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 <u>any</u> collection of neutral particles).
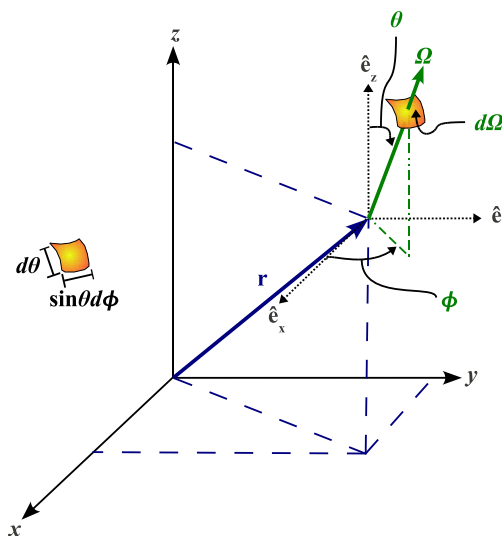
Definitions

Figure 1: Schematic of Phase Space

Spatial logistics

- $d\vec{r} = d^3 r$ = ordinary volume = $r^2 \sin(\theta) d\theta d\varphi dr$

- v = speed (scaler)

- $\vec{v}$ = velocity (vector)

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- $v = \sqrt{(2E)/m}$ 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

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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** ($\sigma_s(E, \hat{\Omega} \to E', \hat{\Omega}')dE'd\hat{\Omega}'$): 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.

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.

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.

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

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.

3.

4.

5.

6.

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

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:

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.

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:

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

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

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.
$s(\vec{r}, E, \hat{\Omega}, t)d^3rdEd\hat{\Omega} \equiv$ 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

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

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.

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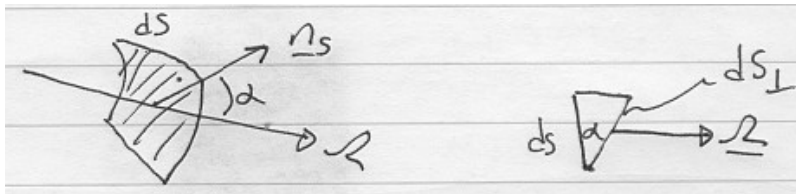
Use the definition of $\vec{j} \to$ the expected number of particles crossing dS along $\hat{e}_S$ with energy
$[E, E + dE]$ and direction $[\hat{\Omega}, \hat{\Omega} + d\hat{\Omega}]$ at time t

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

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

And we can use this identity:

$$\hat{\Omega} \cdot (\nabla f) = \nabla \cdot \hat{\Omega} f \text{ because } \hat{\Omega} \text{ is not a function.}$$
$$\nabla \cdot \hat{\Omega} f = f(\underbrace{\nabla \cdot \hat{\Omega}}_{0}) + \hat{\Omega} \cdot (\nabla f)$$

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

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

Now we have a balance relation that we can rearrange, substituting $\psi(\vec{r}, E, \hat{\Omega}, t) = v n(\vec{r}, E, \hat{\Omega}, t)$, to get what we usually call the Boltzmann Equation for neutron transport
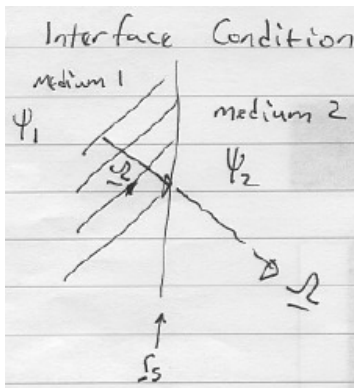
$$\frac{1}{v} \frac{\partial \psi(\vec{r}, E, \hat{\Omega}, t)}{\partial t} + \hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}, t) + \Sigma_t \psi(\vec{r}, E, \hat{\Omega}, t) =$$
$$\int_{4\pi} d\hat{\Omega}' \int_0^{\infty} dE' \Sigma_s(E', \hat{\Omega}' \rightarrow E, \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}', t) +$$
$$\frac{\chi(E)}{4\pi} \int_0^{\infty} dE' \nu(E') \Sigma_f(E') \int_{4\pi} d\hat{\Omega}' \psi(\vec{r}, E', \hat{\Omega}', t) + s(\vec{r}, E, \hat{\Omega}, t)$$

Initial and Boundary Conditions

1. <u>Initial Condition</u>: we start with some initial "known" state:

   for the problem domain. Note, the initial flux can be a functional expression.
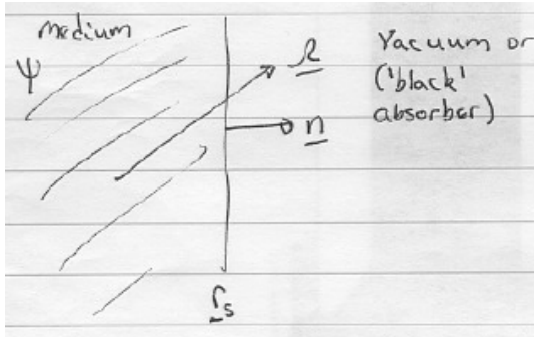
2. <u>Interface Condition</u>: the angular flux must be continuous along $\hat{\Omega}$ at all points, including material interfaces.

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

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

3. <u>Fixed Condition</u>: 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. <u>Reflective Condition</u>: there is mirror symmetry at some surface:

5. <u>Periodic Condition</u>: 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. <u>Finiteness Condition</u>: 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 $s(\vec{r}_0, E, \hat{\Omega}, t)$:

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

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

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

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

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.