
$$n(\vec{r}, \vec{v}, t) = \frac{m}{v} n(\vec{r}, E, \hat{\Omega}, t)$$

7. **particle density**: $(N(\vec{r}, E, t)d^3rdE)$: expected number of particles in d^3r at \vec{r} whose energies are in [E, E + dE] at time t.

$$N(\vec{r}, E, t)d^3rdE = \int_{4\pi} d\hat{\Omega} \, n(\vec{r}, E, \hat{\Omega}, t)d^3rdE$$

- 8. angular flux: $\psi(\vec{r}, E, \hat{\Omega}, t) \equiv vn(\vec{r}, E, \hat{\Omega}, t)$
- 9. scalar flux: $\phi(\vec{r}, E, t) \equiv vN(\vec{r}, E, t)$.

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

10. **interaction rate density**: expected number of j reactions per volume per energy at time t.

$$\int_{4\pi} d\hat{\Omega} \, \Sigma_j v n(\vec{r}, E, \hat{\Omega}, t) = \Sigma_j \phi(\vec{r}, E, t)$$

11. **angular current density** or partial current: $\vec{j}(\vec{r}, E, \hat{\Omega}, t) = \vec{v}n(\vec{r}, E, \hat{\Omega}, t)$;

 $\vec{j}(\vec{r},E,\hat{\Omega},t)\cdot\hat{e}dAdEd\hat{\Omega}$ is the expected number of particles crossing dA along unit direction \hat{e} with energy in [E,E+dE] and direction in $[\hat{\Omega},\hat{\Omega}+d\hat{\Omega}]$ at time t.

12. **net current**: $\vec{J}(\vec{r}, E, t)$ is the net # of particles crossing a unit area per second along a direction normal to that area with energies in [E, E + dE] at time t.

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

Assumptions

- 1. Particles are point objects ($\lambda = h/(mv)$) is small compared to the atomic diameter): its state is fully described by its location, velocity vector, and a given time. This ignores rotation and quantum effects.
- 2. Neutral particles travel in straight lines between collisions.
- 3. Particle-particle collisions are negligible (makes TE linear).
- 4. Material properties are isotropic (generally valid unless velocities are very low).
- 5. Material composition is time-independent (generally valid over short time scales).
- 6. Quantities are expected values: fluctuations about the mean for very low densities are not accounted for.

Derivation

The TE is a <u>detailed</u> balance of the particle population over phase space that is as close to exact as possible.

DRAW a Differential volume picture.

Consider a volume V with surface S. For each point $\vec{r} \in S$, let \hat{e}_S be the outward normal vector.

For a given $\hat{\Omega}$, define S^+ as that part of S for which $\hat{e}_S \cdot \hat{\Omega} > 0$ (outgoing particles) and S^- as that part of S for which $\hat{e}_S \cdot \hat{\Omega} < 0$ (incoming particles).

Then, for this volume V for a fixed E and $\hat{\Omega}$, the general rate equation can be written for particles satisfying $\vec{r} \in V$, energies in [E, E+dE] and direction $[\hat{\Omega}, \hat{\Omega}+d\hat{\Omega}]$ as:

Rate of change of the particle (neutron) population = rate of production - rate of loss

Rate of Change

Recall the definition of n: expected number of particles in volume element d^3r at \vec{r} whose energies are in [E, E + dE] and direction of motion is in $[\hat{\Omega}, \hat{\Omega} + d\hat{\Omega}]$ at time t.

To get the rate of change of particles within the volume, we need to integrate over volume and take the derivative with respect to time:

$$\Big[\int_{V} \frac{\partial}{\partial t} n(\vec{r}, E, \hat{\Omega}, t) d\vec{r} \Big] dE d\hat{\Omega}$$

Production Mechanisms

How can we produce neutrons in volume element d^3r at \vec{r} whose energies are in [E, E+dE] and direction of motion is in $[\hat{\Omega}, \hat{\Omega}+d\hat{\Omega}]$ at time t?

- 1. Inscattering (from some other energy and/or angle into our energy and angle),
- 2. Fission neutrons, or
- 3. Fixed/interior sources.
- 1) Scattering into [E, E + dE] and $[\hat{\Omega}, \hat{\Omega} + d\hat{\Omega}]$

This is the definition of the double differential scattering cross section:

$$\left[\int_{V} d^{3}r \int_{4\pi} d\hat{\Omega}' \int_{0}^{\infty} dE' \, \Sigma_{s}(E', \hat{\Omega}' \to E, \hat{\Omega}) v' n(\vec{r}, E', \hat{\Omega}', t) \right] dE d\hat{\Omega}$$

2) Expected rate of neutron production by fission

Note: fission neutrons are isotropic, thus they are produced at $\frac{1}{4\pi}$ per steradian. This means the fraction within $[\hat{\Omega}, \hat{\Omega} + d\hat{\Omega}]$ is $\frac{d\hat{\Omega}}{4\pi}$ (fyi: including this normalization differs among textbooks and research papers).

