

NE 250, F17
Alternative Derivation for Transport Equation

Definitions

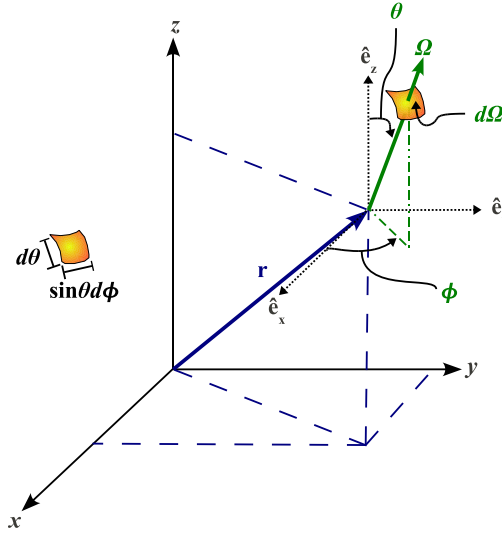


Figure 1: Schematic of Phase Space

Spatial logistics

- $d\vec{r} = d^3r = \text{ordinary volume} = r^2 \sin(\theta) d\theta d\phi dr$
- $v = \text{speed (scaler)}$
- $\vec{v} = \text{velocity (vector)}$
- $d\vec{v} = d^3v = \text{velocity volume} = v^2 \sin(\theta') d\theta' d\phi' dr$
- $v = \sqrt{(2E)/m}$ where m is the rest mass of the particle. Thus, we can relate energy and speed.
- $\hat{\Omega}$: unit directional vector in velocity space, $\vec{v} = v\hat{\Omega}$
- $d\hat{\Omega} = \sin(\theta') d\theta' d\phi' = d^2\Omega$

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** ($\Sigma [cm^{-1}]$): 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:

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

$$n(\vec{r}, v, \hat{\Omega}, t) = v^2 n(\vec{r}, \vec{v}, t)$$

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

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

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

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.

The transport equation

We consider a six-dimensional volume (as a six-dimensional cube) fixed in space, of dimensions $\Delta x, \Delta y, \Delta z, \Delta E, \Delta \theta, \Delta \varphi$. Then, the number of particles within this volume at time t is

$$n(\vec{r}, E, \hat{\Omega}, t) \Delta x \Delta y \Delta z \Delta E \Delta \theta \Delta \varphi = n(\vec{r}, E, \hat{\Omega}, t) \Delta \beta,$$

where all arguments of N are “average” arguments in the increment of six-dimensional phase space $\Delta \beta$. The number of particles in this cube changes with time:

$$\Delta \beta \frac{\partial}{\partial t} n(\vec{r}, E, \hat{\Omega}, t) = \text{time rate of change of the number of particles in the six-dimensional cube } \Delta \beta.$$

This time rate of change is due to five separate processes. One is the rate of streaming of particles out of the volume through the boundaries. The others occur within the six-dimensional “cube”: the rate of absorption; the rate of scattering from $E, \hat{\Omega}$ to all other energies and directions, known as outscattering; the rate of scattering into $E, \hat{\Omega}$ from all other energies and directions, known as inscattering; and the rate of production of particles due to an internal source.

Now, let us consider the surfaces of the cube perpendicular to the x -axis. For the net rate of particles leaving the cube through these two surfaces, we have

$$(\text{Streaming})_x = \dot{x} n(\vec{r}, E, \hat{\Omega}, t) \Big|_x^{x+\Delta x} \Delta y \Delta z \Delta E \Delta \theta \Delta \varphi,$$

where \dot{x} is the x component of the particle velocity, and $\Delta y \Delta z \Delta E \Delta \theta \Delta \varphi$ is the surface area.

Letting Δx go to the differential dx , we rewrite

$$(\text{Streaming})_x = \Delta\beta \frac{\partial}{\partial x} [\dot{x}n(\vec{r}, E, \hat{\Omega}, t)].$$

Using the same procedure for the flow from the cube in the other five “directions”, we obtain

$$\begin{aligned} \text{Streaming} = & \left[\frac{\partial}{\partial x}(\dot{x}n) + \frac{\partial}{\partial y}(\dot{y}n) + \frac{\partial}{\partial z}(\dot{z}n) \right. \\ & \left. + \frac{\partial}{\partial E}(\dot{E}n) + \frac{\partial}{\partial \theta}(\dot{\theta}n) + \frac{\partial}{\partial \varphi}(\dot{\varphi}n) \right] \Delta\beta, \end{aligned}$$

where $n = n(\vec{r}, E, \hat{\Omega}, t)$.

