NE 155, Classes 4-5, S17
TE
January 25 – 27, 2017

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

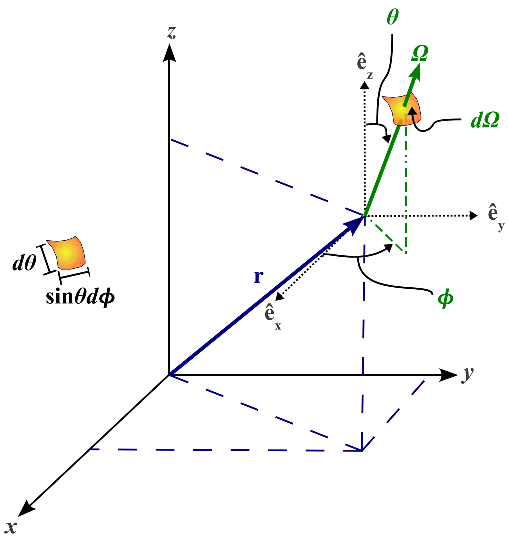


Figure 1: Schematic of Phase Space

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** (σ, [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** ($\sigma_s(E, \hat{\Omega} \rightarrow E', \hat{\Omega}')dE'd\hat{\Omega}'$): 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:

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

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

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

8. **angular flux**: $\psi(\vec{r}, E, \hat{\Omega}, t) \equiv v n(\vec{r}, E, \hat{\Omega}, t)$.

9. **scalar flux**: $\phi(\vec{r}, E, t) \equiv v N(\vec{r}, E, t)$.

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

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: $\vec{j}(\vec{r}, E, \hat{\Omega}, t) = \vec{v} n(\vec{r}, E, \hat{\Omega}, t)$;

    $\vec{j}(\vec{r}, E, \hat{\Omega}, t) \cdot \hat{e}\, dA\, dE\, d\hat{\Omega}$ 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 detailed 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:

$$\boxed{\text{Rate of change of the particle (neutron) population = rate of production - rate of loss}}$$

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:

$$\boxed{\left[\int_V \frac{\partial}{\partial t} n(\vec{r}, E, \hat{\Omega}, t) d\vec{r}\right] dE d\hat{\Omega}}$$

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:

$$\boxed{\Big[\int_V d^3r \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \Sigma_s(E', \hat{\Omega}' \to E, \hat{\Omega}) v' n(\vec{r}, E', \hat{\Omega}', t)\Big] dE d\hat{\Omega}}$$

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

$$\boxed{\frac{\chi(E)}{4\pi}\Big[\int_V d^3r \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE'\, \nu(E')\Sigma_f(E') v' n(\vec{r}, E', \hat{\Omega}', t)\Big] dE d\hat{\Omega}}$$

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

$$\boxed{\Big[\int_V d^3r\, s(\vec{r}, E, \hat{\Omega}, t)\Big] dE d\hat{\Omega}}$$

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?

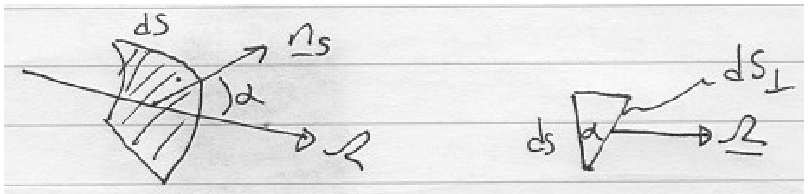
4. Neutrons can collide and exit the phase space (any collision will change its state) or

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.

$$\boxed{\Big[\int_V d^3r \Sigma_t(E) v n(\vec{r}, E, \hat{\Omega}, t)\Big] dE d\hat{\Omega}}$$

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

$$\Big[\int_S \vec{j}(\vec{r}_s, E, \hat{\Omega}, t) \cdot d\vec{S}\Big] dE d\hat{\Omega} \,.$$

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

$$\Big[\int_V d^3r \, \nabla \cdot \big(\underbrace{\vec{j}(\vec{r}_s, E, \hat{\Omega}, t)}_{=\vec{v}n = v\hat{\Omega}n}\big)\Big] dE d\hat{\Omega}$$

And we can use this identity:

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

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

$$\therefore \quad \boxed{\Big[\int_V d^3r \, \hat{\Omega} \cdot \nabla \big(vn(\vec{r}_s, E, \hat{\Omega}, t)\big)\Big] dE d\hat{\Omega}}$$

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

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

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

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

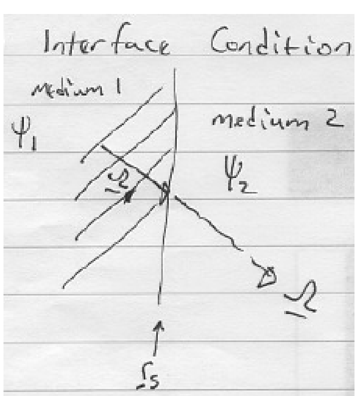
Initial and Boundary Conditions

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.

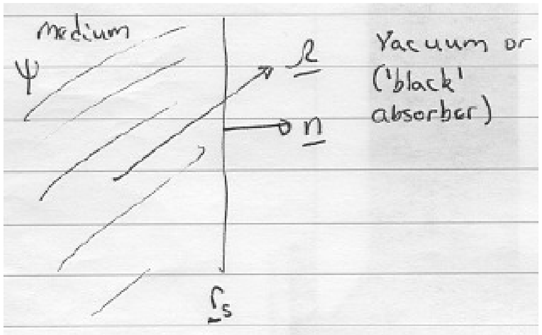
2. Interface Condition: the angular flux must be continuous along $\hat{\Omega}$ at all points, including material interfaces.



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

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

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

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 $d\mu = \sin(\theta)$

$\Omega_x = \cos(\theta) = \mu$

$$\frac{1}{v}\frac{\partial \psi(x, \hat{\Omega}, t)}{\partial t} + \big(\Omega_x \frac{\partial}{\partial x} + \cancel{\Omega_y \frac{\partial}{\partial y}} + \cancel{\Omega_z \frac{\partial}{\partial z}}\big)\psi(x, \hat{\Omega}, t) + \Sigma_t \psi(x, \hat{\Omega}, t) = \int_{4\pi} d\hat{\Omega}' \Sigma_s(\hat{\Omega}' \to \hat{\Omega}) \psi(x, \hat{\Omega}', t) + \frac{\nu \Sigma_f}{4\pi} \int_{4\pi} d\hat{\Omega}' \psi(x, \hat{\Omega}', t) + s(x, \hat{\Omega}, t)$$

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.