Also, recall that $\chi(E)dE$ is the fraction of neutrons born into [E,E+dE]. Thus

$$\frac{\chi(E)}{4\pi} \left[\int_{V} d^{3}r \int_{4\pi} d\hat{\Omega}' \int_{0}^{\infty} dE' \ \nu(E') \Sigma_{f}(E') v' n(\vec{r}, E', \hat{\Omega}', t) \right] dE d\hat{\Omega}$$

3) Production from a fixed source

Sources are fully specified by a function reminiscent of the n definition: $s(\vec{r}, E, \hat{\Omega}, t)$ s.t. $s(\vec{r}, E, \hat{\Omega}, t)d^3r dE d\hat{\Omega} \equiv$ the expected number of particles that are produced at time t inside volume d^3r at \vec{r} with energy [E, E + dE] and direction $[\hat{\Omega}, \hat{\Omega} + d\hat{\Omega}]$.

Rate of production of such particles in V is

$$\Bigg| \Big[\int_{V} d^{3}r \; s(\vec{r}, E, \hat{\Omega}, t) \Big] dE d\hat{\Omega}$$

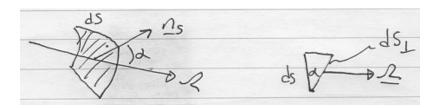
Loss Mechanisms

How can we lose neutrons from volume element d^3r at \vec{r} whose energies are in [E, E+dE] and direction of motion is in $[\hat{\Omega}, \hat{\Omega}+d\hat{\Omega}]$ at time t?

- 4. Neutrons can collide and exit the phase space (any collision will change its state) or
- 5. Neutrons can stream into other locations and/or directions of motion (leakage).
- 4) Total interaction: any collision can lead to (a) absorption or (b) a change in E or $\hat{\Omega}$ or both.

$$\left[\int_{V} d^{3}r \Sigma_{t}(E) v n(\vec{r}, E, \hat{\Omega}, t) \right] dE d\hat{\Omega}$$

5) Net leakage out of phase space



Use the definition of $\vec{j}\to$ the expected number of particles crossing dS along \hat{e}_S with energy [E,E+dE] and direction $[\hat{\Omega},\hat{\Omega}+d\hat{\Omega}]$ at time t

$$= \vec{j}(\vec{r}_s, E, \hat{\Omega}, t) \cdot d\vec{S} dE d\hat{\Omega} ,$$

where \vec{r}_s is a point on the surface and $d\vec{S} = \hat{e}_S dS$.

Thus, the total leakage out of V is

$$\left[\int_{S} \vec{j}(\vec{r}_{s}, E, \hat{\Omega}, t) \cdot d\vec{S}\right] dE d\hat{\Omega}.$$

We can use divergence theorem to rewrite this w.r.t. V (rather than S):

$$\int_{S} \hat{e}_{S} \cdot \vec{F}(\vec{r}) dS = \int_{V} \nabla \cdot \vec{F}(\vec{r}) dV$$

This gives

$$\left[\int_{V} d^{3}r \, \nabla \cdot \left(\underbrace{\vec{j}(\vec{r}_{s}, E, \hat{\Omega}, t)}_{=\vec{v}n = v\hat{\Omega}n} \right) \right] dE d\hat{\Omega}$$

And we can use this identity:

$$\hat{\Omega} \cdot (\nabla f) = \nabla \cdot \hat{\Omega} f \text{ because } \hat{\Omega} \text{ is not a function.}$$

$$\nabla \cdot \hat{\Omega} f = f(\underbrace{\nabla \cdot \hat{\Omega}}_{0}) + \hat{\Omega} \cdot (\nabla f)$$

$$\therefore \left[\int_{V} d^{3}r \, \hat{\Omega} \cdot \nabla \big(vn(\vec{r}_{s}, E, \hat{\Omega}, t) \big) \right] dE d\hat{\Omega}$$

Note: $\hat{\Omega} \cdot \nabla$ represents the derivative along the direction of motion.

All Together Now

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

Suppressing dependencies to save space for the moment

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

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

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

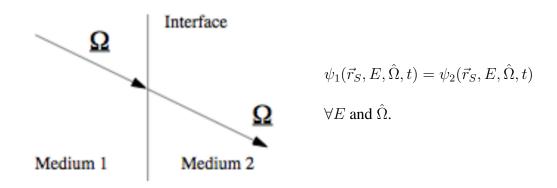
Initial and Boundary Conditions

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

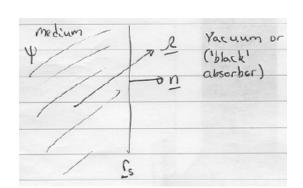
$$\psi(\vec{r}, E, \hat{\Omega}, 0) = \psi_0(\vec{r}, E, \hat{\Omega})$$

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

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



3. Fixed Condition: you can specify incoming flux

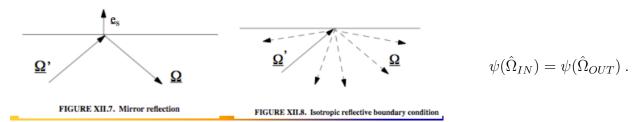


 $\psi(\vec{r}_S, E, \hat{\Omega}, t) = \psi_{IN}(\vec{r}_S, E, \hat{\Omega}, t)$ for $\vec{e} \cdot \hat{\Omega} < 0$: specifying incoming neutrons. Note, the incoming flux can be a functional expression; it can also be zero.