The rate of absorption within the cube is the product of the number of particles in the cube and the probability of absorption per particle per unit of time. This probability is given by the product of the absorption cross section and the particle speed v . That is,

$$\text{Absorption} = v\Sigma_a(\vec{r}, E)n(\vec{r}, E, \hat{\Omega}, t)\Delta\beta.$$

Using similar arguments and the fact that we need to sum the scattering from (to) $E, \hat{\Omega}$ to (from) all other energies and directions $E', \hat{\Omega}'$, we find

$$\begin{aligned} \text{Outscattering} &= \Delta\beta \int_0^\infty \int_{4\pi} v\Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')n(\vec{r}, E, \hat{\Omega}, t)d\hat{\Omega}'dE', \\ \text{Inscattering} &= \Delta\beta \int_0^\infty \int_{4\pi} v'\Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})n(\vec{r}, E', \hat{\Omega}', t)d\hat{\Omega}'dE', \end{aligned}$$

where $\Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$ is the macroscopic differential scattering cross section. Since the distribution function in the integrand of the outscattering term is independent of the integration variables, we can rewrite Outscattering as $\Delta\beta v\Sigma_s(\vec{r}, E)n(\vec{r}, E, \hat{\Omega}, t)$. Finally, we need to consider the internal source of particles. We quantify this source by introducing the function $S(\vec{r}, E, \hat{\Omega}, t)$ such that the rate of introduction of particles into the cube is given by

$$\text{Source} = S(\vec{r}, E, \hat{\Omega}, t)\Delta\beta.$$

In order to build the transport equation, we sum these equations with appropriate signs for loss and gain, to the overall rate of change. Letting $\Delta\beta$ approach a differential element and canceling it, we

obtain

$$\begin{aligned}
\frac{\partial n}{\partial t} = & - \left[\frac{\partial(\dot{x}n)}{\partial x} + \frac{\partial(\dot{y}n)}{\partial y} + \frac{\partial(\dot{z}n)}{\partial z} + \frac{\partial(\dot{E}n)}{\partial E} + \frac{\partial(\dot{\theta}n)}{\partial \theta} + \frac{\partial(\dot{\varphi}n)}{\partial \varphi} \right] \\
& - v\Sigma_a(\vec{r}, E)n \\
& + \int_0^\infty \int_{4\pi} v'\Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})n(\vec{r}, E', \hat{\Omega}', t)d\hat{\Omega}'dE' \\
& - \int_0^\infty \int_{4\pi} v\Sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')n(\vec{r}, E, \hat{\Omega}, t)d\hat{\Omega}'dE' \\
& + S(\vec{r}, E, \hat{\Omega}, t),
\end{aligned} \tag{1}$$

where $n = n(\vec{r}, E, \hat{\Omega}, t)$. Since particles travel in a straight line between collisions, $\dot{\theta} = \dot{\varphi} = 0$. Furthermore, $\dot{E} = 0$ because particles stream with no change in energy. Finally, performing the outscattering integral:

$$\begin{aligned}
& \frac{1}{v} \frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) + \hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}, t) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, E, \hat{\Omega}, t) \\
& = \int_0^\infty \int_{4\pi} \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})\psi(\vec{r}, E', \hat{\Omega}', t)d\hat{\Omega}'dE' + S(\vec{r}, E, \hat{\Omega}, t).
\end{aligned} \tag{2}$$