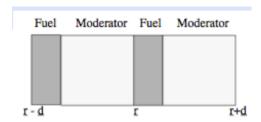
This is equivalent to specifying the incoming partial current,

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

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



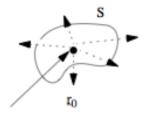
5. Periodic Condition: you know there is a repetition in the system



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

- 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 <u>Source Condition</u>: localized sources are introduced as mathematical singularities at the location of the source.

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



$$\begin{split} &\lim_{\vec{r}\to\vec{r_0}}\int_S dS \; \vec{e}\cdot\hat{\Omega}\psi(\vec{r},E,\hat{\Omega},t) = s(\vec{r_0},E,\hat{\Omega},t)\;,\\ &s(\vec{r},E,\hat{\Omega},t) = s(\vec{r_0},E,\hat{\Omega},t)\delta(\vec{r}-\vec{r_0})\;. \end{split}$$

Simplified Forms

One Speed

Assume all particles are at the same speed, so we no longer need energy dependence.

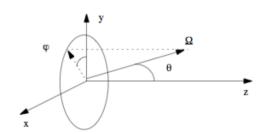
$$\frac{1}{v} \frac{\partial \psi(\vec{r}, \hat{\Omega}, t)}{\partial t} + \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, t) + \Sigma_t \psi(\vec{r}, \hat{\Omega}, t) =
\int_{4\pi} d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \to \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}', t) + \frac{\nu \Sigma_f}{4\pi}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

One Speed, One Dimensional

We'd like to simplify even farther by only worrying about one dimension, so we'll get rid of y and z.

$$\vec{r} = (x, y, z) \, d\hat{\Omega} = \sin(\theta) d\theta d\varphi = d\mu d\varphi$$

Note $\mu = \cos(\theta)$ so $d\mu = \sin(\theta)$
 $\Omega_x = \cos(\theta) = \mu$
(in the image mentally swap y and z to get the notation we are using)



$$\frac{1}{v} \frac{\partial \psi(x, \hat{\Omega}, t)}{\partial t} + \left(\Omega_x \frac{\partial}{\partial x} + \Omega_y \frac{\partial}{\partial y} + \Omega_z \frac{\partial}{\partial z}\right) \psi(x, \hat{\Omega}, t) + \Sigma_t \psi(x, \hat{\Omega}, t) =$$

$$\int_{4\pi} d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \to \hat{\Omega}) \psi(x, \hat{\Omega}', t) + \frac{\nu \Sigma_f}{4\pi} \int_{4\pi} d\hat{\Omega}' \psi(x, \hat{\Omega}', t) + s(x, \hat{\Omega}, t)$$

Using this idea we can write things more cleanly:

$$\frac{1}{v_0} \frac{\partial \psi(x, \hat{\Omega}, t)}{\partial t} + \mu \frac{\partial}{\partial x} \psi(x, \hat{\Omega}, t) + \Sigma_t \psi(x, \hat{\Omega}, t) =
\int_0^{2\pi} d\phi \int_{4\pi} d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) \frac{\psi(x, \mu', t)}{2\pi} + \frac{1}{4\pi} \nu \Sigma_f \int_0^{2\pi} d\phi \psi(x, \mu, t) + s(x, \mu, t)$$

If scattering is also isotropic:

$$\Sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) = \frac{\Sigma_s}{4\pi}$$

And we get the 1-group, 1-D, isotropic neutron TE:

$$\frac{1}{v_0} \frac{\partial \psi(x, \mu, t)}{\partial t} + \mu \frac{\partial}{\partial x} \psi(x, \mu, t) + \Sigma_t \psi(x, \mu, t) =
\frac{1}{2} \Sigma_s \int_{-1}^1 d\mu' \psi(x, \mu', t) + \frac{1}{2} \left(\nu \Sigma_f \phi(x, t) + S(x, t) \right)$$

Steady State

If we get rid of time dependence.

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \Sigma_t \psi(x, \mu) = \frac{1}{2} \Sigma_s \int_{-1}^1 d\mu' \psi(x, \mu') + \frac{1}{2} \left(\nu \Sigma_f \phi(x) + S(x) \right)$$

And very finally - we can have the unrealistic case of purely absorbing media:

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \Sigma_a \psi(x, \mu) = \frac{1}{2} \left(\nu \Sigma_f \phi(x) + S(x) \right)$$

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.