We can easily generalize this equation to include nuclear fission. To do that, we must revisit our treatment of Σ_a ; there are two main processes responsible for the absorption of particles in the system: *radiative capture* and *nuclear fission*. Now, we define

$$\Sigma_\gamma(\vec{r}, E)ds = \text{probability of capture}$$

and

$$\Sigma_f(\vec{r}, E)ds = \text{probability of a fission event},$$

such that

$$\Sigma_a(\vec{r}, E) = \Sigma_\gamma(\vec{r}, E) + \Sigma_f(\vec{r}, E).$$

While a captured neutron is simply removed from the system, a neutron with energy E that induces a fission event causes the target nucleus to split into two smaller daughter nuclei, and

$$\nu(E) = \text{the mean number of fission neutrons that are released}.$$

Of this number, $\nu(E)[1 - M(E)]$ are *prompt* fission neutrons (being emitted within 10^{-15} seconds of the fission event). These fission neutrons are emitted isotropically, with an energy distribution given by the fission spectrum $\chi_p(E)$. Also, $\nu(E)M(E)$ *delayed* fission neutrons (being released roughly 0.1 to 60 seconds after the fission event) are created; a delayed neutron is produced when a radioactive daughter nucleus undergoes a radioactive decay process in which a neutron is emitted.

Assuming (for simplicity) that the number of delayed neutrons emitted by fission is very small [$M(E) \ll 1$], we can neglect the delayed neutron terms and rewrite the transport equation as

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t}(\vec{r}, E, \hat{\Omega}, t) + \hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}, t) + \Sigma_t(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}, t) \\ = \int_0^\infty \int_{4\pi} \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\ + \frac{\chi_p(E)}{4\pi} \int_0^\infty \int_{4\pi} \nu(E') \Sigma_f(\vec{r}, E') \psi(\vec{r}, E', \hat{\Omega}', t) d\hat{\Omega}' dE' \\ + S(\vec{r}, E, \hat{\Omega}, t). \end{aligned} \quad (3)$$

These equations require both spatial and temporal boundary conditions. Assuming that the physical system of interest is nonreentrant (convex) and characterized by a volume V , it is sufficient to specify the flux of particles at all points of the bounding surface of the system in the incoming directions. This implies

$$\psi(\vec{r}_s, E, \hat{\Omega}, t) = \psi_b(\vec{r}_s, E, \hat{\Omega}, t), \quad \mathbf{n} \cdot \hat{\Omega} < 0,$$

where ψ_b is a specified function at the boundary, \vec{r}_s is a point on the surface, and \mathbf{n} is the unit outward normal vector at this point. In the time variable, we assume the range of interest $0 \leq t < \infty$ and specify the initial condition at $t = 0$, such that

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

where ψ_0 is a specified function.

It is common to make extra assumptions in order to obtain a simpler version of these equations. For instance, in the case of time-independent, monoenergetic particle transport in a homogeneous

medium with a known interior isotropic source:

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, \hat{\Omega}) = \int_{4\pi} \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}' + \frac{S(\vec{r})}{4\pi},$$

and

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, \hat{\Omega}) &= \int_{4\pi} \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}' \\ &+ \frac{\nu \Sigma_f}{4\pi} \int_{4\pi} \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}' + \frac{S(\vec{r})}{4\pi}. \end{aligned}$$

Both the equations above need a spatial boundary condition, which is given by

$$\psi(\vec{r}_s, \hat{\Omega}) = \psi_b(\vec{r}_s, \hat{\Omega}), \quad \mathbf{n} \cdot \hat{\Omega} < 0.$$

In steady-state reactor calculations, one often sees a version of these equations in which the inhomogeneous source $S(\vec{r})$ and the boundary source $\psi_b(\vec{r}_s, \hat{\Omega})$ are set to zero, and the fission source is modified by a constant factor $1/k$:

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}) + \Sigma_t \psi(\vec{r}, \hat{\Omega}) &= \int_{4\pi} \Sigma_s(\hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}' \\ &+ \frac{\nu \Sigma_f}{4\pi k} \int_{4\pi} \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}', \\ \psi(\vec{r}_s, \hat{\Omega}) &= 0, \quad \mathbf{n} \cdot \hat{\Omega} < 0. \end{aligned}$$

These equations always have the zero solution $\psi = 0$; the goal is to find the largest value of k such that a nonzero solution ψ exists. The resulting k is called the *criticality* (or *criticality eigenvalue*) of the system. If a system has a fissile region, it can be shown that k always exists, and the corresponding (eigenfunction) ψ is unique and positive.